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2024
Conference

The 5th International Electronic Conference on Applied Sciences

04–06 December 2024 | Online



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The 5th International Electronic Conference on Applied Sciences

04–06 December 2024 | Online



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Welcome from the Chair

We are pleased to announce the 5th International Electronic Conference on Applied Sciences. This international conference is sponsored by MDPI OA journal *Applied Sciences* (ISSN: 2076-3417), will bring together scientists from different areas to discuss important recent developments in a number of fields. It represents an opportunity to gather an interdisciplinary community to discuss applied sciences. More specifically, after the success of the first four editions, this year's edition will focus on eight thematic areas of applied nature sciences:

1. Applied Biosciences and Bioengineering
2. Nanosciences, Chemistry and Materials Science
3. Computing and Artificial Intelligence
4. Electrical, Electronics and Communications Engineering
5. Mechanical and Aerospace Engineering
6. Energy, Environmental and Earth Science
7. Food Science and Technology
8. Applied Physical Science

We expect that participants of this conference will exchange novel provocative ideas by presenting short oral presentations on research and development discoveries. Posters can be presented without an accompanying proceedings paper and will be available on this website during and after the e-conference.

Specifically, you do not need to seek financial support for travel, purchase air tickets, leave your house, office, and family, make a hotel room reservation, take a trip, or adjust to the time zone where the conference takes place during the entire conference period.

Under the virtual conference settings, there are additional advantages: (1) engagement tools that keep energy levels high, (2) participants are given a voice, (3) far stronger attention is received while one is talking, (4) Q&A through "Chat" is also possible if you do not wish to raise your question verbally, (5) polls, (6) feedback through Chat, (7) use of symbols under the "Reactions" function to show your voice, appreciation, or request, (8) greater reach with a remote audience, and (9) the ability to deliver live and pre-recorded presentations simultaneously.

Please find the best oral award and best poster award by clicking the following link: <https://sciforum.net/event/ASEC2024?section=#awards>

Extended and expanded versions of the conference proceedings papers can be submitted to a Special Issue in the journal *Applied Sciences* after the conference, with a **20%** discount on the article processing charges.

Applied Sciences is an international, peer-reviewed, open access journal on all aspects of applied natural sciences. It is published semimonthly online by MDPI.

We hope the community will share our enthusiasm and help to make this 5th edition a success, and that there will be many more conferences in the future.



Prof. Dr. Nunzio Cennamo

Professor of Electronics at
University of Campania Luigi
Vanvitelli, Naples, Italy



Dr. Stefano Toldo

Robert M. Berne Cardiovascular
Research Center, University of
Virginia, Charlottesville, USA



applied sciences

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Impact Factor: 2.5 (2023); 5-Year Impact Factor: 2.7 (2023)

Keynote Speaker



Prof. Dr. Gabriele Cervino

**Università degli Studi di
Messina, Messina, Italy**

Invited Speakers



Prof. Dr. Armando Ricciardi

Department of Engineering,
University of Sannio, Benevento,
Italy



Dr. Enza Panzardi

Department of Information
Engineering and Mathematics,
Università degli Studi di Siena,
53100 Siena, Italy



Dr. Emanuela Stampone

Department of Precision
Medicine, University of
Campania "Luigi Vanvitelli",
80138 Naples, Italy



Dr. Lihua Lou

Department of Mechanical
Engineering, Clemson University,
Clemson, USA



Prof. Dr. Silvia De la Flor

Mechanical Engineering,
Mechanics of Materials,
Universitat Rovira i Virgili (URV),
Tarragona, Spain



Dr. Giuseppe Trusso

University of Catania,
Catania, Italy



Dr. Xiaobo Wu

Fralin Biomedical Research
Institute at Virginia Tech,
Blacksburg, USA



Dr. Sara Tombelli

Istituto di Fisica Applicata Nello
Carrara – CNR, Florence, Italy



Dr. Laura Pasquardini

Indivenire srl, Trento, Italy



Professor Giuseppina Roviello

University of Naples
Parthenope, Naples, Italy



Prof. Dr. Robert Gourdie

Fralin Biomedical Research
Institute, Virginia Tech Carilion,
Roanoke, USA



Dr. Adolfo Gabriele Mauro

Department of Pediatrics,
Division of Pediatric Cardiology,
Virginia Commonwealth
University, Richmond,
VA 23298, USA



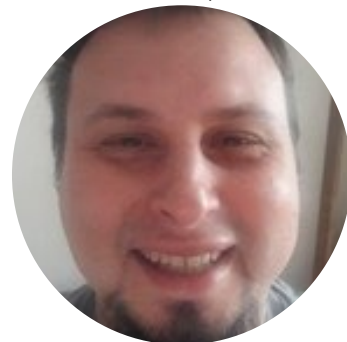
Dr. Mario Acunzo

Virginia Commonwealth
University, Richmond, USA



Dr. Christos Boutopoulos

Department of Ophthalmology,
Faculty of Medicine | University
of Montreal, Montreal, Canada



Prof. Dr. Michal Pawlak

Institute of Physics, Nicolaus
Copernicus University, Toruń,
Poland



Prof. Dr. Rocío Moriche Tirado

Universidad de Sevilla, Seville,
Spain



Dr. Regis Orobtschouk

Institut des Nanotechnologies
de Lyon, Université de Lyon,
INSA Lyon, CNRS, UMR 5270,
Lyon, France



Dr. Josephin Giacomini

University of Camerino,
Camerino, Italy



Mr. Graziano Zappalà

University of Messina,
Messina, Italy

Program at a Glance

	Morning	Afternoon
Day 1	Session 1. Applied Biosciences and Bioengineering	Session 2. Nanosciences, Chemistry and Materials Science
Day 2	Session 2. Nanosciences, Chemistry and Materials Science Session 7. Food Science and Technology	Session 1. Applied Biosciences and Bioengineering Session 3. Computing and Artificial Intelligence
Day 3	Session 2. Nanosciences, Chemistry and Materials Science Session 4. Electrical, Electronics and Communications Engineering Session 5. Mechanical and Aerospace Engineering	Session 8. Applied Physical Science Session 6. Energy, Environmental and Earth Science

ASEC 2024 Program

4th December 2024 (Wednesday)

Session 1. Applied Biosciences and Bioengineering

Time: 9:00 (CET, Basel) | 03:00 (EDT, New York) | 16:00 (CST Asia, Beijing)

Time in CET	Speaker	Title
09:00-09:10	Prof. Dr. Nunzio Cennamo Event Chair	Opening Speech
09:10-09:15	Prof. Dr. Paola Saccomandi Session Chair	Welcome from the session chair
09:15-09:45	Prof. Dr. Gabriele Cervino Keynote Speaker Dr. Graziano Zappalà Invited Speaker	Treatment Of Sea Turtle Shell Fractures: A Novel Approach By Using Bis-Gma-Free Dental Composites
09:45-10:05	Dr. Giuseppe Trusso Invited speaker	Detection of Human Stress Biomarkers by Optical Array
10:05-10:20	Chitaranjan Mahapatra Selected oral speaker	In Silico Electrophysiological Analysis Highlights Cardiac Toxicity of Ibrutinib in B-Cell Lymphoma Therapy through Sodium Current Inhibition
10:20-10:35	Maria Manuela Lageiro Selected oral speaker	Applicability assessment of a proteolytic fermentation broth to leather tanning and protein stain removal
10:35-10:50	Luca Fiorillo Selected oral speaker	Addressing Scientific Misconduct in Dental Publications: From Predatory Journal to Artificial Intelligence Misuse
10:50-11:05	Gergely Kali Selected oral speaker	Novel glutathione-responsive polyrotaxanes with enhanced cellular uptake
11:05-11:20	Jose Alejandro Amezcua Garcia Selected oral speaker	Evaluation of the Effect of Electrode Displacement on Hand Movement Classification
11:20-11:35	Rohit Malik Selected oral speaker	Ethnopharmacological role of plant phytoconstituents (Acteoside) in treatment of Alzheimer's disease
11:35-11:50	Leonardo Bianchi Selected oral speaker	Optical and thermal properties of lung tissue undergoing thermal treatment
11:50-14:00	BREAK	

Session 2. Nanosciences, Chemistry and Materials Science

Time: 14:00 (CET, Basel) | 08:00 (EDT, New York) | 21:00 (CST Asia, Beijing)

Time in CET	Speaker	Title
14:00-14:05	Prof. Dr. Alberto Jiménez Suárez Session Chair	Welcome from the Session Chair
14:05-14:25	Dr. Lihua Lou Invited Speaker	Mechanistic Insights into the Structural and Mechanical Properties of Quantum Dot-Doped Nanofibers
14:25-14:45	Prof. Dr. Sílvia De la Flor Invited Speaker	Some insights into covalent adaptable networks as reversible and recyclable adhesives
14:45-15:05	Dr. Michal Pawlak Invited Speaker	High Accuracy and Precision Method for Measuring Anisotropy in Thin Layers
15:05-15:25	Prof. Dr. Rocío Moriche Tirado Invited Speaker	The effect of Ba _{0.77} Ca _{0.18} Zr _{0.08} Ti _{0.92} O ₃ on the piezoelectric response of flexible PVDF-TrFE-based nanogenerators

15:25-15:40	Francesco Arcadio Selected oral speaker	A low-cost and portable biosensor array for the simultaneous multi-analyte monitoring employed in health and athletic performance exploiting a multi-channel surface plasmon resonance platform based on plastic optical fiber
15:40-15:55	Yurly Garbovskiy Selected oral speaker	Tuning the Electrical Resistivity of Molecular Liquid Crystals for Electro-Optical Devices
15:55-16:10	Matilde de Simão Marques Selected oral speaker	Thermoresponsive Hydrogel Loaded with Clobetasol Piga Nanoparticles for the Treatment of Inflammatory Skin Diseases: Formulation Development and Characterization
16:10-16:25	Erika Saccullo Selected oral speaker	Kojic-Acid-Driven Innovation: Developing Biocompatible and Versatile Catalysts for Sustainable CO ₂ Conversion
16:25-16:40	Antónios Kelarakis Selected oral speaker	Photoluminescent Carbon dots: synthesis, properties and applications

5th December 2024 (Thursday)

Session 2. Nanosciences, Chemistry and Materials Science
Session 7. Food Science and Technology

Time: 9:30 (CET, Basel) | 03:30 (EDT, New York) | 16:30 (CST Asia, Beijing)

Time in CET	Speaker	Title
09:30-09:35	Dr. Antonios E. Koutelidakis Session Chair	Welcome from the session chair
09:35-09:55	Dr. Laura Pasquardini Invited speaker	Natural nanostructures to realize nanoplasmonic biochips for single-molecule detection
09:55-10:15	Dr. Emanuela Stampone Invited Speaker	Measurement of Hepcidin-25 in human serum: development of an intrinsic SPR-based biosensor combining biochemistry and engineering
10:15-10:30	Patricia Iweka Selected oral speaker	Impact of Individual Cow Milk Quality Measurement on Accuracy of Calibration Models Using Near-infrared Spectroscopy
10:30-10:45	Christos Avramopoulos Selected oral speaker	Sour beer fermentation without using bacteria
10:45-11:00	Jong H. Kim Selected oral speaker	Repurposing of natural compound derivatives for control of foodborne fungi and mycotoxins
11:00-11:15	Carina Félix Selected oral speaker	From Sea to Farm: Using Seaweed Extracts for Sustainable Control of Fungal Diseases in Rocha Pear
11:15-11:30	Ana Augusto Selected oral speaker	Apple-Based Biodegradable Film Packaging: A Zero-Waste Solution
11:30-11:45	Ana Gonçalves Selected oral speaker	Extraction of Tannins from Chestnut By-Products for Incorporation Into Chestnut Flour
11:45-14:00	BREAK	

Session 1. Applied Biosciences and Bioengineering
Session 3. Computing and Artificial Intelligence

Time: 14:00 (CET, Basel) | 08:00 (EDT, New York) | 21:00 (CST Asia, Beijing)

Time in CET	Speaker	Title
14:00-14:05	Dr. Eugenio Vocaturo Session Chair	Welcome from the Session Chair
14:05-14:25	Dr. Adolfo Gabriele Mauro Invited Speaker	Hydrogen Sulfide Donors in Cardiovascular Health
14:25-14:45	Dr. Christos Boutopoulos Invited Speaker	NIR laser photothermal immunotherapy of melanoma
14:45-15:05	Dr. Xiaobo Wu Invited Speaker	Detection, Isolation and Quantification of Myocardial Infarct with Four Different Histological Staining Techniques
15:05-15:25	Dr. Robert Gourdie Invited Speaker	Oral Delivery of Therapeutic Peptides for Treatment of Ischemic Heart Disease
15:25-15:45	Dr. Mario Acunzo Invited Speaker	microRNA post-transcriptional modifications: Novel biomarkers and their role in cancer
15:45-16:00	Héctor Penadés Selected oral speaker	A comparative analysis of metric combinations in face verification with machine learning techniques
16:00-16:15	Giacomo Nalli Selected oral speaker	Using clustering of biometric data in evaluating virtual reality experiences

6th December 2024 (Friday)

Session 2. Nanosciences, Chemistry and Materials Science
Session 4. Electrical, Electronics and Communications Engineering
Session 5. Mechanical and Aerospace Engineering

Time: 9:00 (CET, Basel) | 03:00 (EDT, New York) | 16:00 (CST Asia, Beijing)

Time in CET	Speaker	Title
09:00-09:05	Prof. Dr. Stefania Campopiano Session Chair	Welcome from the session chair
09:05-09:25	Prof. Dr. Giuseppina Roviello Invited Speaker	Geopolymers: from sustainable construction materials to environmental remediation
09:25-09:40	Mimimorena Seggio Selected oral speaker	An innovative POF-based device for real-time monitoring of binding processes at ultra-low concentrations via a plasmonic sensor combined with a microcuvette chip
09:40-09:55	Marcello Asciolla Selected oral speaker	Estimating Relativistic Errors in Satellite-Based Geolocation Algorithms with Passive Sensors
09:55-10:10	Fabio Salmeri Selected oral speaker	Evaluating the Environmental Impact of 3D Printing: A Comparative LCA of Electron Beam Melting and Material Extrusion with Metal-Filled Filament
10:10-10:25	Massimiliano Chillemi Selected oral speaker	Design and Evaluation of Aerodynamic Appendages for a Racing Motorcycle Prototype
10:25-10:40	Kevin Kilobocishta Selected oral speaker	Thermal and Mechanical Performance of Cement Mortar Containing Microencapsulated Phase Change Material
10:40-10:55	Daniele Ferrara Selected oral speaker	An Overview of Innovative Space Propulsion Systems: Current Directions and New Technologies
10:55-11:10	Daniel Gomez Lendinez Selected oral speaker	Computational Analysis and Simulation of Polylactic Acid Extrusion in 3D Printing
11:10-14:00	BREAK	

Session 8. Applied Physical Science
Session 6. Energy, Environmental and Earth Science

Time: 14:00 (CET, Basel) | 08:00 (EDT, New York) | 21:00 (CST Asia, Beijing)

Time in CET	Speaker	Title
14:00-14:05	Dr. Cosimo Trono Session Chair	Welcome from the Session Chair
14:05-14:25	Prof. Dr. Armando Ricciardi Invited Speaker	Optoelectronics on Fiber Technology
14:25-14:45	Dr. Enza Panzardi Invited Speaker	Dual Detection of NO ₂ and CO ₂ in Combustion Exhaust Using a Photoacoustic Measurement System
14:45-15:05	Dr. Sara Tombelli Invited Speaker	Surface chemistries and receptors in fiber optic biosensors
15:05-15:25	Dr. Regis Orobtcchouk Invited Speaker	Half etch slot waveguide new platform for Si photonics sensing applications
15:25-15:45	Dr. Josephin Giacomini Invited Speaker	Numerical modeling of coffee extraction
15:45-16:00	Carlos Andrés Rosero-Zambrano Selected oral speaker	Portable, Energy-Autonomous Electrochemical Impedance Spectroscopy (EIS) System Based on Python and Single-Board Computer
16:00-16:05	Dr. Grazia Leonzio Session Chair	Welcome from the Session Chair
16:05-16:20	Mariana Marques da Cunha Selected oral speaker	A Comparison Between Methanol and Carbon Nanotube Production from CO ₂ Inside a Cement Industry

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16:20-16:35	Angelos Alamanos Selected oral speaker	A Cellular Automata Markov (CAM) model for land use change prediction using GIS and Python
16:35-16:50	Michail-Christos Tsoutsos Selected oral speaker	Natural Hazards and Spatial Data Infrastructures (SDIs) for Disaster Risk Reduction

Session 1. Applied Biosciences and Bioengineering

sciforum-103957: In vitro antibacterial activity of native and encapsulated mangiferin against ESKAPE bacteria

Vladislava I. Klimshina *, Roman O. Shaikenov, Svetlana N. Morozkina and Petr P. Snetkov

ITMO University, 197101, Russia

Nowadays, one of the major healthcare problems is the strong increase in the prevalence of resistant bacterial infections. The ESKAPE group (*Enterococcus faecium*, *Staphylococcus aureus*, *Klebsiella pneumoniae*, *Acinetobacter baumannii*, *Pseudomonas aeruginosa* and *Enterobacter* spp) is defined among clinically relevant bacteria, as these pathogens cause the majority of nosocomial infections and have increasing multidrug resistance and virulence. One of the options for alternative treatment of resistant bacterial infections is the use of natural bioactive agents derived from plants with antibacterial properties. The effectiveness of these natural compounds consists in their chemical composition, which allows them to affect multiple sites of bacterial cells and disrupt their essential biological processes. In addition, due to their diverse mechanisms of action, plant secondary metabolites are less likely to induce resistance in pathogens.

Mangiferin is a unique xanthone derivative, one of the main sources of which is *Mangifera indica*. Besides antibacterial activity, this secondary metabolite has numerous pharmacological effects, including antioxidant, antiviral, antidiabetic, anticancer, immunomodulatory, hepatoprotective, analgesic and anti-aging properties.

In vitro studies have shown that mangiferin has a synergistic effect when used with existing antibiotics and/or exhibits an independent inhibitory effect against almost all ESKAPE group bacteria. In addition, there is an opportunity to improve the antibacterial properties of secondary metabolites using various methods, including loading them into polymer matrix-based delivery systems.

In this work, we collected information on the antibacterial properties of mangiferin against the ESKAPE group of pathogens. This review will contribute to future antimicrobial studies of this bioactive compound and to the search for methods of its encapsulation to improve these properties.

This research was funded by the Russian Science Foundation, project number 24-23-00269. Link to information about the project: <https://rscf.ru/en/project/24-23-00269/>



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sciforum-106377: Are 24 bits too high of a resolution for wearable sEMG devices? What open datasets say

Alexandra Gomez Caraveo ^{1,2,*}, Miguel Bravo Zanoguera ^{1,2}, Guillermo Galaviz ¹, Jose Alejandro Amezcua Garcia ^{1,2} and Fabian N. Murrieta Rico ²

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The surface electromyography (sEMG) signal is used in the medical field for treating various diseases related to muscular conditions, as well as in other applications such as video games, gesture detection for smart devices, motion pattern recognition, and monitoring muscle activity in athletes. The proper acquisition, processing, and handling of this signal are important for data reliability. There are specialized devices that digitize the sEMG signal, but since there is no established standard resolution, the resolution varies from one device to another. Currently, semiconductor companies are marketing remarkable 24-bit data acquisition chips. This higher resolution should provide better diagnostics but also demand memory storage and bandwidth resources, which are limited for a wearable device to be practical and realizable. At any rate, it is important to ensure the accuracy of the data for applications requiring the use of the sEMG signal. This article delves into the real resolution used to develop sEMG-based applications by first investigating the open access sEMG database accuracy and comparing it with the claimed resolution. A methodology is proposed for resolution evaluation. Additionally, hand gesture evaluation was conducted using classification algorithms attempting to ascertain the suitability of using 24-bit versus a lower resolution performance. And finally, an investigation of the wireless transmission required for eight high-resolution sEMG channels is presented. Preliminary results of hand gesture evaluation demonstrated a better classification when using 24-bit resolution but only for an accuracy improvement of 0.44% to 1.6% over the 16-bit data resolution. Some of the conditions under which this high resolution may be relevant are identified.



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sciforum-107218: In Silico Structural Analysis of a Putative Class IA Phospholipase A2 from the Brazilian Coral Snake, *Micrurus corallinus*

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³ Centro Bioindustrial, Instituto Butantan, São Paulo 05503-900, Brazil

Introduction: The venom of the coral snake species *Micrurus corallinus* is highly potent and exerts neurotoxic effects through presynaptic enzymes such as class IA phospholipases. However, due to the difficulty in obtaining the venom and the fact that most collected venom is used for antivenom production in Brazil, pharmacological studies of these toxins are scarce. Previous studies have already characterized the primary structure of *M. corallinus* PLA2. With the advent of tools like AlphaFold2 and recent improvements in tools like CHARMM-GUI, in silico studies of these molecules have become more accessible and accurate. This study proposes the *in silico* characterization of *M. corallinus* PLA2, comparing its structure with other characterized elapid PLA2s, evaluating both catalytic and presynaptic toxicity-related residues. **Methods:** The alignment of primary structures of PLA2s from *Micrurus altirostris* (F5CPF0), *Micrurus nigrocinctus* (P81166), *Naja atra* (P00598), and *Pseudechis australis* (P04056 and P04057) was performed using ClustalW. The three-dimensional structure of *M. corallinus* PLA2 was modeled using AlphaFold2. The interactions of the enzyme with its substrates (phospholipid or tridecanoic acid) were analyzed using the CHARMM-GUI web interface and the PPM 2.0 server. All molecular representations were created using the PyMOL molecular graphics software package. **Results:** *Micrurus corallinus* PLA2 presents all residues necessary for catalytic action: CCXXH48D49XC in the active site and GCY28CG30X32GXG in the Ca²⁺ binding loop. Both catalytic mechanisms, the single-water mechanism and the assisted-water mechanism, were evaluated, with the latter being more likely due to the large distance observed between His48 and the Ca²⁺ ion. **Conclusion:** The results indicate that *M. corallinus* PLA2 possesses all the necessary residues to exert its catalytic effects, supporting the possibility that this toxin is responsible for the presynaptic action observed in *M. corallinus* venom.



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sciforum-107697: A Comparative Analysis on Bioethanol production from degradation of Glutinous Rice Straw and Soybean Hull using *Colletotrichum gloeosporioides*

Alexzandrei Gacusan Rara, Julia Irish Remulla Cruz, Lorraine Sofia Dacoscos Geronimo and John Jobert Arlos Sarmiento *

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The Philippines, as a predominantly agricultural country and a leading exporter of agricultural products in Southeast Asia, generates significant agricultural waste each harvest season. Most of these wastes are straws and hulls, which are usually burned, decomposed, and dumped. This presents an opportunity to repurpose these wastes through bioethanol production that can be used in various applications such as in vehicle engines, energy generation, and as an effective industrial solvent. However, the potential of bioethanol from degraded glutinous rice straw and soybean hull using *Colletotrichum gloeosporioides* has not yet been explored. Therefore, this study will evaluate the use of the said fungal plant pathogen, causing leaf rot extracted from mango leaves to convert the agricultural wastes into bioethanol and determine which material produces the higher yield. Both the collected glutinous rice straw and soybean hull will be sun-dried and granulated before *Colletotrichum gloeosporioides* will be introduced to accelerate their biodegradability and to increase their sugar yields in preparation for simultaneous hydrolysis and fermentation (SHF). The collected mixture from SHF will then be distilled to isolate bioethanol yield from the raw materials. The findings of this study will demonstrate the potential for sustainable bioethanol production using local agricultural residues. The application of *Colletotrichum gloeosporioides* for degradation will offer an eco-friendly and cost-efficient alternative to traditional methods. These results will support the country's renewable energy objectives and contribute to environmental sustainability. Furthermore, the study will encourage further exploration of microbial-based renewable energy technologies, highlighting their promising future for bioethanol production.



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sciforum-107629: Insights into Tumors: Morphological Analysis of Spheroidal Tissue Models

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Spheroids are three-dimensional models that play a crucial role in the study of tissues and tumors. Advances in technology have enabled the automated generation of spheroids with various experimental parameters, but the manual analysis of such data is time-consuming and prone to inaccuracies. Therefore, a robust and rapid solution for the morphological analysis of these models is required. This study presents a Python-based algorithm for the quantified analysis of 3D tumor spheroids (PANC1 cell line) produced through a robotic-enabled platform. The pipeline includes sharp image detection, instance segmentation, and contour analysis, using a YOLO (You Only Look Once) machine learning model to identify key morphological features of the tumor models, such as their shape, area, and circularity. The model is custom-trained on a dataset comprising 518 images of 3D tumor spheroids. Its accuracy is validated by comparing its results with manual annotations performed by experts on the test dataset. The model achieved an F1 score of 0.872 in training results, indicating a strong balance between precision and recall in its classification of morphological features. Furthermore, the algorithm facilitates the rapid and reproducible analysis of large datasets, reducing the workload and improving the overall quality of morphological assessment. This contributes to better insights into tumor behavior and the effects of drug treatments.



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sciforum-103604: "Dentomics": Current State of the Literature on Omics in Dentistry

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'Omics' technologies provide a comprehensive understanding of biological systems by analyzing the collective characterization and quantification of pools of biological molecules that translate into the structure, function, and dynamics of an organism. The integration of 'omics' technologies in dentistry has opened new avenues for personalized medicine, particularly in bone regeneration and osseointegration. This review synthesizes the current literature on the application of genomics, proteomics, transcriptomics, and metabolomics in dental research to evaluate their impact on understanding molecular mechanisms and improving clinical outcomes in dental implantology. A comprehensive search was conducted across PubMed, Scopus, and Web of Science, focusing on studies published in the last decade. Key findings highlight the significant potential of omics to personalize treatment strategies based on individual genetic and proteomics profiles, optimize implant surface properties, and elucidate critical signaling pathways involved in bone healing. The review underscores the transformative impact of omics on dental research, driving innovations that enable more precise diagnostics and tailored therapeutic approaches. Six studies meeting all criteria were included for detailed discussion, revealing the critical role of omics in personalizing treatments and enhancing bone regeneration and osseointegration outcomes. By leveraging these technologies, personalized treatment strategies can be better tailored to individual healing profiles, potentially enhancing clinical outcomes. This review concludes that the transformative impact of omics on dental research holds promise for the future of personalized dental medicine.



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sciforum-107340: Anemia in patients with end-stage renal disease: a comparison between hemodialysis and peritoneal dialysis

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Introduction: Anemia is a common complication in patients with end-stage renal disease, especially those on dialysis. Several factors, such as consumed erythropoietin production, iron deficiency, and inflammation, contribute to anemia in these patients. The treatment of anemia differs between hemodialysis (HD) and peritoneal dialysis (PD). HD is associated with blood loss through the extracorporeal circuit, while PD patients generally have better residual renal function and do not experience blood loss. These differences suggest that PD patients may have better control of anemia. Since the care for patients on dialysis has improved in recent years and there are no Brazilian data in this field, we aimed to compare the prevalence of anemia between PD and HD patients.

Methods: This was a cross-sectional study. The laboratory variables evaluated were hemoglobin, ferritin, and the transferrin saturation index. We included all patients who had been on dialysis for at least two months between September 2022 and September 2023. Anemia was defined as hemoglobin level 10mg/dL.

Results: We included 58 patients on PD and 146 on HD. Comparison between PD and HD revealed no difference in age ($p=0.104$) or sex distribution ($p=0.565$). Hemoglobin levels were lower among patients on HD than PD, although this was not significant (10.5 ± 1.7 vs. 11.0 ± 1.7 mg/dL, $p=0.069$). There was no difference in iron or transferrin saturation between groups. Serum ferritin was higher among patients on HD [372 (184, 643) vs. 121 (64, 392) ng/mL, $p=0.008$]. Repeated measures over the year showed no significant change in hemoglobin levels among patients on PD ($p=0.492$) but this was not the case in those on HD ($p0.001$). The prevalence of anemia was similar between HD and PD (35.0% vs. 25.5%, respectively, $p=0.200$).

Conclusion: We found a similar prevalence of anemia and hemoglobin levels between patients on HD and PD, despite higher levels of ferritin among patients on HD. This result suggests the need for a more intense supplementation of iron in patients on HD to target hemoglobin levels.



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sciforum-094630: Bioengineered Neural Interfaces: Pioneering Neurotechnologies for Enhanced Brain-Machine Interactions

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Abstract: Introduction: Bioengineered neural interfaces represent a revolutionary frontier in neuroscience and bioengineering, facilitating seamless communication between the brain and external devices. This research article explores novel advancements in bioengineered neural interfaces, highlighting their transformative potential in enhancing brain-machine interactions and unlocking new capabilities for individuals with neurological disorders. **Methods:** A comprehensive synthesis of recent literature and cutting-edge research findings was conducted, focusing on emerging trends in bioengineered neural interfaces. Key methodologies and technologies, including neural prosthetics, brain-computer interfaces, and neuromodulation techniques, were explored to elucidate their applications in restoring motor function, facilitating communication, and augmenting cognitive abilities. **Results and Discussion:** The findings underscore the transformative impact of bioengineered neural interfaces, with breakthroughs in areas such as neuroprosthetics for limb control, brain-computer interfaces for communication and control, and neuromodulation for treating neurological disorders. From the development of minimally invasive implantable devices to the integration of machine learning algorithms for decoding neural signals, interdisciplinary collaborations are driving unprecedented progress in neural engineering and neurotechnology. **Conclusions:** Bioengineered neural interfaces offer a paradigm shift in neurotechnologies, providing individuals with neurological disorders newfound independence and autonomy. By harnessing the power of neuroengineering and bioinformatics, researchers and practitioners can bridge the gap between the brain and external devices, enabling seamless brain-machine interactions and enhancing quality of life for individuals with neurological impairments. This research article highlights the transformative potential of bioengineered neural interfaces and emphasizes the importance of continued innovation in neuroengineering to address unmet needs in neurological care.



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sciforum-105630: Chemical-Sensing Molecules represented by Two Chromophore Groups used for Accurate Visible (VIS) Spectrophotometric Analysis of Levodopa in a Pharmaceutical

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Levodopa, or L-3,4-dihydroxyphenylalanine, is an amino acid directly obtained from phenylalanine and a medicine widely used for the effective treatment of Parkinson's disease. The main aim of this work was to clearly highlight and develop two quantitative synthesis methods of two new azo dyes possessing chromophore groups, which were obtained by the color reactions of Levodopa with two main chromogenic agents—alpha-naphthol 0,1% and beta-naphthol 0,1 % alcoholic alkalized solutions—in the presence of NaNO₂ 5% and HCl 15%-20%. Following the first color reaction of Levodopa with alpha-naphthol, an intensely bright yellow azo dye was quantitatively obtained and showed a maximum absorption at $\lambda = 418 \text{ nm}$. In the second case, as a result of the second quantitative reaction of Levodopa with beta-naphthol, an intense orange azo dye with a reddish tint at $\lambda = 478 \text{ nm}$ was synthesized. Both azo dyes quantitatively obtained from Levodopa had the azo- **-N=N- reactive groups as color-generating chromophores directly assigned to the signaling moieties of two chemical sensors**. In the first reaction, the azo group was directly linked to alpha-naphthol, and in the second reaction, the azo group was linked to the beta-naphthol aromatic cycle. An important objective of this research was to accurately quantitatively analyze Levodopa in a pharmaceutical following these two new color reactions of L-Dopa with alpha-naphthol 0,1% and beta-naphthol 0,1 %. According to these reactions, two new azo dyes were quantitatively obtained from Levodopa and could be spectrophotometrically dosed at $\lambda = 418 \text{ nm}$ for the intensely bright yellow azo dye and $\lambda = 478 \text{ nm}$ for the intense orange azo dye with a reddish tint. Through the spectrophotometric quantitative analysis of the two azo dyes formed at $\lambda = 418 \text{ nm}$ and $\lambda = 478 \text{ nm}$, it was possible to successfully and accurately quantify Levodopa in a pharmaceutical.



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sciforum-104183: Clinical and surgical indications and current guidelines on the surgical avulsion of third molars.

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Third molar surgery, commonly known as wisdom tooth surgery, is a dental procedure frequently performed to remove these teeth located at the back end of the mouth. Often, third molars do not find enough space to erupt properly, resulting in partial or complete impaction. This condition can cause pain, infection, cysts, tooth decay, and damage to adjacent teeth. The decision to remove third molars is based on a clinical and radiographic evaluation, considering factors such as angulation, depth of impaction and the presence of symptoms. The surgical procedure varies in complexity from simple extraction to more complex procedures that require opening the gum tissue and removing some of the surrounding bone. Local anesthesia is commonly used, but in some cases general anesthesia or sedation may be used. The post-operative period may include swelling, pain and bleeding, managed with pain relievers and antibiotics. Possible complications include infection, nerve damage, and the formation of dry socket. However, with proper planning and surgical technique, most third molar extractions occur without significant problems. Collaboration between dentists, oral surgeons and patients is crucial for the success of the procedure and for rapid recovery, because often, non-cooperation of patients leads to very severe failures and discomfort.



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sciforum-103879: Digital design can be simplified in routine clinical practice: A hybrid digital–analogue technique for maxillary overdenture fabrication.

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This article describes a hybrid digital–analogue workflow for the fabrication of a maxillary overdenture prosthesis, as opposed to an implant-based overdenture. This procedure provides a predictable and accurate technique in five visits by integrating digital and analogue workflows, guided prosthetic surgery, 3D printers and classical total denture techniques.

The introduction of digital technology into the dental world has enabled 3D programming in surgery, prosthetics and orthodontics.

The combined use of intra-oral scanners (IOS), facial scanners and cone beam computer tomography (CBCT) enables the virtual reconstruction of the patient and the design of surgical guides for implant-supported prostheses by means of various types of computer-aided design (CAM) software. The use of optical impressions makes it possible to decrease patient discomfort, as well as speed up and improve communication with the dental laboratory. However, optical impressions present challenges in reporting the resilience characteristics of the mucosa in edentulous patients. A possible solution to improve the performance of the digital workflow is the integration of the analogue technique. The implant-retained overdenture of the upper jaw allows for a significant improvement in chewing ability, speech, sociability and the psychological well-being of patients compared to mucosa-only restorations, with a lower cost of the overdenture.

The overdenture prosthesis is a viable therapeutic choice for all patients in need of total rehabilitation. The use of a hybrid digital–analogue protocol allows for the advantages of both protocols to be combined with speed, precision, comfort, reliability, reproducibility and efficiency.



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sciforum-105272: Ethnopharmacological role of plant phytoconstituents (Acteoside) in treatment of Alzheimer's disease

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Background: Alzheimer's disease is a progressive neurological disorder that primarily affects memory and cognitive function, mostly affecting the elderly population. Although there are currently no disease-modifying treatments for such neurological disorders, there are a number of ways to reduce the risk of Alzheimer's through appropriate diagnosis and by using of natural plant products.

Aim(s): The goal of this research study was to see how the main plant phytoconstituents (Acteoside) overcome Alzheimer's type dementia in rodents by activating the cholinergic system, anti-oxidants, and the protection of neuronal death in the hippocampus region of the brain.

Methods: Investigating the extraction method initially, followed by an in vitro and in vivo investigation in rodent models, and a phytoconstituents analysis using a variety of analytical techniques. Numerous criteria, including behavioral, biochemical, and histological examination, are examined during rodent modeling, using different groups. Subsequently, a standard group including a marketed formulation was used to assess each group.

Results: The hot continuous percolation (Soxhlet) method is used in the preliminary evaluation to determine the percentage yield, which measures 14.10%. Strong antioxidant properties are also shown by the plant extract in the early stages.

Conclusion: The current study suggested that the plant extract in in vivo experiments to prevent related oxidative stress-mediated problems. Further studies are needed to explore the potential medicinal applications of this plant.



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sciforum-107756: Exploring the Bioactive Benefits of Hops for Skincare and Health Applications

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Hops (*Humulus lupulus* L.) have been extensively investigated for their multifunctional properties across various industries, including food, cosmetics, and pharmaceuticals. This study collected samples from several hop cultivars (Nugget, Cascade, Chinook) and wild-type hops from the Bragança region, Portugal. The plant materials studied comprised cones, stems, and leaves, while in the case of the Nugget byproduct, additional plant parts such as seeds, bracts, and vegetative tissue were also analyzed.

The main goal was to use UV-VIS and HPLC spectrophotometric techniques to assess the chemical composition and pharmacological features of hydromethanolic hop extracts. The presence of several phytochemicals, including flavonoids, phenolic acids, alkaloids, and terpenes was associated with the antibacterial, antioxidant, and anti-inflammatory actions of the key bioactive characteristics evaluated. Using enzymatic inhibition tests that target the enzymes tyrosinase, elastase, collagenase, and hyaluronidase, the extracts' sun protection factor (SPF) and dermatological bioactivity were further assessed. Human fibroblast (HFF-1) and keratinocyte (HaCaT) cell lines were used to test in vitro cytotoxicity. The hydromethanolic extracts were found to contain bioactive phenolic compounds, including isoquercetin, kaempferol, rutin, and apigenin. Outstandingly, the extracts exhibited potent antibacterial activity against *Cutibacterium acnes* and demonstrated significant elastase-inhibitory effects.

These bioactivities highlight the potential of hops as a valuable source of bioactive compounds for future applications in pharmaceutical, cosmetic, and nutraceutical development.



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sciforum-104247: Neuro-Fusion: A Unified Approach for Cognitive Workload Classification Using Electroencephalogram (EEG) Data

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In a world marked by perpetual change and constant evolution, the pursuit of optimizing human performance transcends traditional boundaries. Central to this relentless quest is the precise assessment of cognitive workload—an essential element in unlocking and enhancing human potential. Neuro-Fusion represents a pioneering approach poised to revolutionize cognitive workload classification. This innovative methodology seamlessly integrates advanced neural network models with EEG (electroencephalogram) data, merging the capabilities of LSTM (Long Short-Term Memory) and GRU (Gated Recurrent Unit) models into a unified, adaptive framework designed for accurate cognitive workload assessment. At the core of our research lies the real-time application of the Neuro-Fusion model in cognitive workload assessment, powered by EEG data from the STEW dataset. Rigorous EEG data preprocessing facilitated feature extraction, channeling these processed data into the innovative LSTM-GRU hybrid architecture, giving rise to the formidable Neuro-Fusion model. The Neuro-Fusion model achieved remarkable cognitive workload classification accuracy, boasting an impressive 96%. This precision underscores the substantial potential of our approach in providing dependable cognitive assessments, especially in scenarios demanding precision. The implications of our research extend across diverse practical applications. Neuro-Fusion promises to offer invaluable insights into cognitive workloads, facilitating more informed decision-making and enhanced human performance optimization. Its practical implications span various sectors, promising efficiency, productivity, and safety improvements. Neuro-Fusion, merging neural networks with EEG data, revolutionizes cognitive workload assessment, with implications for diverse sectors.



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sciforum-103605: The Future of Dental Care: Integrating AI, Metaverse, Augmented Reality/Virtual Reality, Teledentistry, Computer-Aided Design, 3D Printing, Blockchain, and CRISPR Innovations

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Advancements in technology are revolutionizing the field of dental care, offering unprecedented improvements in diagnostic accuracy, treatment planning, and patient outcomes. This paper explores the transformative potential of integrating cutting-edge technologies such as Artificial Intelligence (AI), Metaverse, Augmented Reality (AR), Virtual Reality (VR), Teledentistry, Computer-Aided Design (CAD), 3D Printing, Blockchain, and CRISPR in dentistry. AI enhances diagnostic precision, particularly in detecting dental caries and periodontitis and planning orthodontic treatments, by analyzing vast datasets and enabling the early identification of oral health issues. AR and VR are reshaping dental education and clinical practice, providing immersive and interactive environments for both training and patient care, thereby improving educational methodologies and reducing patient anxiety. Teledentistry extends dental services to underserved populations, overcoming access barriers and reducing healthcare costs. CAD and 3D Printing streamline the production of dental prosthetics, ensuring precision, efficiency, and customization. Blockchain technology secures patient data, enhancing privacy and enabling seamless information sharing across platforms. CRISPR, a groundbreaking genome editing tool, offers the potential to treat genetic disorders, combat oral cancers, and prevent dental caries. This comprehensive review underscores the importance of balancing these technological advancements with traditional oral hygiene practices to maintain overall oral health. The integration of these technologies heralds a new era in dental care, promising enhanced diagnostic capabilities, efficient treatment processes, and improved patient satisfaction. Dental professionals must stay abreast of these developments and consider their implications for future practice.



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sciforum-105810: The Use of Software in Dental Practice Management: Predictable Tools to Improve Economic Performance.

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Introduction: Today, through management programs, dentists have data at their disposal that can be useful for measuring and planning strategies to better manage their practice. This study aims to analyze the digital benefits and possible outcomes of using new IT solutions. **Materials and Methods:** First and foremost, it must not be taken for granted that all dental practices have a management program and, above all, that they correctly enter the information intended to allow for the subsequent monitoring of their center's performance. Constant monitoring is to be carried out under the logic of analyzing the two macro-areas of management control, namely effectiveness and efficiency. **Results:** Today, the amount of information available to dental practices is truly substantial, but it is only truly usable if it is correctly entered into a management system or other electronic support: the quality of the data is fundamental since imprecise, partial, inconstant, or uncoded data do not allow for subsequent processing and render the great compilation efforts made by the entire team useless. The first step along the path of computerizing a dental practice is to determine the objectives to be achieved. **Conclusion:** It is fundamental to avoid criticalities that are rarely attributable to the software itself, but to the process of change that must be implemented within the practice. Computerization is a radical change and involves an investment in terms of time and commitment on the part of the staff involved.



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sciforum-107311: Unlocking neural networks: Explainability techniques for enhanced performance in automatic peripheral blood cell recognition

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Introduction and objectives:

Automatic classification systems have significantly advanced in hematology, enabling the identification of over 80% of hematological diseases through peripheral blood cell analysis. However, their black box nature complicates adaptation to new images with variability, affecting precision and reliability. This study proposes a methodology using explainability techniques, such as LIME and Saliency Map, to enhance model performance in the identification of leukocytes and other cell types.

Methods:

A dataset of 12298 leukocyte images, labeled by clinical pathologists and divided into five classes, basophils (1218), eosinophils (3117), lymphocytes (1214), monocytes (1420), and neutrophils (3329), was used to train a VGG19 convolutional neural network, achieving 98% accuracy on the test set. The model was then evaluated on a second dataset comprising neutrophils (416), lymphocytes (104), monocytes (43), and eosinophils (10), where accuracy dropped to 83%. Analysis of the 100 best- and 100 worst-classified images from both sets revealed that, in correctly classified images, Saliency Map showed high pixel activation across the entire cell except the nucleus, whereas misclassified images focused on the nucleus. LIME indicated a dependency on image borders.

Results:

To address this, zoom-based data augmentation was applied, reducing the model's reliance on superior and inferior borders. Progressive layer unfreezing revealed that adjusting the fourth convolutional block reduced focus on the nucleus and improved cell-wide activation. After re-training, performance significantly improved, achieving 99.4% accuracy, 99.8% precision, 99.6% sensitivity, 99.9% specificity, and a 99.6% F1-score on the second dataset.

Conclusion:

The proposed approach demonstrates that integrating LIME, Saliency Map, and layer unfreezing can effectively identify and adjust specific layers impacting model interpretability and accuracy. This integration enhances adaptability and interpretability in diverse clinical contexts, supporting improved model performance under varying data conditions.



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sciforum-104390: 3D Motion Capture in Tennis: A Markerless Approach with MocapMe for Biomechanical Analysis

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Tennis requires precise and rapid movements, making biomechanical assessments essential for optimizing player performance and preventing injuries. Traditional motion capture methods, while effective, are often expensive, highlighting the need for markerless alternatives. This study presents a dual-camera setup for 3D motion capture, expanding on previous research in this field. The system was tested using videos of tennis players recorded at a provincial Tennis Club, with MocapMe, a framework built on DeepLabCut and OpenPose.

The dataset includes synchronized recordings from two cameras capturing tennis strokes such as serves, forehands, and backhands, providing a robust foundation for analysis. A ResNet152 architecture was fine-tuned on this dataset to enable accurate 3D pose estimation. Preliminary tests indicate high accuracy in detecting key points, especially during complex movements like serves, and demonstrate the system's stability across multiple trials. Although exact performance metrics are still being finalized, early results suggest that the system's accuracy is expected to significantly outperform previous 2D models, showing lower error rates and greater consistency.

This system offers rapid performance analysis and valuable insights for technique improvement and injury prevention. It holds significant potential for applications in sports biomechanics research, offering a practical solution for 3D biomechanical analysis in tennis. Future work will expand the dataset and integrate additional machine learning models to further enhance the system's capabilities.



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sciforum-103525: 3D STS Motion Analysis Using MocapMe DeepLabCut-Based Approach

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The Sit-to-Stand (STS) motion is a critical functional activity often analyzed in clinical and biomechanical studies. This research examines the application of MocapMe (DeepLabCut-Based approach), a robust pose estimation tool, trained with data processed through OpenPose, for accurate STS motion analysis. By employing a two-camera setup, the author achieves a more comprehensive three-dimensional reconstruction of the movement, enhancing the accuracy and reliability of the kinematic data. OpenPose provides initial pose estimations, which are subsequently refined and filtered to eliminate noise and improve landmark detection accuracy. These refined data sets are then used to train MocapMe (DeepLabCut-based approach), leveraging its capability to adapt to specific datasets for more precise tracking. The dual-camera system captures the STS motion from different angles, allowing for a more complete understanding of the biomechanical nuances involved in the transition. This setup significantly improves the robustness of the pose estimation by reducing occlusions and providing a fuller representation of body movements. The combined approach improves the accuracy of movement analysis and facilitates the identification of subtle variations in motor patterns, which are crucial for clinical assessments and rehabilitation monitoring. The results demonstrate that integrating OpenPose and DeepLabCut with a two-camera system can offer an effective, low-cost solution for detailed biomechanical analysis in both research and clinical settings, advancing the accuracy of human movement studies.



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sciforum-106632: A Custom Convolutional Neural Network Model-Based Bioimaging Technique for Enhanced Accuracy of Alzheimer's Disease Detection

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Alzheimer's disease (AD), an intense neurological illness, severely impacts memory, behaviour, and personality, posing a growing concern worldwide due to the aging population. Early and accurate detection is crucial as it enables preventive measures and personalized healthcare strategies that can significantly improve patient conditions. However, current diagnostic methods are often inaccurate in identifying the disease in its early stages, which is essential for effective treatment. Although deep learning-based bioimaging has shown promising results in medical image classification, challenges remain in achieving the highest accuracy for detecting AD. Existing approaches such as ResNet50, VGG19, InceptionV3, and AlexNet have shown potential, but they often lack reliability and accuracy due to several issues. To address these gaps, this paper proposes a new bioimaging technique by developing a custom Convolutional Neural Network (CNN) model for AD detection. This model is designed with optimized layers to enhance feature extraction from medical images, which are pivotal in identifying subtle biomarkers associated with AD. The experiment's first phase involves the construction of the custom CNN model with three convolutional layers, three max-pooling layers, one flatten layer, and two dense layers. The Adam optimizer and categorical cross-entropy are adopted to compile the model. The model's training is carried out on 100 epochs with the patience set to 10 epochs. The second phase involves augmentation of the dataset images and adding a dropout layer to the custom CNN model. In addition, fine-tuned hyperparameters and advanced regularization methods were integrated to prevent overfitting. A comparative analysis of the proposed model with conventional models was performed on the dataset both before and after data augmentation. The experimental results demonstrate that the proposed custom CNN model significantly outperforms the pre-existing models, achieving a training accuracy of 100% and a testing accuracy of 99.79%, with a low training loss of 1.0148×10^{-5} and a testing loss of 0.0205.



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sciforum-104240: A Hexa-Band Refractive Index Sensor Using a Symmetrical Boss-Cross Terahertz Metamaterial Absorber with Biomedical Applications

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Terahertz (THz) metamaterial absorbers have become a prominent research topic in recent years. In this paper, a hexa-band metamaterial absorber is designed for bio-medical sensing applications. The design can detect changes in the surrounding medium's refractive index and operates in the refractive index range of 1.3 – 1.4, with six prominent absorption peaks. The proposed structure comprises a square ring resonator made up of gold with a boss-cross structure at the center, on top of a Gallium Arsenide (GaAs) substrate with a thickness of 8 μm . When the surrounding medium's refractive index is 1.4, it offers six absorption peaks at 0.537 THz, 2.573 THz, 3.025 THz, 3.146 THz, 3.493 THz, and 3.739 THz, with corresponding peak absorptions of 75%, 92.9%, 98.4%, 95.3%, 94.1%, and 97.7%, respectively. The structure was designed at $n = 1.4$ instead of $n = 1$, as several biological specimens, such as blood, breast cells, etc., have a refractive index in the range of 1.3 - 1.4, and it offers six bands for $n = 1.4$. This choice was made because many biomedical applications have a refractive index around 1.4. The design parameters were selected through a parametric analysis so as to achieve maximum absorption peaks. The design was also tested with different polarization angles, and it was discovered that the absorber is polarization-insensitive. This design can inspire future research on the biomedical application of THz absorbers.



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sciforum-104033: A Novel Method for Transferring Ideal Incisor Position from Cephalometric Analysis to Virtual Set-Up

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Introduction. This scientific contribution aims to describe a new methodology to improve diagnosis and treatment planning in daily orthodontic practice.

Methods. The proposed methodology is described by reporting a series of cases that were assessed before treatment according to the standardized digital workflow reported below. Cephalometric analyses of the included cases were performed using the “WebCeph” platform (Software Version: 1.5.0, Assemble Circle Corp., Republic of Korea), and the buccolingual inclinations of the upper incisors were assessed. Using individualized templates, the ideal position and inclination of the upper incisors were determined on the cephalometric tracing, and linear and angular differences of the incisors were measured and compared to pre-treatment values. A virtual set-up of the case was generated with a 3Shape Ortho System 2022 (3Shape, Copenhagen K, Denmark). As the first step of the virtual set-up, the positions and inclinations of the upper incisors were adjusted according to the cephalometric differences previously evaluated. Subsequently, the final set-up was defined according to the planned position of the central incisors.

Results. For the first time in the orthodontic literature, this new method describes the following workflow: planning the position of the upper incisors with respect to the cranial base structures, transferring this position to the virtual set-up, and obtaining a set-up that realistically shows the real orthodontic movements in the anteroposterior direction. This method clearly and immediately defines the ideal anchorage management, thereby facilitating the ideal biomechanical case management.

Conclusions. This article outlines an original method that combines patient data derived from cephalometric analysis with data obtained from study model analysis. This combination is used to identify the ideal position and buccolingual inclination of the upper incisors on cephalometric tracing and to transfer this position to an ideal orthodontic virtual set-up.



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sciforum-104024: A Single-Dose Treatment of *Alstonia boonei* Stem Bark Extract Elicits Anti-inflammatory Effect *in vivo*

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Introduction: This study aimed to investigate the anti-inflammatory effect of methanol extract of *Alstonia boonei* stem bark in a lipopolysaccharide (LPS)-induced model of inflammation.

Methodology: Twenty Wistar albino rats were divided into five groups (n=4). Group 1 served as the normal control, while groups 2-5 were induced with 10 mg/kg b.wt of LPS dissolved in normal saline. Thirty minutes after lipopolysaccharide (LPS) induction, group 3 (standard control) and groups 4 and 5 (*Alstonia boonei* groups) were treated with the standard drug (50 mg/kg of ibuprofen) and 250 mg/kg and 500 mg/kg (AB₂₅₀ and AB₅₀₀) of the *Alstonia boonei* extract, respectively. Blood was collected from the animals six hours post-treatment for biochemical analysis.

Results: The acute toxicity study demonstrated a high safety profile of the extract, with an LD₅₀ exceeding 5000 mg/kg body weight in mice. Phytochemical analysis of the *Alstonia boonei* methanol extract revealed the presence of diverse bioactive compounds, including pomiferin, quercetin, ellagic acid, rutin, coumarin, stilbenes, catechol, and gallic acid, amongst others. The *in vivo* results showed that the untreated group had a significantly higher (p < 0.05) increase in Interleukin-6 (IL-6), Nuclear factor kappa B-p65 (NFKB-p65), and Interleukin 1 beta (IL-1 β) activities in the untreated group compared to the normal control group. In the treatment groups, both doses of the extract (AB₂₅₀ and AB₅₀₀) caused significant reductions in IL-6 and IL-1 β levels but not NFKB-p65.

Conclusion: This result highlights the rich bioactive store of *A. boonei* stem bark and its potential to modulate inflammatory responses *in vivo*.



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sciforum-103866: Addressing Scientific Misconduct in Dental Publications: From Predatory Journal to Artificial Intelligence Misuse

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Scientific misconduct and the misuse of artificial intelligence (AI) pose significant threats to the integrity of academic research, particularly in the field of dental publications. This paper provides a comprehensive review of various forms of malpractice, including citation doping, the proliferation of predatory journals, inappropriate citation requests, and the unethical application of AI in research and publication processes. These malpractices undermine the credibility and reliability of scientific outputs, compromising the advancement of knowledge and evidence-based practices. This review highlights the impact of citation doping, a practice where authors manipulate citation counts to enhance their academic profiles unethically. Additionally, the rise of predatory journals, which prioritize profit over scholarly integrity, is discussed. Inappropriate citation requests, where authors are pressured to include unnecessary citations to inflate the impact factors of certain journals, are examined for their detrimental effects on research quality. The misuse of AI, including the generation of fraudulent data and plagiarism, is critically analyzed. By drawing on international guidelines and best practices, this paper proposes a robust framework to promote ethical research and publication practices. The measures recommended aim to enhance the quality and credibility of research in the dental field, ensuring that scientific contributions are both trustworthy and valuable.

Scientific integrity is the cornerstone of academic research, yet recent trends have highlighted significant issues of misconduct within the field of dental publications. These malpractices include citation doping, the use of non-peer-reviewed journals, predatory publishing, and the emerging misuse of artificial intelligence (AI) in research processes. This paper aims to discuss these issues, summarize expert interventions, and propose a set of guidelines to combat scientific misconduct and AI misuse.



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sciforum-103926: Advancing Dental Diagnostics with AI: UNet for Precision in Treatment and Anatomy Mapping

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Medical imaging methods are crucial in dental patient care for diagnosing pathologies related to teeth and surrounding structures. Radiological techniques, such as cone-beam computed tomography (CBCT), are vital for orthodontic diagnosis, treatment planning, and monitoring. With the increasing number of radiological examinations, there is a growing need for comprehensive diagnostic tools. To address this, Artificial Intelligence (AI)-based systems have emerged. Machine Learning (ML) has significantly impacted medical specialties, including orthodontics, offering promising results. ML enables early screening, accurate diagnosis, appropriate treatment, and prediction of treatment-associated toxicity for maxillofacial cysts and tumors. Additionally, ML models are valuable for planning, evaluating, and improving dental implants. The purpose of this work was to develop an algorithm for dentistry aimed at recognizing pathologies observable in second-level instrumental investigations, to present them in a simplified way both to expert dentists and those who intend to approach image reading. Six patients (3M, 3F, ages 29-61) with various dental treatments were selected. UNet was used for segmentation, performing pixel-wise classification to localize and distinguish the edges of structures in the images. The model's architecture allows the input and output to share the same dimensions, facilitating accurate delineation of dental structures. The training utilized a dataset of annotated images to enhance the model's capacity to identify and differentiate various dental treatments and conditions. Once training was complete, the neural network was tested on a separate dataset known as the test set, which consisted of data not used during the former phase. This testing phase aimed to evaluate the neural network's performance in practical scenarios and provide an objective estimate of its segmentation capabilities. UNet effectively demonstrated its ability to precisely identify and highlight structures of interest, including those that are smaller in size, thereby reducing the manual workload of dental operators.



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sciforum-103848: Affective Temperaments and Depressive Rumination in an Italian-Spanish sample with bruxism

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Introduction

Bruxism, a condition characterized by teeth grinding or clenching, is a complex issue influenced by various factors. From a mental health perspective, bruxism has been linked to psychopathological variables, i.e., anxiety, depression and ruminative thinking. The aim of this study is to investigate the psychological traits associated with affective components in an Italian-Spanish sample with bruxism.

Method

In total, 581 subjects were examined and data were collected through online survey including the Ruminative Response Scale (RRS) and the Brief Italian Version of the TEMPS-A (Temperament Evaluation of Memphis, Pisa, Paris, and San Diego Autoquestionnaire). Differences between the groups were assessed using Student's t-test for independent samples. In addition, a linear regression analysis was performed, in which the Ruminative Response Scale variable was considered the dependent variable, and all the TEMPS-A factors were included in the equation, to assess which temperamental dimensions could act as specific predictors of depressive rumination in patients with bruxism.

Results

The analyses revealed statistically significant gender differences concerning Depressive, Cyclothymic, Hyperthymic, and Anxious temperaments, as well as components of Depressive Rumination. Furthermore, linear regression analysis showed that Depressive, Cyclothymic, and Anxious temperaments are predictive of the Depressive Rumination variable.

Conclusions

These preliminary results suggest the relevance of affective temperaments and Depressive Rumination in the clinical population of patients with bruxism.



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sciforum-107370: Antimicrobial Screening of Soil Filamentous Fungi: A Search for New Bioactive Agents

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Introduction: The increasing resistance of microorganisms to antibiotics has highlighted the urgent need for new antimicrobial agents. Filamentous fungi, commonly found in soil, are known producers of bioactive compounds, including antimicrobial agents. This study aimed to isolate and evaluate the antimicrobial activity of filamentous fungi found in soil samples, with the objective of identifying potential new sources of antimicrobial compounds that may offer alternatives to conventional antibiotics.

Methods: Soil samples were collected from a biological garden on the University Lusófona campus to isolate filamentous fungi using selective media. The isolated fungi were then subjected to antimicrobial activity tests using the agar well diffusion method against two pathogenic bacterial strains: *Escherichia coli* (Gram-negative) and *Staphylococcus aureus* (Gram-positive). The fungi that exhibited the most promising results were selected for DNA analysis. To accurately identify the fungal species, DNA extraction and polymerase chain reaction (PCR) amplification were performed. Sequencing data were analysed using the BLAST algorithm to confirm the identities of the isolated fungi.

Results: Several filamentous fungi were successfully isolated from the soil samples, including *Penicillium pimateouiense* and *Aspergillus niger*. Both fungi exhibited significant antimicrobial activity, as demonstrated by the formation of inhibition halos in the presence of *E. coli* and *S. aureus*. These results indicate these fungi's potential to produce antimicrobial compounds effective against *S. aureus* and *E. coli*, two of the most representative pathogenic bacteria.

Conclusion: This study supports the potential of soil microbiota, particularly filamentous fungi, as a rich resource for discovering new antimicrobial compounds. The findings highlight the importance of further research to explore the mechanisms of action of these compounds and to develop them for clinical applications. The isolated fungi, namely *P. pimateouiense* and *A. niger*, show promise as sources of new antimicrobial agents that could help combat antibiotic resistance and pathogenic bacteria.



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sciforum-104439: Applicability assessment of a proteolytic fermentation broth to leather tanning and protein stain removal

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The use of alkaline microbial proteases makes the industry more eco-sustainable, both in terms of reducing the consumption of chemical products and in terms of lowering effluent treatment costs.

A proteolytic *Bacillus* strain isolated from a tannery alkaline bath was used to produce extracellular proteases by submerged fermentation in bioreactor and the produced proteolytic broth was applied in leather tanning and protein stain removal.

The tanning process application consisted of using fermentation broth with 780 LVU (Löhlein-Volhard Unit) proteolytic activity on half-skin tanning, and the other half-skin was tanned using a commercial enzymatic bate (OROPON) with same proteolytic activity and tanning conditions.

The physical properties of the hide tanned using proteolytic broth and the hide tanned with commercial bate were assessed in terms of bursting load (kg) and bursting elongation (mm) for hides with two different leather thicknesses (2.4 mm and 1.6 mm). The hide tanned with the produced broth showed better physical tests of bursting (with elongation till 6.8 mm before bursting) than the one tanned with commercial proteases (elongation only till 6.3 mm) for same bursting load of 19 kg and 1.6 mm leather thickness. The thicker leather (2.4 mm) showed the same bursting elongation of 10 mm for a higher load (54 Kg) for the hide tanned with bulk proteases than commercial proteases.

Protein stain removal from cotton fabric (squares of cotton fabric with 4 cm sides with the centre stained with egg, blood, soya sauce and English sauce) was tested using the produced proteolytic broth and compared with the use of water (blank), or a commercial detergent, under the same agitation at room temperature. The proteolytic broth showed better blood and egg stain removal than water or the detergent.

Produced proteases can be used in protein residue and effluent treatments. Applications showed potential for use in the bioeconomy and for green chemistry.



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sciforum-095944: Bacterial Infection Models In Mice Used In The Research Of Antimicrobial Compounds

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Antimicrobial resistance represents one of the main threats to global health due to some pathogens being extremely resistant to existing antibiotics. In this scenario, it is necessary for new drugs to become promising. To this end, in vivo nonclinical trials are an important step in the development of new drugs due to their relatively low cost, the possibility of mimicking pathological conditions in living organisms, and the fact that they provide relevant data on toxicity and antibacterial activity. However, there is no homogeneity in the studies regarding the techniques and protocols used to achieve the desired clinical conditions. This is a narrative review, the objective of which is to evaluate which models are used to induce sepsis in mice. The research was carried out using the PubMed and Virtual Health Library databases, with the descriptors “models of bacterial infection”, “mus musculus”, “sepsis”, and “in vivo”, using the AND and OR connectors. Twenty-seven articles were selected, of which 40% used the intraperitoneal technique—with the species *Escherichia coli* and *Staphylococcus aureus* being the most commonly used—33% were performed with cecal puncture ligation (CPL), and in the other 26%, the administration route was intravenous, preferably via the caudal route. In most studies, the final disease induced was sepsis, differing in relation to the focus, which varied between urinary, abdominal, and pulmonary. The main organs removed were the spleen, lungs, liver, and kidneys, which were subjected to histopathological examination and bacterial count. Thus, it is concluded that the most commonly used models are obtained via the intraperitoneal administration route and CPL and that there is a wide range of protocols used for confirmation.



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sciforum-105130: Bispecific Antibodies in Oncology with Dual-Targeting, Immune System Activation, Enhanced Tumor Specificity, Adaptive Immune Engagement, and Novel Linker Technologies for Advanced Precision Cancer Immunotherapy

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The emergence of bispecific antibodies (BsAbs) represents a groundbreaking advancement in oncological therapeutics, offering innovative approaches for precision cancer immunotherapy. These specialized antibodies are engineered to bind simultaneously to two distinct antigens, thereby facilitating dual-targeting strategies that enhance therapeutic precision and efficacy. This dual engagement not only improves the targeting of malignant cells but also addresses limitations observed with conventional monoclonal antibodies. One of the most compelling features of BsAbs is their capacity to modulate the immune system in a more sophisticated manner. By simultaneously interacting with tumor-associated antigens and immune cell receptors, BsAbs orchestrate a more potent and directed immune response against cancer cells. This immune modulation addresses the challenge of immune evasion employed by tumors, potentially leading to improved therapeutic outcomes. Enhanced tumor selectivity is another significant advantage of bispecific antibodies. By directing therapeutic activity towards specific tumor antigens, BsAbs minimize off-target effects and reduce collateral damage to normal tissues, thereby improving the safety and efficacy profiles of cancer treatments. This selectivity is further refined by cutting-edge linker technologies that optimize the stability, pharmacokinetics, and overall performance of BsAbs. The dynamic nature of the adaptive immune engagement enabled by BsAbs facilitates interactions with various immune system components, including T cells and natural killer (NK) cells. This review delves into the innovative landscape of bispecific antibodies in oncology, emphasizing their dual-targeting capabilities, immune modulation, and tumor selectivity, and the role of advanced linker technologies. By examining these advancements, this review aims to illuminate the transformative potential of BsAbs in advancing precision cancer immunotherapy and improving patient outcomes.



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sciforum-104006: Color Stability of PET-G in Clear Aligners: Impact of Prolonged Exposure to Everyday Substances and its Psychological and Social Implications

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Introduction: The transparency and aesthetics of clear aligners are critical factors that influence patient satisfaction and psychological and social well-being. Based on our previous research on the chemical-physical characterization of polyethylene terephthalate glycol (PET-G) aligners exposed to staining agents and cleaning solutions, this study aimed to evaluate the color stability of PET-G after prolonged exposure to everyday substances, potentially due to chemical interactions affecting aligner transparency.

Methods: Twenty-five sheets of PET-G and a truncated pyramid-shaped thermoforming mold were used to obtain flat samples (n = 220). These samples were immersed in various substances (coffee, tea, Coca-Cola, red wine, colloidal silver-based disinfectant, nicotine, artificial saliva, cigarette smoke, and three saliva solutions mixed with plain, coffee, and nicotine). Immersion times of 10 (n = 110) and 15 days (n = 110) were randomized. L*a*b* parameters were measured before and after immersion for colorimetric assessment, and the total color change (ΔE) was calculated for evaluation. Statistical analysis included nonparametric tests, with significance set at P 0.05.

Results: Significant colorimetric changes were detected in PET-G samples exposed to acidic or polyphenol-rich substances, suggesting that chemical interactions may drive discoloration. Pairwise comparisons highlighted significant differences between ΔE values for groups exposed to different substances, particularly coffee, tea, and Coca-Cola, at both immersion durations. In addition, highly significant colorimetric changes were demonstrated between the two times, particularly for samples exposed to coffee, tea, and Coca-Cola. Clinical evaluations revealed slight to noticeable color changes, with Coca-Cola causing more pronounced changes, especially after 15 days.

Conclusions: Prolonged exposure to certain substances significantly affects PET-G's color stability, likely due to chemical adherence and degradation mechanisms, which has important psychological and social implications for patients undergoing orthodontic treatment. This study underscores the need for proactive strategies to maintain aligner transparency and enhance patient satisfaction.



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sciforum-103607: Comparative Evaluation of Composite Splinting and Thermoformed Removable Splints in Managing Dental Mobility Due to Periodontitis: A Clinical and Quality of Life Assessment

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Periodontitis associated with dental mobility is an inflammatory disease of the periodontium that leads to the deterioration of the supporting tissues of the teeth, resulting in a loss of stability and subsequent dental mobility. The primary objective of this study was to evaluate the clinical efficacy and patient-reported quality of life associated with replacing conventional composite splinting for dental mobility with removable thermoformed splints through a literature review of clinical studies. Conventional composite splinting, although mechanically stabilizing teeth, often exacerbates gingival conditions and complicates oral hygiene maintenance. This study hypothesizes that removable splints would improve periodontal health and hygiene practices while offering comparable esthetic and social benefits. Clinical assessments included periodontal status and dental mobility measurements, while patient-reported outcomes focused on oral hygiene, esthetic satisfaction, and overall quality of life. Patients using thermoformed splints reported significantly better oral hygiene practices due to the ease of removal and cleaning of the splints. Clinically, a reduction in periodontal inflammation and plaque accumulation was observed in patients using removable splints compared to those with composite splinting. The esthetic and social aspects of the thermoformed splints were rated higher by patients, with improved satisfaction in social interactions and phonation. Additionally, the composite splints showed a higher propensity for bacterial proliferation due to their material properties and deterioration over time. Thermoformed removable splints offer a viable alternative to conventional composite splinting for managing dental mobility due to periodontitis. They facilitate better oral hygiene, reduce periodontal inflammation, and enhance patient satisfaction in the esthetic and social domains.



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sciforum-105257: Comparative evaluation of images of alveolar bone loss using panoramic images and artificial intelligence

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Aim: The present study aimed to employ a VGG-16 convolutional neural network (CNN) system to determine alveolar bone loss and periodontal disease/health status from dental panoramic radiography images.

Materials and Methods: This study was conducted with a dataset of panoramic images obtained from an institution. The training dataset contained 1874 panoramic images, of which 953 were of bone loss cases and 921 were of periodontally healthy cases. The presence/absence of resorption at the bone crest was recorded in consideration of the distance between the enamel-cementum junctions of the teeth and the alveolar bone crest. Radiographs showing bone resorption with a horizontal/vertical shape or bone defects were included in the bone loss group. Images with artefacts, image distortion, and blur were excluded. All images in the dataset were resized to 1472 x 718 pixels, followed by preprocessing for arbitrary sequence formation using python language along with OpenCV, NumPy, Pandas, and Matplotlib libraries to generate an image dataset. The dataset was divided into a testing set and validation set. The validation dataset was used to validate the model. The Feature Extraction approach **strategy with 10–20 epochs and learning rate 1e-4 (0.0001) for trainable layers were used.** Training and validation datasets were used to predict and generate optimal weight factors for this CNN.

Results: Of 100 bone loss cases, the CNN system evaluated 92 correctly and 8 incorrectly. Further, of 100 periodontally healthy cases, it evaluated 89 correctly and 11 incorrectly. The sensitivity, specificity, precision, accuracy, and F1 score were 0.8317, 0.8683, 0.8918, 0.8927, and 0.8615, respectively.

Conclusion: The CNN model was successful in assessing the alveolar bone loss and periodontal disease status using panoramic radiographs. This study resulted in effective image segmentation which can more accurately predict grading of periodontal bone loss, avoiding user interpretation for overlapping on periodontal classification.



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sciforum-105728: Computational approaches for molecular characterization, structure-based functional elucidation, and drug design of uncharacterized transcriptional regulator Rv0681 protein of *Mycobacterium tuberculosis*

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Microorganisms belonging to the *Mycobacterium tuberculosis* (MTB) complex cause tuberculosis (TB), a contagious respiratory illness. While MTB is mainly associated with lung infections, it has the potential to cause illness in several other organs and tissues. MTB infection can progress from a state of containment within the host, where the bacteria remain confined to granulomas (latent TB infection), to a communicable stage, marked by the manifestation of symptoms. Recently, there have been worries over novel strains of MTB and multidrug-resistant tuberculosis. Consequently, experts have expressed worries regarding efforts to suppress MTB as a means to enhance healthcare administration and avert TB. This study aims to characterize the uncharacterized HTH-type transcriptional regulator Rv0681 protein, examine its physicochemical properties, investigate protein--protein interactions, document functional annotations, anticipate its structure, and design a computational drug to prevent potential protein infections. The instability index has identified this protein as stable. The protein is predicted to be involved in the transcriptional regulation of the TetR family. It has an HTH-type TetR domain. Gene ontology studies demonstrated that this protein is involved in both molecular and biological processes. The enzyme and pathway databases indicate that this protein participates in a reaction that phosphorylates Rv0681, resulting in the production of phosphorylated Rv0681 and ADP. To predict the 3D structure of the protein, three different servers were employed and were used to compare the outcomes, with AlphaFold being documented as the best structure-predicting server. Maestro software was used to perform molecular docking between the drug molecule (proflavine) and the selected protein, resulting in a docking energy of -8.151 kcal/mol.



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sciforum-106554: Computational approaches to find inhibitors for human papillomavirus-induced cervical cancer

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Human papillomavirus infection is the cause of cervical cancer. The majority of human papillomavirus (HPV) infections are benign and resolve on their own. However, there is a risk of chronic infection with high-risk strains of HPV. Human HPV turns on the E6AP ubiquitin-protein ligase (E3), which makes it easier for the p53 tumor suppressor protein to break down in cervical cancer. The p53 tumor suppressor protein is a governing protein that inhibits tumorigenesis by regulating cell division and facilitating DNA repair mechanisms. The p53 protein resides in the nucleus of cells across the organism. Human malignancies often display this mutation, which may confer resistance to oncological therapies. A third type of enzyme, called an E3 ubiquitin-protein ligase, takes ubiquitin from an E2 ubiquitin-conjugating enzyme as a thioester and moves it to its target proteins. In this study, we prepared the protein and potential ligand molecules for molecular docking studies. We also applied computational strategies to demonstrate the pharmacokinetic properties in five different stages of the selected ligands that describe the drug's journey through the body. The objective of this study is to identify nature-derived compounds that have the ability to inhibit the E6AP-UbcH7 protein complex. These compounds have the potential to inhibit the harmful effects of HPV on the p53 tumor suppressor in cervical cancer. After performing docking between the ligand molecules and the receptor protein molecule, we determined the molecular docking scores. We found that kaempferol required the least energy to interact with the protein (docking score of -5.896 kcal/mol). The molecular docking and ADMET test results indicate that kaempferol is the most promising therapeutic candidate compared to the other compounds.



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sciforum-104650: Cultivation of green microalgae in the air

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Microalgae are cultivated for a broad range of applications, from food to cosmetics, and from biofuel to biotechnology. While usually grown in suspension in bioreactors, this technique poses several challenges regarding processing, especially with respect to illumination, and harvesting. Alternatively, some microalgae can be cultivated on suitable substrates in the form of a biofilm to solve the problem of harvesting. In this case, however, a constant and sufficient light intensity on the microalgae without overheating the medium is still problematic. A previous project has thus investigated the possibility of letting green microalgae grow on a suitable substrate outside a bioreactor, i.e., in the air, under regular wetting, which would improve illumination and ease harvesting. Here, we report the growth of the green microalgae *Chlorella vulgaris*, which is often used as dietary supplement or for cosmetics on textile substrates outside a bioreactor. We show how the first setup was improved in terms of fixing the textile, ensuring regular watering and increasing the available light on the substrates. Our comparison between *C. vulgaris* grown on identical textile fabrics in a bioreactor, in a petri dish, and in the air show that the latter leads to a significantly higher microalgae growth than both the more common methods, and that cultivation of microalgae at the air should thus be optimized further in future studies.



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sciforum-107306: Deep learning improves the identification of neutrophil abnormalities in immune and inflammatory conditions

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Introduction

The identification of inflammatory and immunological diseases, which affect millions of people, requires accurate and early diagnosis to optimize treatment. However, these diagnoses often rely heavily on visual analysis by expert clinical pathologists, delaying timely intervention.

Neutrophils, the most important immune cells, are critical in defending against infections and regulating the inflammatory response. While conventional morphological analysis systems can identify normal neutrophils, they have difficulty detecting specific alterations, such as those seen in bacterial infections, severe inflammation, and autoimmune disorders. This limitation poses a significant challenge to timely and accurate diagnosis.

Objective

This work aims to develop an automated deep-learning-based system to differentiate normal neutrophils from those with abnormalities characteristic of various pathologies, including bacterial infections, severe inflammation, and autoimmune disorders.

Methodology

The images were obtained at the Core Laboratory of the Hospital Clínic de Barcelona using the Cellavision DM96 morphological analysis system. Pathologists validated 5,492 images: normal neutrophils (4,595), hypogranulated neutrophils (494), and neutrophils with inclusions (Döhle bodies: 139, cryoglobulins: 191, bacteria: 73).

To address imbalance, the Pareto rule was applied, starting with the smallest group (bacteria), generating 138 training images and oversampling to 276. This value balanced each neutrophil class in training and proportionally divided the dataset into training (828), validation (216), and test (4,622) sets. Data Augmentations (rotation, zoom, mirroring) were applied. Two ResNet152-based models A and B classify general categories and inclusions.

Results

The deep learning system showed high accuracy: 99% in Model A and 85% in Model B for classifying normal neutrophils and those with inclusions. It effectively identified normal, hypogranulated neutrophils, and those containing bacteria, cryoglobulins, and Döhle bodies, demonstrating its clinical value.

Conclusion

The proposed system effectively identifies normal neutrophils and those linked to bacterial infections, severe inflammation, and autoimmune disorders, showing potential for enhancing hematological disease diagnosis.



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sciforum-107308: Detection of neutrophil hypogranulation as an early marker of Myelodysplastic Syndrome using deep learning models

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Introduction and objectives

Myelodysplastic syndrome (MDS) is a blood disorder marked by abnormal blood cell production and a high risk of leukemia. Neutrophils, a type of leukocyte, can exhibit hypogranulation, an early indicator of MDS. While automated analyzers can identify leukocyte types, they cannot distinguish between normal and hypogranulated neutrophils, a challenge that deep learning techniques can address.

The objective of this work is to develop a two-stage identification system using convolutional neural networks (CNNs). The first stage classifies five types of leukocytes, including normal and hypogranulated neutrophils, while the second stage distinguishes between normal and hypogranulated neutrophils.

Methods

Images were collected at the Hospital Clínic de Barcelona using the CellaVision DM96 analyzer, resulting in a dataset of 500 images of basophils, lymphocytes, eosinophils and monocytes, and 5089 images of neutrophils (4595 normal and 494 hypogranulated). The dataset was split into training sets (320 images per leukocyte type, with 160 normal and 160 hypogranulated neutrophils), validation and test sets, and the rest for the test set. Two CNN-based models were developed: the first one with VGG19 architecture to differentiate leukocyte types and the second one with ConvNeXt architecture to distinguish normal from hypogranulated neutrophils. A final proof-of-concept was performed with 1000 images of neutrophils from MDS patients to simulate real clinical conditions.

Results

The test set results showed 99.57% accuracy for the first model and 99.32% for the second, identifying 4415 normal and 282 hypogranulated neutrophils. In the proof of concept, accuracies were 96.7% for the first model and 80% for the second, with sensitivities of 87.9% for hypogranulated neutrophils.

Conclusion

The proposed system showed high accuracy in testing and acceptable performance in the proof of concept for detecting neutrophil hypogranulation in MDS patients. However, its clinical performance is lower, indicating a need for more diverse data and refinement for improved accuracy in real-world applications.



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sciforum-107392: Determination of Macro- and Microelement Composition in *Alhagi maurorum* Using Inductively Coupled Plasma Mass Spectrometry (ICP-MS)

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Alhagi maurorum, a plant species widely distributed in the arid regions of Uzbekistan, is known for its diverse therapeutic properties. Understanding its elemental composition is essential for assessing its nutritional value and potential medicinal applications. This study aims to quantify the macro and microelements present in various parts of *Alhagi maurorum*, specifically seeds and leaves, collected from the Qashqadaryo and Xorazm regions. The focus is on elements critical to human health, such as calcium, magnesium, sodium, and iron. Elemental analysis was conducted using Inductively Coupled Plasma Mass Spectrometry (ICP-MS). Samples of *Alhagi maurorum* seeds and leaves were collected, dried, and digested in a microwave system with nitric acid and hydrogen peroxide. The digested solutions were analyzed using ICP-MS to determine the concentrations of 61 elements. Standard calibration and control samples were used to ensure accuracy and precision during the analysis. The study found significant variations in the concentrations of macroelements between the seeds and leaves. Calcium was found in the highest concentration in the leaves (100,000 mg/kg), while magnesium and sodium also showed elevated levels, with concentrations up to 14,000 mg/kg and 4,200 mg/kg, respectively. Trace elements such as scandium, lithium, and cobalt were present in lower concentrations, generally below 0.5 mg/kg. Samples from the Xorazm region exhibited higher levels of iron, reaching up to 1,558 mg/kg. This study highlights the rich elemental composition of *Alhagi maurorum*, particularly its high calcium and magnesium content in the leaves, which may have implications for its use in nutritional supplements or pharmaceuticals. The regional differences in elemental concentrations suggest that environmental factors influence the uptake of these elements. ICP-MS proved to be an effective method for the precise quantification of both macro- and microelements in plant matrices.



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sciforum-107367: Development of Novel DNA Fluorescence In Situ Hybridization Probes for Rapid Detection of Microbial Contaminants in Cosmetic Products

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Introduction: Microbial contamination in the cosmetic industry represents a significant risk to product safety, potentially causing health issues for consumers and leading to costly recalls. Common contaminants, such as *Escherichia coli*, *Pseudomonas aeruginosa*, and *Staphylococcus aureus*, can be introduced during manufacturing or consumer use, resulting in contaminations and product spoilage. Conventional detection methods commonly used, like plate counting, are slow, often taking up to a week to yield results, which delays quality control processes and increases analysis costs. The Fluorescence In Situ Hybridization (FISH) technique offers a faster, specific, and sensitive alternative for directly detecting microorganisms in cosmetic products. This study aims to design and validate new DNA-FISH probes, optimized to function without formamide, for the rapid identification of cosmetic microbial contaminants.

Methods: In silico probes targeting *E. coli*, *P. aeruginosa*, and *S. aureus* were designed using the DECIPHER program, which included sequence alignment, as well as assessments for specificity and efficiency. The 23S ribosomal RNA gene was selected due to its high variability and functional relevance, making it an ideal target for specific identification. Probes were evaluated both in silico and experimentally with target and non-target microorganisms. The FISH procedure was optimized to exclude formamide, a commonly used but toxic solvent in FISH protocols, thereby enhancing safety and usability.

Results: The designed probes demonstrated high specificity and efficiency for detecting the target microorganisms in both in silico and experimental conditions. Experimental validation confirmed that the probes could reliably identify *E. coli*, *P. aeruginosa*, and *S. aureus* in controlled cultures, producing fluorescent signals without the need for formamide.

Conclusions: This study successfully developed formamide-free DNA-FISH probes for the rapid identification of key microbial contaminants in cosmetic products. The proposed method addresses the limitations of traditional microbiological testing by providing quicker, safer, and more reliable results, thereby improving quality control processes and product safety in the cosmetic industry.



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sciforum-102177: Effect of catheter contact force on lesion volume in pulsed field ablation: A computational study

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Cardiac arrhythmia is one of the most common disorders affecting millions of people globally. More recently, pulsed-field ablation (PFA) has received FDA approval and emerged to be a safe and effective treatment modality for treating different types of cardiac arrhythmia. Unlike other ablative techniques like radiofrequency ablation, PFA is non-thermal-energy approach based on irreversible electroporation phenomena for attaining highly selective cellular injury by administering microsecond-scale, high-voltage electrical pulses. Despite numerous feasibility studies highlighting PFA's safety and efficacy, the exact mechanisms of action remain elusive. Substantial research efforts are essential to comprehensively understand PFA technology, leveraging its potential for sustainable health improvements. The objective of the present study is to quantify the relationship between the electrode–tissue proximity and the applied contact force on the shape and size of lesions induced during PFA. A coupled computational model was developed, incorporating electrical, thermal, mechanical, and fluid dynamics, simulating cardiac tissue as a hyper-elastic material. This study examined both the monopolar and bipolar electrode configurations. The outcomes were analyzed on the basis of ablation volume, as well as maximum temperature rise within the cardiac tissue and blood. It was found that the lesion dimensions induced during PFA are strongly correlated to the contact force at the electrode–tissue interface. Statistical correlations were developed to predict the lesion volume based on contact depth for monopolar and bipolar electrode configurations.



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sciforum-106266: Effects of Alloxan Monohydrate-Induced Cognitive Decline Associated with Diabetes in Wistar Rats

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Introduction: Untreated chronic diabetes can lead to the formation of amyloid plaques in the brain, reflecting signs of Alzheimer's disease. Effective treatment of chronic diabetes does not fully resolve cognitive problems.

Objective: To assess the cognitive decline associated with alloxan monohydrate-induced diabetes in Wistar rats.

Material and methods: This study involved 24 Wistar rats weighing between 150 and 300 g. They were divided into three groups: (1) normal rats, (2) untreated diabetic rats and (3) diabetic rats treated with D-erythrodihydrosphingosine. The rats were given glucose and food overnight to prevent hypoglycaemia. Behavioural experiments were carried out using object recognition and radial arm maze tests.

Results: The results showed a significant difference between the groups in terms of weight, with a significant decrease observed from day 7. Behavioural analysis revealed significant differences in the time spent exploring familiar and novel objects in the rats. The study also assessed the cognitive impact of diabetes by evaluating spatial learning in an eight-branch radial maze. The results showed that diabetes affects working memory and that SPK1 and 2 inhibitors do not improve it in diabetic rats.

Conclusion: Working memory is impaired and spatial learning is difficult. Nevertheless, our results would help to understand the link between cognitive decline and hyperglycaemia and highlight the importance of comprehensive management of diabetic patients with neurocognitive problems.



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sciforum-107683: Epidermal $\alpha 3\beta 1$ is required for efficient wound healing and is downregulated in aged skin

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Introduction

Epidermal integrin $\alpha 3\beta 1$ has emerged as a promising therapeutic target in impaired wound healing as it has been shown to be highly expressed during wound healing and has been linked to keratinocyte migration *in vitro*. However, its role in re-epithelialization *in vivo* has remained unclear. This study aims to clarify this role by using a novel inducible epidermis-specific $\alpha 3$ knockout ($\alpha 3eKO$) murine model.

Methods

Young (8-week-old) and aged (22-month-old) $\alpha 3eKO$ mice were treated topically with tamoxifen (4OHT) to induce $\alpha 3$ knockout, or with vehicle control (acetone) 5 and 3 days prior to wounding. The backs of the mice were shaved, disinfected, then wounded with 4mm full-thickness biopsy punches. Frozen sections were prepared and immunostained with anti-integrin $\alpha 3$, anti-K14, anti-Ki67, and DAPI. Keratinocyte proliferation and wound re-epithelialization were assessed in each age group.

Results

Young 4OHT-treated mice exhibited markedly reduced wound re-epithelialization compared to their vehicle-treated counterparts ($p < 0.0001$). Keratinocyte proliferation was also decreased in wound-distal hair follicles in young animals ($p = 0.0235$), suggesting a lack of proliferating keratinocytes contributes to the reduced wound re-epithelialization. Keratinocyte proliferation was similarly decreased in aged mice, and 4OHT treatment did not further reduce healing parameters. Additionally, our findings indicate that epidermal $\alpha 3\beta 1$ levels naturally decline with advanced murine age, and preliminary results indicate that this may also occur during human aging. Therefore, we hypothesize that reduced levels of $\alpha 3\beta 1$ contribute to reduced capacity for wound healing observed in the aged population.

Conclusions

Overall, our work indicates that integrin $\alpha 3\beta 1$ promotes wound re-epithelialization and declines with chronological age, suggesting that wound healing mechanisms may be impaired in the elderly due to a natural decrease in $\alpha 3\beta 1$ levels. Future studies will reveal whether therapeutic promotion of integrin $\alpha 3\beta 1$ function will aid in wound closure in the elderly and/or in hard-to-heal wounds, in general.



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sciforum-103871: Evaluating the Failure Rates of Dental Crowns on Endodontically Treated Teeth: A Comprehensive Review of Contributing Factors and Clinical Outcomes

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A comprehensive review of the literature was conducted, focusing on clinical studies, retrospective analyses, and systematic reviews that reported the failure rates of crowns placed on endodontically treated teeth. Factors such as the type of crown material, quality of root canal treatment, crown-to-root ratio, occlusal forces, and the presence of residual tooth structure were examined. Data were synthesized to identify common patterns and potential predictors of failure. This review revealed that the failure rates of crowns on endodontically treated teeth vary widely, with mechanical failures such as crown dislodgement, fractures, and secondary caries being the most prevalent. Factors such as inadequate root canal obturation, poor crown fit, insufficient ferrule effect, and high occlusal stress were strongly associated with increased failure rates. Additionally, the use of certain crown materials, such as metal–ceramic and all-ceramic crowns, showed different performance outcomes based on the clinical scenario. The success of crown restorations on endodontically treated teeth is highly dependent on multiple factors, including the quality of endodontic treatment, crown design, material selection, and proper case management. To reduce failure rates, clinicians should focus on ensuring optimal root canal therapy, using appropriate crown materials, and adhering to principles such as achieving a sufficient ferrule. Continued research and advances in dental materials and techniques are essential to further enhance the outcomes of these rehabilitations.



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sciforum-102841: Evaluation of Adaptive Laboratory Evolution (ALE) Using the *Comamonas* sp. C10 Strain for the Enhancement of Polyhydroxybutyrate (PHB) Degradation Capability

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In recent years, biodegradable plastics have increasingly been adopted as alternatives to petroleum-based plastics to mitigate environmental pollution. Among these, polyhydroxybutyrate (PHB) is particularly favored due to its considerable strength and durability. However, the anticipated mass production and widespread use of biodegradable plastics may introduce new environmental challenges related to their decomposition. To address this issue, we isolated *Comamonas* sp. C10, an aerobic microorganism, from wood fragments around Mt. Kurodake in Japan and confirmed its capability to degrade PHB. While genetic modification could enhance degradation, it raises ecological concerns when applied to natural ecosystems. Recent findings by Cao et al. (2024) suggest that biodegradable microplastics may have equal or greater ecotoxicity than traditional plastics, making their rapid decomposition a pressing issue. This study employed Adaptive Laboratory Evolution (ALE) to investigate enhancements in PHB degradation. We incrementally increased PHB concentrations to 0.2%, 0.5%, and 0.8% during ALE. Once degradation rates exceeded 80% at each concentration, we conducted further degradation experiments using adapted cultures at higher PHB concentrations. The ALE-induced samples exhibited a degradation rate exceeding 60% within 48 hours, while the non-ALE-induced samples showed a degradation rate of approximately 36% over the same period. These results indicate that the degradation rate of ALE-induced samples is approximately 1.7 times higher than that of non-ALE-induced samples, highlighting the effectiveness of ALE. Additionally, experiments comparing the degradation rates with and without ALE induction using crude extracellular enzymes from strain C10 demonstrated that PHB degradation was consistently faster in the presence of ALE induction across all concentrations. This suggests that the enhanced degradation rate of strain C10 induced by ALE is attributable to the increased activity of its extracellular enzymes. In conclusion, our findings indicate that the ALE method is effective in enhancing the PHB degradation activity of *Comamonas* sp. C10, presenting a promising approach for improving the environmental performance of biodegradable plastics.



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sciforum-106683: Evaluation of the Effect of Electrode Displacement on Hand Movement Classification

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Muscle electrical control has been extensively documented in the pursuit of methodologies to extract pertinent information for the artificial reproduction of natural movements. Nevertheless, the physiological phenomena underlying this process are complex. The system comprises a finite set of actuators, each responsible for generating electrical impulses that propagate throughout the muscular tissue. The use of superficial electrodes for signal acquisition introduces an additional layer of complexity due to cross-talk phenomena. Consequently, the precise positioning of electrodes is imperative to enhance the quality of the extracted information. In this study, we evaluate the impact of electrode placement on movement recognition rates using a quadratic discriminant classifier, as well as the influence of unintended electrode displacement as a determining factor. This investigation utilizes a high-definition open-access database. Root Mean Square (RMS) values were computed from measurements obtained from 128 electrodes, and a sequential feature selection (SFS) algorithm was employed to identify the optimal subset of features. Recognition rates were calculated for each participant and for the overall sample of 18 participants to derive intersubject and intrasubject results. Furthermore, three displacement scenarios were developed: longitudinal displacement, transverse displacement, and diagonal displacement, aligned with muscle fiber orientation. The results encompass evaluations using the top four to ten most significant features identified via SFS, the feature subset, and all electrode measurements. This study shows that electrode positioning significantly impacts movement classification, with random displacement (7.5–12.54 mm) causing variations up to 17.16% within and 24% between subjects. RMS values per electrode were analyzed using the 4 to 10 most relevant features, revealing variations of 10.92% and 9.6% (4 features) and 6.4% and 7.6% (10 features). Cross-validation was employed to ensure that results were independent of data partitioning, and ANOVA was used to confirm statistically significant differences between group means.



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sciforum-104355: Exploiting the SuperPred Tool for the Target Deconvolution of Novel Bioactivities of Drug-Like Secondary Metabolites from Aglaia Species

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Several alkaloids, terpenoids, limonoids, steroids, lignans and flavaglines have been isolated from the genus *Aglaia*. A significant number of them have not been tested for any biological activities, while those already screened for activities may have limited phenotypic targets, are under-utilized or may require validation. This study exploited the SuperPred tool for prospective and retrospective drug target fishing for novel bioactivities of drug-like molecules derived from *Aglaia* species. A total of 291 secondary metabolites were obtained from a review of the literature. The simplified molecular input line entry system (SMILES) canonical strings were subjected to drug-likeness prediction using the SwissADME tool. The anatomical therapeutic chemical class and potential targets of the compounds were deconvoluted by SuperPred logistic regression machine learning models, based on Morgan fingerprints with a length of 2048 and with a probability and model accuracy cut-off of $\geq 90\%$. Of the 291 secondary metabolites, 25 displayed the most favourable pharmacokinetic, physicochemical and toxicological properties. The 25 drug-like compounds comprised a lignan (lariciresinol acetate), a triterpenoid (17,24-epoxy-20 α ,25-dihydroxy-21-norbaccharan-3-one), three flavaglines (pyrimidinone, dihydropyrimidinone and rocagloic acid) and steroids ((E)-aglawone, 2 β ,3 β ,4 α -trihydroxypregnan-16-one and androst-1,4-dien-3,17-dione), five sesquiterpenoids and twelve alkaloids. The compounds were found to interact with many targets, such as the NF- κ B p105 subunit, cannabinoid CB2 receptor, MAP kinase ERK2, hypoxia-inducible factor 1 α , G-protein coupled receptor 55, tyrosyl-DNA phosphodiesterase 1, p53-binding protein Mdm-2, cathepsin D, COX-1 and arachidonate 12-lipoxygenase. The target fishing of the secondary metabolites provided insights into the potential novel activities, polypharmacology and possible unintended off-target binding of *Aglaia* molecules.



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sciforum-106130: Expression of Tryptophanyl-tRNA Synthetase (WARS) and Indoleamine 2,3-Dioxygenase-1 (IDO1) in the Prediction of Bladder Cancer Staging

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Introduction

Bladder cancer (BC) is one of the most common neoplasms in the world. Like other types, BC can produce the enzyme indoleamine 2,3-dioxygenase-1 (IDO1), which, by modulating the immune system, protects the tumor and favors its progression. When present, IDO1 degrades tryptophan in the microenvironment, producing kynurenine catabolites. This situation blocks the local immune response but does not affect the IDO1-producing cell itself. The mechanisms for this resistance remain unknown, but there is evidence that reserves are generated by the enzyme tryptophanyl-tRNA synthetase (WARS), which loads tRNA with the amino acid, ensuring protein synthesis and the cell cycle.

The objective of this study was to verify if the expression of IDO1 and WARS is associated with BC staging.

Materials and Methods

The study included BC specimens extracted from 165 patients, 88 with non-muscle invasive BC (NMIBC) and 77 with muscle invasive BC (MIBC). The project was approved by the ethics committee (49446515.0.0000.5511). The expression of IDO1 and WARS was evaluated by immunohistochemistry in both neoplastic and inflammatory cells. Correlation analysis (Spearman) and ROC curve were used.

Preliminary Results

Although no correlation was detected between IDO1 and WARS, the expression of both proteins was effective in predicting NMIBC.

Preliminary Conclusion

It is possible that the enzymes IDO1 and WARS play a role in the pathophysiology of BC and have predictive power in disease staging. This study is ongoing for further clarification.

Funding

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sciforum-102498: Features of the Clammy locust (*Robinia viscosa* Michx. ex Vent.)'s naturalization into semi-natural and cultivated phytocenoses as potential sources of its raw materials

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Robinia viscosa, whose natural habitat is localized in North America, is used mainly as an ornamental plant species and for the restoration of degraded areas. Among the metabolites found in the Clammy locust's glandular trichomes, there is a significant content of mucus and pectins [2]. Therefore, it should be considered also a potential medicinal plant with antioxidant and antibacterial activities.

The field experiment method was used. *R. viscosa* specimens were planted in semi-natural and cultivated phytocenoses in the north of Ukraine (plant resistance zone 5a: from -28.9°C to -26.1°C).

R. viscosa demonstrated a high degree of drought resistance in conditions of moisture deficit and high temperatures (up to +42°C), as well as a high degree of winter and frost resistance (tolerating temperatures as low as -28°C). It did not demonstrate the ability to reproduce through seeds. In the conditions of the cultivated phytocenosis, it had the ability to grow intensively due to root shoots: one 5–7-year-old *R. viscosa* plant produced 13±4 root sprouts per growing season at a distance of 1–8 m from the mother plant.

A. Konarska [1] notes that *R. viscosa* is a valuable melliferous species. Its nectar productivity is 1000 kg or more from 1 ha (according to oral reports from Ukrainian beekeepers). *R. viscosa* blooms after *R. pseudoacacia* L., which extends the period of a good honey harvest until September. In light of this, places where the Clammy locust is naturalized in the north of Ukraine should be considered potential sources of *R. viscosa*'s raw materials.

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sciforum-107338: Implementation of federated learning for peripheral blood cell identification across different clinical centers

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Introduction and objectives:

Morphological analysis of peripheral blood is essential for diagnosis 80% of hematological diseases. Although automatic classification systems in morphological analyzers support diagnosis, image variability caused by differences in reagents, sample preparation, and analyzer optics between centers affects their performance. To address this challenge, this study proposes using federated learning, a collaborative training approach that adapts to the specific characteristics of each center while maintaining high performance despite image variability.

Methods:

The reference center, the Core Laboratory of the Hospital Clínic de Barcelona, provided 10298 images with five leukocyte classes: basophils, eosinophils, lymphocytes, monocytes, and neutrophils. Four public datasets were used as external centers in the federated learning approach: C1 (14514 images), C2 (2513), C3 (5000), and C4 (11353). Data were divided into training, validation, and test sets.

Initially, a VGG16 network was trained with the reference center data, achieving 99.4% accuracy. However, accuracy dropped significantly when evaluated on the external centers: 58.6% in C1, 93.2% in C2, 60.3% in C3, and 69.82% in C4.

The model's performance was evaluated using precision, recall, specificity, and F1 score:

C1: 0.736, 0.586, 0.942, 0.657.

C2: 0.944, 0.932, 0.983, 0.931.

C3: 0.803, 0.603, 0.901, 0.562.

C4: 0.711, 0.698, 0.952, 0.785.

To improve generalization, a federated learning approach was used. The first three convolutional blocks of VGG16 were frozen, the remaining blocks were unfrozen to perform fine-tuning with the training sets of each centre, averaging the adjusted weights using the FedDyn technique. This resulted in a Final Global Model that is better adapted to the variability between centers.

Results:

The test sets from all four centers were evaluated again with the Final Global Model, showing significant increases in classification accuracy, 96.18% in C1, 99.6% in C2, 99.5% in C3, and 84.75% in C4, with corresponding metric improvements:

C1: 0.964, 0.952, 0.992, 0.958.

C2: 0.992, 0.992, 0.998, 0.992.

C3: 0.974, 0.973, 0.993, 0.973.

C4: 0.884, 0.888, 0.992, 0.885.

Conclusion:

Federated learning can effectively fine-tune classifiers in multicenter settings, making the model more robust to the variability between different datasets. This approach shows potential as a tool for automatic recognition in multicenter contexts.



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sciforum-104083: In silico Analysis of a Three-Finger Toxin from *Micrurus corallinus* Suggests Anticoagulant Potential through Structural Homology with *Hemachatus haemachatus* Toxins

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Introduction: Three-finger toxins (3FTx) are a diverse group of non-enzymatic polypeptides found in snake venoms, known for their broad range of biological activities. This study focuses on a specific 3FTx from the venom of the coral snake *Micrurus corallinus* (C6JUP0_MICCO). The objective is to identify potential biological targets for this toxin using advanced bioinformatics tools. **Methods:** The bioinformatics tools employed in this study include AlphaFold2, the DALI server, and Rosetta docking. AlphaFold2 was used to predict the three-dimensional structure of the toxin. The DALI server was then utilized to compare this structure with other known proteins to identify potential structural homologs. Finally, Rosetta docking was applied to predict the toxin's ability to interact with three specific receptors: the nicotinic acetylcholine receptor (nAChR), the muscarinic M1 acetylcholine receptor (M1mAChR), and the $\alpha 7$ nicotinic acetylcholine receptor ($\alpha 7$ nAChR). **Results:** The structural analysis using AlphaFold2 revealed that the 3FTx from *Micrurus corallinus* shares significant similarity with toxins from *Hemachatus haemachatus*, specifically a cytotoxin homolog (3SOE_HEMHA) and Ringhalexin (3SO1_HEMHA). DALI protein structure comparison confirmed these similarities, suggesting a possible shared functional role. However, the Rosetta docking results indicated that the *Micrurus corallinus* 3FTx does not establish significant interactions with nAChR, M1mAChR, or $\alpha 7$ nAChR, which are common targets for many neurotoxic 3FTx. **Conclusion:** The *Micrurus corallinus* 3FTx exhibits structural similarities to toxins with known anticoagulant properties rather than neurotoxic effects. This suggests a potential anticoagulant action for this toxin, which aligns with the functional characteristics of its structural homologs from *Hemachatus haemachatus*. Further experimental studies are required to validate these findings and elucidate the exact biological activities of this 3FTx.



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sciforum-104585: In Silico Electrophysiological Analysis Highlights Cardiac Toxicity of Ibrutinib in B-Cell Lymphoma Therapy through Sodium Current Inhibition

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Background:

Ibrutinib, a small-molecule drug inhibiting Bruton's tyrosine kinase, is widely used for treating B-cell lymphoma. However, its potential cardiac toxicity is not fully understood. This study aims to examine how different concentrations of Ibrutinib affect cardiac electrophysiological properties.

Methods:

Using an in-silico electrophysiological model of the sinoatrial node (SAN), we analyzed the effects of Ibrutinib (ranging from 0.1 $\mu\text{mol/L}$ to 10 $\mu\text{mol/L}$) on the conductance of voltage-gated sodium channels (Nav1.5) over a 200 ms period. Electrophysiological activities were recorded using both current-clamp and voltage-clamp techniques.

Results:

Application of varying current stimuli (0.1-0.10 nA) and durations (10-50 ms) generated action potentials (AP) in the SAN. The current-voltage (I-V) relationship of Nav1.5 under different Ibrutinib concentrations demonstrated a significant reduction in inward current, with a 26% decrease at 10 $\mu\text{mol/L}$. The I-V curve shifted positively by 20%, and the half-activation potential increased by 28%. This change in inward current was then integrated into a whole-cell model, revealing prolonged AP repolarization and decreased firing frequency at 10 $\mu\text{mol/L}$ Ibrutinib.

Conclusions:

Our findings indicate that high concentrations of Ibrutinib reduce the frequency of spontaneous AP firing by inhibiting Nav1.5 currents, suggesting a risk of cardiac toxicity. Careful dosage management of Ibrutinib is recommended, and further clinical trials are needed to explore its detailed subcellular mechanisms.



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sciforum-104011: In Vivo Toxicity and In Silico Molecular Docking of NXH8, a Post-Synaptic Three-Finger Toxin from *Micrurus corallinus*, in Comparison to α -Bungarotoxin.

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Introduction: Coral snakes of the genus *Micrurus*, primary representatives of the family Elapidae in the Americas, contain potent neurotoxins, making envenomation highly dangerous. In Brazil, *M. corallinus* and *M. frontalis* cause most bites. Recently, NXH8, a three-finger toxin (3FTx) with antagonistic activity on nicotinic acetylcholine receptors (nAChR), was characterized. **Methods:** Anti-NXH8 antibodies were produced in Balb/c mice. In vivo toxicity was assessed in mice receiving 3 LD₅₀ of *M. corallinus* venom (control) or synthetic NXH8. The neutralizing capacity of anti-NXH8 antibodies was tested in mice injected with venom pre-incubated with saline (G1), antivenom (G2), anti-NXH8 antibodies (G3), and post-treated with Varespladib (VPL) intramuscularly after intraperitoneal administration of venom pre-incubated with saline (G4) or pre-incubated with anti-NXH8 antibodies (G5). Survival was monitored for 48 hours. **Results:** Mice injected with venom pre-incubated with saline (G1) died in 6.00 ± 1.22 hours, while those injected with venom pre-incubated with antivenom (G2) survived for more than 48 hours. Anti-NXH8 antibodies (G3) resulted in a survival time of 7.2 ± 0.84 hours, with no significant difference from G1 ($p = 0.108$). VPL administration post-venom (G4) increased survival to 10.2 ± 0.45 hours ($p = 0.05$). VPL post-venom pre-incubated with anti-NXH8 (G5) increased survival to 11.0 ± 1.22 h, not significantly different from G4 ($p = 0.207$). Docking simulations indicated that NXH8 binds to nAChR but lacks crucial residues for effective interaction, explaining its low toxicity. **Conclusion:** NXH8's low toxicity in vivo is likely due to structural differences from α -bungarotoxin, suggesting that other venom toxins, including presynaptic β -neurotoxins such as Phospholipase A₂ (PLA₂), may contribute to lethality. This study was conducted under Animal Ethics Committee Protocol 4463100419 with financial support from H.R.-R. (FAPESP: 2017/18398-1) and S.H. (CNPq: 406816/2022-0).



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sciforum-103565: Intelligent Microrobots for versatile applications in Biomedicine.

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With the recent advancements in biomaterials and biomanufacturing, the concept of miniaturized yet minimally invasive surgical procedures has emerged in biomedicine. In this regard, microrobots have been transforming the natural ways of diagnosis, treatments, and real-time monitoring of biosignals even from intricate organs (such as the Brain and the Gastrointestinal Tract) of the human body. However, due to the available scientific studies being limited, there has been a significant research gap in exploring the different types and applied clinical areas of intelligent microrobots. Therefore, herein, artificial, biological, and biohybrid microrobots are systematically categorized to develop the theoretical background for diversified medical procedures. A well-comprehended discussion on the design and fabrication of these miniaturized agents is considered to explore the practicality of micro-engineered biomedical solutions. These microrobots are controlled by applying different mechanisms, primarily including but not limited to external magnetic fields, acoustic waves, electrical fields, and optical tweezers. Furthermore, self-propelled, untethered, and autonomous features of the microrobots contribute to intelligent yet targeted biomedical operations (such as navigating through complex bio-fluidic environments, locating tumors, and delivering drugs). The utility of these microrobots has also been seen in several in vitro as well as in vivo applications, aiding medical scientists to transform precision surgery and lab-on-chip diagnostics. Based on the findings, this article provides the scientific community with a micro-robotics foundation to explore their well-connected theoretical interpretations, design, manufacturing, intelligent control, and utility in several areas of biomedicine. It is highly recommended to further explore the practical limitations of these biocompatible robots to optimize futuristic medical Interventions.



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sciforum-107453: It's not “Machine against Man” but “Machine for Man”: a case study on the use of robotics by vegetable farmers from the South-24 Parganas district of West Bengal, India

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The implementation of digitized farming technologies along with site-specific precision management are possible responses to ever-increasing expectations from the agri-food industry. The field of robotics is demonstrating significant potentials and benefits when integrated into the modernized agriculture. Although still in the prototype stage, automation in agriculture has a bright future. Agri-robots are capable of performing various farming operations such as seeding, pruning, spraying, pest and disease detection, harvesting and weed control. The present study was designed to recognize the utility of multi-functional robots across vegetable fields in Baruipur, Sonarpur and Jaynagar blocks of the South-24 Parganas district, West Bengal, India. Seeding robots could offer precision in seeding functionary by augmenting plant densities to increase yield. Robotic application in disease and pest management (both detection and control) would probably contribute towards reductions in economic damage. Plant-detection robots utilizing high-quality sensors are highly reliable for estimations of crop volume and area, thereby determining the appropriate amount of fertilizer required. Such robots could also distinguish between crops and weeds on fields. The usage of such robots for crop estimation in the study area would also help in determining the accurate amount of weedicides required, thereby preventing damage caused by blanket spraying. The utilization of harvesting robots by farmers could assist them in localizing the most appropriate state of fruit and its careful handling without damaging the crop. Thus, the evolution and development of robotics could play a vital role in paving the path towards complete automation in agriculture sector with minimal human involvement.



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sciforum-104825: Mitigating enzyme and bacterial functions in diabetic ulcer environments using WAAPV-containing electrospun fibers

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Diabetic ulcers are often worsened by elevated levels of human neutrophil elastase (HNE) and bacterial infections, both of which impede healing. To address these challenges, polycaprolactone (PCL)/polyethylene glycol (PEG) electrospun fibers infused with elastase-targeting peptides, AAPV and WAAPV, were engineered. The fibers were designed to exert multiple actions, including the inhibition of HNE. WAAPV's effectiveness in regulating proteolytic enzymes was verified by its ability in inhibiting HNE activity. The incorporation of PEG into the fibers enhanced their wettability, although it also accelerated degradation. However, the inclusion of WAAPV mitigated this effect, resulting in a sustained release of peptides over 24 hours.

Peptide loading within the fibers was confirmed through thermal stability and hydration capacity analyses, and the peptide concentrations were determined by mass/dimension ratios in approximately 51.1 $\mu\text{g}/\text{cm}^2$ and 46.0 $\mu\text{g}/\text{cm}^2$ for AAPV, and 48.5 $\mu\text{g}/\text{cm}^2$ and 51.3 $\mu\text{g}/\text{cm}^2$ for WAAPV, within PCL and PCL/PEG matrices, respectively. Both peptides effectively inhibited HNE, with PEG showing potential to enhance this inhibition by interacting with the peptides and forming peptide-PEG complexes. The fibers containing PCL and peptides achieved approximately 10% HNE inhibition after 6 hours of incubation, while PCL/PEG fibers showed $\approx 20\%$ inhibition after 4 hours testing.

Peptide-loaded fibers demonstrated significant antibacterial activity, inhibiting the growth of *Staphylococcus aureus* by up to 78% and *Escherichia coli* by up to 66%, with peak efficacy observed after 4 and 2 hours of incubation, respectively. These findings suggest that WAAPV-loaded fibers hold promise for inhibiting HNE and bacterial activity, and thus for treating diabetic ulcers.



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sciforum-099993: Monitoring cobalt presence in the hair of young individuals from Alcalá de Henares, Spain: effect of age and sex.

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Background: Cobalt (Co) is increasingly used in green technology development. Recently, our group detected Co in the scalp hair of 73 out of 97 monitored adolescents born and residing in Alcalá de Henares (Spain), suggesting some exposure. We studied Co presence in young children, owing to their greater susceptibility.

Methods: Co was analysed by ICP-MS, after the appropriate removal of exogenous contamination, in scalp hair from 120 children (6 to 9 years old; 70 females) who met strict inclusion criteria.

Results: Data were processed using the NADA statistical package owing to the level of censored values (26.05%; LoD=0.0034 µg/g), which was similar to the percentage observed in adolescents' hair (24.73%). Co levels were slightly higher in children's hair [data presented as medians and ranges, in µg/g: 0.0062 (0.0036-0.0437) vs. 0.0036 (0.0016-0.0817)], suggesting a minor dependency of detoxification on young age. This effect was also reported in an study carried out with individuals living in the city of Madrid and in a village in the NE; thus, significantly higher levels of Co were detected in children's hair (aged 6-10 years) versus the hair of teenagers aged 11-15 years (0.0172 vs. 0.0141 µg/g). Similarly to what was observed in the adolescent cohort, Co presence in children's hair was sex-dependent; it was significantly higher in female participants [p-value=0.00087; median and range, in µg/g: 0.0074 (0.0037-0.0437) vs. 0.0047 (0.0036-0.0157)], which is also in agreement with what was observed in individuals living in Madrid.

Conclusions: The results suggest some exposure to Co, which would be mostly from dietary sources, as little Co has been detected in the environment of Alcalá de Henares. Tentative reference values for Co, i.e., the 95% confidence interval of the 95th population percentile (CI-PP95), are proposed for girls (0.0199-0.0356) and boys (0.0083-0.0144), as age and sex have been shown to affect the levels of Co in human hair. These ranges could be used to detect exposure to Co in children living in the same city.



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sciforum-099992: Monitoring iron in Spanish adolescents' scalp hair: potential effect of age and sex

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A monitoring study conducted on young adults (20-24-years old) from the Madrid region (Spain) revealed a lower iron (Fe) status in this demographic, particularly in women. Given the potential adverse effects of suboptimal iron status on academic performance, we monitored iron status in adolescents through analyzing it in hair. This approach could be advantageous because it is not affected by rapid fluctuations due to dietary intake, which can complicate the interpretation of iron status assessments based on other biological samples. Scalp hair was collected from 97 adolescents (13- to 16-years-old; 68 girls) living in Alcalá de Henares (Madrid). Fe was monitored by ICP-MS (LoD=1.148 µg/g). Contrarily to the results observed in young adults, Fe hair concentrations did show sex dependency, being significantly higher in female adolescents [p -value=0.000057; median and ranges; all in µg/g: 5.524 (3.167-13.262) vs. 4.464 (2.666-6.173)]. The observed effect of sex might be reflective of the endocrine system, which usually becomes active earlier in females with the onset of adolescence. Thus, the levels of Fe did not show statistical differences according to the four areas of residency (p -value=0.370) distributed in relation to Alcalá's environmental characteristics: 5.230 (green spaces), 5.197 (urban), 5.522 (traffic), and 6.225 (industrial). The levels of Fe were similar to those detected in young adults (5.157 vs. 5.054) but were much lower than those detected in individuals 11-15-years-old (14.8; all in µg/g) living in the Madrid region. Previous studies have documented a decline in iron in hair with age, which could explain our observations. Although our results have shown a similar trend in relation to the effects of age and sex reported in the literature, they might highlight a lower Fe status in Alcalá's adolescent population, which should be further investigated to increase public health interventions to enhance the status of iron in the population monitored.



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sciforum-104413: Multimodal Immersive Environment for Evaluating Reaction Time and Decision-Making in Sport Situations: A Pilot Study on Time Analysis and Learning Effects

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Introduction: The assessment of motor performance in athletes is a multifaceted endeavor, with methods varying across sports, each requiring assessment techniques tailored to its specific characteristics. Sports science research aims to establish reliable methods that depend on the complexity of the instruments. Athletes have been studied in controlled laboratory settings, immersive virtual reality, and real-world scenarios. However, there are inherent limitations in translating findings from controlled laboratory environments to practical sports applications. To bridge this gap, this study introduces a mixed modality, combining virtual immersion with physical objects. We present a quantitative assessment based on time analysis.

Methods: This pilot study evaluated male athletes performing motor reaction tasks, moving their hands in response to visual stimuli under a go/no-go protocol. The same protocol was carried out in a quiet laboratory environment (QLE) and a multimodal immersion environment (MIE). The QLE lacked noise or visual distractions other than the task stimuli. The MIE included a 180°-enveloping screen with sport-specific video and audio noise and the same task stimuli as the QLE. Motion capture and EMG data from the upper limbs were collected. Reaction time (RT) and decision-making time (DM) were used to compare the athletes' performance.

Results and Discussion: The two-way ANOVA showed no significant differences for RT and DM between left- and right-hand performance across environments, consistent with previous findings. The RT in the MIE was significantly shorter, ~10% ($p < 0.001$, $ES = 0.52$), than in the QLE. The DM showed no differences between environments. While the absence of changes in DM suggests consistent processing speed in both environments, the improved RT performance in the MIE indicates a potential advantage for using combined scenarios in future assessments.

Conclusion: A multimodal immersion environment could allow the introduction of specific stimuli for physical training and assessment, thereby improving the transferability of findings to real-world sports situations.



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sciforum-104457: Newly Developed Quantitative Spectrophotometric Analysis in the Visible Range (VIS) of Lisinopril that belongs to angiotensin-converting enzyme inhibitors

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Lisinopril is a dipeptide containing an **L-Proline** group and an **L-Lysine** residue. It is an antiarrhythmic medication belonging to the family of angiotensin-converting enzyme (ACE) inhibitors. It effectively treats arterial hypertension (first-line treatment), heart failure, and heart attacks; it also prevents kidney problems in people with diabetes mellitus. The main purpose of this work consisted of the dosage of Lisinopril as a single active substance from pharmaceutical tablets. A new method for the quantitative analysis of Lisinopril using visible spectrophotometry (VIS) was found, optimized, and applied in laboratory practice. This method was based on the diazotization of the free primary amino group $-NH_2$ of Lisinopril in cold conditions for 25 minutes at 1-5 degrees Celsius, in the presence of sodium nitrite 5 % and hydrochloric acid 10%-15%, followed by the quantitative coupling of the obtained diazonium salt with alpha-naphthol from an alkalized 0.2 % alcoholic solution. An intense orange azo dye with a reddish shade was dosed at the wavelength corresponding to the absorption maximum, $\lambda = 489 \text{ nm}$, in relation to double-distilled water, which was used as a blank. The amount of pure Lisinopril found per tablet was **19.60 mg / coated tablet**. This value was very close to the official reference value of **20 mg pure Lisinopril/tablet**. The average percentage deviation was only **2.00%** compared to the officially declared content of the active substance; this fell perfectly within the normal limits of the average percentage deviation allowed by the Romanian Pharmacopoeias 10th Edition and European Pharmacopoeias ($\pm 7.5\%$). The method proposed to be applied for the visible spectrophotometric analysis of Lisinopril from pharmaceutical tablets presented a very good linearity over the entire chosen concentration range of **0.41 $\mu\text{g/mL}$ - 12.24 $\mu\text{g/mL}$** . The linear regression coefficient was $R^2 = 0.999085$, which fit perfectly within the normal range of values, $R^2 \geq 0.9990$. The proposed method was then statistically validated.



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sciforum-104409: NIR photothermal immunotherapy of melanoma

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Near-infrared (NIR) photothermal therapy (PTT) of solid tumors utilizes localized heat to induce the immunogenic death of tumor cells. The combination of PTT with checkpoint inhibitor therapy can further amplify the immune response and improve the therapeutic outcome in what is known as photothermal immunotherapy. Here, we introduce a triple therapy, where photothermal immunotherapy is further amplified by the pharmacological silencing of tumor-infiltrating sensory neurons, an approach that was recently shown to affect tumor immunosurveillance as a standalone treatment .

For our model, B16F10-OVA melanoma cells were injected subcutaneously in mice. Once the tumors reached approximately 200 mm³, they were treated by NIR laser irradiation, with a local silencing of nociceptors using an lidocaine derivative (QX-314), and immunotherapy alone (aPDL1) or in combination.

We employed mathematical modeling to predict heat distribution and necrotic tissue in mice bearing melanoma tumors. Our model utilized experimentally defined parameters, such as tissue optical properties, tumor size, laser beam size and power, and irradiation time. The model was experimentally validated using data on tumor temperature increases. We found that the tumor size is a key determinant of temperature increase, which underscores the need for personalized treatment conditions . We determined optimal treatment conditions (808 nm, 0.3 W/cm², 3 min) for mice bearing 200 mm³ tumors.

Laser treatment was subsequently applied either alone (Laser+) or in combination with immunotherapy (aPDL1+) and neuronal silencing (QX-314+). When compared to control groups, the triple therapy (Laser+, QX-314+, and aPDL1+) significantly decreases tumor progression (p=0.0003) and increases survival time. Specifically, it resulted in complete ablation in 42% of the treated mice. Tumor re-growth was observed in only 16% of rechallenged mice, suggesting an immune memory effect.

Our results indicated that triple treatment can lead to a significant reduction in tumor growth and could complete tumor ablation in a significant fraction of the treated mice.



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sciforum-106307: Novel glutathione-responsive polyrotaxanes with enhanced cellular uptake.

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Polyrotaxanes are supramolecular assemblies composed of polymers, threaded macrocycles, and bulky stopper molecules to inhibit the decomposition of the first two. Cyclodextrin (CD)-based polyrotaxanes are promising therapeutic agents for lysosomal storage disorders, as they can transport CDs into the cells to normalize the intracellular trafficking of lipids, such as glycolipids or even cholesterol. Even though the important application of these supramolecular polymeric assemblies, their application is highly hindered by the costly, multistep synthesis methods, as well as the low aqueous solubilities of the non-modified polyrotaxanes. We have developed a simple one-pot synthesis of CD-based polyrotaxanes with poly(ethylene glycol) (PEG) and poly(ϵ -caprolactone) (PCL) axes using glutathione-sensitive disulfide-connected stopper molecules. This new synthetic pathway provides high threading efficacy and, due to the versatility of threaded CDs, also tunable water solubilities. In the case of PCL polyrotaxanes, high biodegradability was also detected, using lipase as a model enzyme. Cellular uptake studies on the Caco2 cell line showed up to 52-fold enhanced cellular internalization of these supramolecular assemblies compared to free CDs. In addition, the glutathione-triggered reductive removal of the stopper molecules showed the potential decomposition of these polyrotaxanes in target cells. Based on these results, the synthesized polyrotaxanes with disulfide stopper molecules might be promising supramolecular excipients for cellular delivery of α -CD and its derivatives.



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sciforum-104119: Optical and thermal properties of lung tissue undergoing thermal treatment

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Minimally invasive photothermal and thermal ablation techniques represent promising strategies for the treatment of tumors affecting lung tissue. In order to monitor and increase the effectiveness of these therapies, it is pivotal to characterize the optical-thermal response of lung tissue as a function of thermal treatment. In this study, we present the analysis of the optical and thermal properties of ex vivo calf and porcine lung tissue samples undergoing a homogenous thermal treatment from room to ablative temperature.

Optical properties, specifically the absorption coefficient (μ_a) and reduced scattering coefficient (μ'_s), were estimated over a broadband spectral range from 657 nm to 1107 nm, using time-domain diffuse optical spectroscopy. Furthermore, the transient hot-wire technique was utilized for the measurements of the thermal properties, i.e., thermal conductivity (k) and thermal diffusivity (D), by means of a dual needle probe.

Concerning optical properties, the thermal treatment induced changes in the μ_a spectra, such as the rise of two more evident peaks at the wavelengths of 770 nm and 830 nm and a dip at ~910 nm at temperatures >75 °C. Conversely, for μ'_s , related to the lung microstructure, minimal variations were observed during the thermal treatment.

Regarding thermal properties, both k and D experienced an exponential increment with tissue temperature. At ablative temperatures (~90 °C), the measured thermal properties reached average values more than 13 times higher than the nominal values estimated for the tissue samples at room temperature.

Overall, the characterization of the optical and thermal response of lung tissue subjected to thermal treatment could represent a step forward in the optimization of photothermal and thermo-ablative techniques for pulmonary tissue treatment.



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sciforum-102785: Phenol degradation and production of PHA using phenol degradation products as substrates

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Polyhydroxyalkanoates (PHAs), which are alternatives to plastics, are derived from microorganisms and are environmentally friendly due to their biodegradable nature. However, they typically have high production costs. Therefore, the conversion of low-cost harmful substances into high-value-added products such as PHA represents a promising approach to potentially reducing production costs. Phenol is one of the organic pollutants found in industrial wastewater. It is discharged by producers in industries such as textile processing, petroleum, pharmaceuticals, and resins. Even at low concentrations, phenol exhibits strong toxicity to all forms of life and is classified as a priority pollutant by the U.S. Environmental Protection Agency (EPA). Therefore, this study targeted phenol as the substance of interest. This study employed a two-stage process for PHA production. In the first stage, phenol degradation by the phenol-degrading bacterium *Comamonas* sp. C1 was conducted, and in the second stage, PHA was produced by *Bacillus* sp. CYR1 using phenol degradation products as substrates. Phenol (500 mg/L) was repeatedly added three times in a conical flask, resulting in the production of 2000 mg/L of phenol degradation products. These degradation products were added to the media, adjusted to pH 7, sterilized, and used as PHA production media. Results showed an increase in pH under all conditions, possibly due to the consumption of organic acids such as cis,cis-muconic acid, which is generated during phenol degradation. PHA production of 54.5 mg/L with a PHA yield of 30.2% was observed, suggesting that the conversion of harmful phenol degradation products to PHA is feasible.



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sciforum-103614: Polymeric matrices for target delivery of mangiferin

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Mangiferin is a bioactive substance extracted from the plant *Mangifera indica*. Mangiferin has many properties, such as antiviral, antitumor, anti-inflammatory, anti-viral qualities, among others, so it has attracted much attention as a potential drug. However, one of the problems with using mangiferin for therapeutic purposes is its poor water solubility and, consequently, low bioavailability.

However, it has been found that drug matrices such as films or fibers significantly increase the bioavailability and stability of drugs and attenuate side effects. This is also true for mangiferin: several types of drug delivery matrices have been developed in recent years.

These include nanospheres made of biodegradable and biocompatible materials, lipid-based micelles, nanoemulsions of hyaluronic acid aqueous solution, and gold nanoparticles and other systems.

Some of the delivery systems have already been tested in preclinical *in vivo* and *in vitro* trials and have shown positive effects in the treatment of cancer, kidney disease, and inflammatory diseases.

The systematization of data on drug delivery systems will accelerate their study and may develop new matrices. In this work, we have compiled information on the major systems involving mangiferin and their efficacy in disease control.

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sciforum-107883: Portable, Energy-Autonomous Electrochemical Impedance Spectroscopy (EIS) System Based on Python and Single-Board Computer

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The widespread use of organophosphorus pesticides, such as chlorpyrifos, in agriculture has raised significant environmental and health concerns due to their persistence and toxic effects. To address these challenges, we present the development of a portable, solar-powered, and energy-autonomous system for the detection of chlorpyrifos in water using Electrochemical Impedance Spectroscopy (EIS). The system integrates an EmstatPico card for electrochemical measurements, a Raspberry Pi Zero 2W as a wireless data server, and Python-based software to control and execute the EIS tests. Powered by a lithium-ion battery charged via a solar panel, this setup is suitable for field applications without the need for external power sources.

The detection of chlorpyrifos is achieved through a commercial amperometric electrochemical biosensor based on acetylcholinesterase (AChE), which is sensitive to neurotoxic inhibitors such as chlorpyrifos. Nine water samples containing different concentrations of chlorpyrifos were prepared to evaluate the system's performance. EIS measurements were conducted with a frequency sweep ranging from 200 kHz to 20 Hz and an alternating signal amplitude of 15 mV. The results showed an inverse relationship between the chlorpyrifos concentration and impedance, along with a decrease in the phase angle as the analyte concentration increased.

By utilizing Python and a Raspberry Pi, this system opens possibilities for integrating machine learning and artificial intelligence algorithms, enabling real-time data analysis, pattern recognition, and predictive modeling to further enhance the accuracy and adaptability of pesticide detection.

The findings suggest that this portable, energy-autonomous system is a simple, efficient, and sensitive tool for detecting chlorpyrifos in liquid samples. It has potential applications in environmental monitoring and public health, offering an alternative to traditional analytical techniques that are often costly and complex and require extensive sample preparation.



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sciforum-098263: Preliminary assessment of temperature as a relevant factor in the pyrolysis process, for the valorization of corn cob waste (*Zea mays*).

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The implementation of Thermogravimetric Analysis (TGA) laboratory tests allowed us to determine the thermal stability and degradation of corn cob waste (*Zea mays*); it was observed that corn cob waste should not be exposed to a temperature higher than 240 °C because when exceeding this temperature, a mass loss of around 50% is observed. At this temperature, we removed traces of moisture and some low-molecular-weight aromatic molecules after the drying stage.

Subsequently, the corn cob residues were degraded by pyrolysis in a nitrogen (N₂) atmosphere at different temperatures (500, 550, and 600 °C). Tests were performed on each solid product obtained to determine its stability.

Finally, FTIR tests were applied to decode the signals and generate spectra that allowed the identification and quantification of the materials present in the samples. The results of comparing the tests before and after the pyrolysis of the corn cob residues show the conservation of the CO, CH, C=C, C=O, CO and CH bonds, which are common in ethers and aromatic compounds that include hydroxyl groups.

In conclusion, corncob pyrolysis represents a promising technology for the valorization of agricultural residues and the production of sustainable bioproducts. Through this process, it is possible to contribute to the transition towards a circular economy and to the mitigation of climate change.



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sciforum-106951: Purification of Fc-fusion proteins without Chromatography, polymers, membranes or specific ligands

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We introduce a new concept and a potentially general platform for the purification of Fc-fusion proteins that does not rely on any resins, chromatographic media, membranes or specific ligands but, rather, makes use of aromatic [metal–chelator] complexes. We modified and significantly expanded our existing technology which was used to purify antibodies in our previous studies. **Our fully aromatic complex is composed of the chelator bathophenanthroline (batho) and metal ions (zinc or copper ions) to form [(batho)₃:Zn²⁺] or [(batho)₃:Cu²⁺] complexes.** Our technology captures the target proteins quantitatively via [cation–π] and [π–π] interactions and allows for their recovery at high yields (>80%, by densitometry) and purity (≥90%, by SDS-PAGE) while preserving their secondary structure, enzymatic activity and monomeric state. The entire process is performed at pH 7, thereby avoiding the complications that derive from exposure to harsh acidic conditions (e.g., aggregation or partial denaturation). The monomeric dispersity was preserved after the elution and evaluated by DLS (dynamic light scattering) and native page gel electrophoresis. The secondary structure of the target protein was not affected during the purification process and was confirmed by the technique of CD (Circular Dichroism). The biological activity of the purified protein was assessed and was preserved. Its cost-effectiveness and simple integration into the future industrial-scale downstream processing of therapeutic-grade biopharmaceuticals will be discussed. In future, we are planning to apply the same purification technology to different types of therapeutic proteins as an efficient purification platform while applying the necessary modifications.



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sciforum-107429: Sensor ensemble for patient stress monitoring using CNT-based temperature sensor and GSR sensor

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Introduction: This study presents the fabrication of a carbon nanotube-based temperature sensor and the development of a multiparameter patient monitoring system. The system integrates the temperature sensor with a galvanic skin response (GSR) sensor to monitor temperature, breath rate, and electrolyte profile, providing insights into the patient's stress and physiological status.

Methods: The temperature sensor is fabricated using a stencil-printing method on a paper-based substrate, followed by encapsulation and calibration for temperature detection. The sensor is integrated into a system built around an Arduino Nano microcontroller, combined with a GSR module. The setup, designed as a chest band, includes an extended temperature sensor embedded in the patient's mask for breath monitoring. Data on skin conductivity, temperature, and breath rate are wirelessly transmitted via a Bluetooth module.

Results: The carbon nanotube-based sensor demonstrated successful temperature detection, and the GSR sensor effectively monitored changes in skin resistance, indicating electrolyte levels. The system transmitted all collected data wirelessly, validating its functionality for real-time monitoring.

Conclusions: The developed system offers a simple yet effective solution for patient monitoring, particularly in settings lacking advanced equipment. By wirelessly tracking body temperature, breath rate, and electrolyte profile, it provides essential data for assessing patient stress and overall health, improving accessibility and patient comfort.



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sciforum-103632: Study of the antimicrobial activity of new 1,3,5-triazine derivatives

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Introduction: 1,3,5-triazine derivatives are an important class of heterocyclic compounds that have a wide range of biological activities, including exhibiting strong antimicrobial activity. Thus, the preparation of new compounds based on a triazine core, as well as the study of their antimicrobial activity, is an urgent task. **Methods:** The target compounds were obtained by the recyclization of 2-aryl-4-hydroxy-5-methyl-6H-1,3-oxazin-6-ones (**1-3**) with ethanimidamide and benzenecarboximidamide, which are 1,3-binucleophilic reagents. The reaction was carried out in the presence of an amount of sodium propoxide equimolar to the nucleophile in boiling n-propanol for 2-5 hours. The structure of the obtained compounds (**4-9**) was proven using modern physico-chemical methods of analysis: ¹H and ¹³C NMR spectroscopy, IR spectroscopy, and mass spectrometry. The antimicrobial activity potential of the synthesized compounds was determined by computer analysis using the AntiBac Pred online service. Experimentally, the antimicrobial activity of the compounds was studied by the method of serial dilutions against Gram-positive (Staphylococcus aureus, Bacillus subtilis) and Gram-negative (Escherichia coli, Pseudomonas aeruginosa) test cultures of microorganisms. **Results and conclusions:** The target compounds were obtained in 58-88% yield. As a result of in silico computer screening using the AntiBac Pred online service, data on the potential antimicrobial effect of the target compounds were obtained. Using experimental microbiological studies, it was shown that the studied compounds have moderate antimicrobial activity against the test cultures studied. Analyzing the structure-activity relationship, it was found that compounds that have a methyl group in position 2 of the triazine ring have the strongest inhibitory effect. The inhibitory activity against Gram-negative strains (Escherichia coli, Pseudomonas aeruginosa) is strongest for triazines that have a methyl group in position 2 and electron-donating substituents in the benzene ring.



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sciforum-104352: The Role of Genetic Polymorphisms in Modulating Beta-Blocker Response: A Comprehensive Review

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Introduction: Genetic variation significantly influences individual responses to beta-blockers, a class of medications commonly used to manage cardiovascular conditions such as hypertension and heart failure. Understanding these genetic differences is crucial for optimizing treatment efficacy and minimizing adverse effects.

Methods: We conducted a systematic review using three online databases: PubMed, Scopus, and Web of Science. The search strategy included terms such as "genetic polymorphisms," "beta-blockers," "ADRB1," "ADRB2," and "CYP2D6." After removing duplicates, we screened 921 titles and abstracts for relevance. Full-text articles of 111 studies were assessed for eligibility based on the inclusion criteria, which required studies to report on genetic polymorphisms affecting beta-blocker response in human subjects. A quality assessment was performed using a modified Cochrane RoB1 tool, evaluating aspects such as study design, sample size, and statistical analysis.

Results: Out of the 111 full-text articles assessed, 95 studies met the inclusion criteria and were included in the final analysis. Of these, 16 studies were excluded due to poor quality or insufficient data. The 95 included studies provided comprehensive baseline data on the pharmacogenomics of beta-blockers. Key findings indicated that polymorphisms in the ADRB1 gene, particularly the Ser49Gly and Arg389Gly variants, significantly affected the therapeutic response to beta-blockers in hypertensive patients. Variants in the ADRB2 gene, such as Gly16Arg and Gln27Glu, were associated with differential responses in heart failure patients. Furthermore, CYP2D6 polymorphisms influenced the metabolism of beta-blockers, affecting drug plasma levels and clinical outcomes.

Conclusions: Our findings underscore the importance of genetic testing in the personalized prescription of beta-blockers. Genetic variations in ADRB1, ADRB2, and CYP2D6 genes were particularly influential, affecting drug efficacy and safety profiles. Incorporating pharmacogenomic data into clinical guidelines can enhance therapeutic outcomes for patients receiving beta-blockers by tailoring treatments based on individual genetic profiles.



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sciforum-103592: The Treatment of sea turtle shell fractures: a novel approach using Bis-GMA-free dental composites

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Aim/Introduction: This paper aims to investigate the use of Bis-GMA-free dental composite as a valid method of repairing Sea Turtle shell fractures.

Materials and methods: One shell with multiple fractures from a *Caretta caretta* (Linnaeus, 1758) turtle, donated by the Veterinary Department of University of Messina, was used to perform the investigation. An expert operator repaired the shell using Bis-GMA-free ENAMEL plus HRI® BIO FUNCTION composites, MICERIUM S.p.A., Avegno (GE). The repairing protocol consisted of six stages: preparation, adhesion, composite layering, polymerization, finishing and polishing, and immersion. Microscopic and macroscopic analysis was performed after polishing (T0) and after 24h immersion in sea water (T1) using a SEM microscope and a Canon EOS 90D photographic device.

Results and Discussion: The SEM analysis shows a good interface between the composite and the shell at both T0 and T1, with no relevant differences being noted in adhesion. The macroscopy at T0 demonstrates the good mimetic ability of the BIS-GMA-free composite. At T1, the repaired area looks a little bit different in colour (different value, same hue and chroma). This change is due to the rehydration process. Current guidelines for shell repair recommend resins, adhesives, synthetic materials, and biocompatible fabrics. Repair methods range from mechanical fixation to adhesive use, or a combination, depending on the damage's severity and nature. The complete healing of the chelonian shell requires long periods of time (1-2 y.), so the role of covering materials is to protect the underlying granulation bed, ensuring a longer healing process.

Conclusions: Using Bis-GMA-free composites offers an aesthetically pleasing and safe alternative to traditional materials. The combination of the physical and optical properties of Bis-GMA-free composites allows for long-lasting and natural results, faithfully reproducing the structure and colour of the chelonian shell. These results require further and in vivo investigations to optimise shell repair and to ensure the survival of these fascinating creatures.



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sciforum-103940: Unveiling the Link: How Personality Traits Influence Central Serous Chorioretinopathy Through OCT and Psychological Assessment

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Central Serous Chorioretinopathy (CSCR) is a retinal condition characterized by the accumulation of subretinal fluid, leading to visual disturbances. Although the exact pathophysiology remains unclear, its etiology can be considered multifactorial, with stress and personality traits being significant contributors. This study involved 44 participants, half having been diagnosed with CSCR and the other half serving as controls. Comprehensive data, including medical history, symptomatology, and corticosteroid use, were collected. Psychological assessments were conducted using the Personality Inventory for DSM-5–Brief Form (PID-5-BF) and TEMPS-A-brief. Optical coherence tomography (OCT) was used to evaluate choroidal thickness, photoreceptor alteration, pigment epithelium detachment, and macular edema. The results indicated a higher prevalence of CSCR in men (male-to-female ratio of 1:10) with an average age of 50.55 years. A correlation between increased choroidal thickness and age was noted, with older patients showing higher values and complications like secondary choroidal neovascularization. Corticosteroid use did not correlate with increased choroidal thickness. Psychological assessments revealed no significant correlation between CSCR and specific personality domains; however, a trend towards higher negative affectivity was observed in CSCR patients. In conclusion, the study's epidemiological findings align with those in the existing literature, emphasizing a higher prevalence of CSCR in males and increased choroidal thickness with age. Although no direct correlation between personality traits and CSCR was statistically validated, a trend towards negative affectivity suggests a potential link. The interplay between psychological factors and CSCR warrants further investigation, and understanding the role of mental states in CSCR's onset and progression could inform integrated management strategies. The results underscore the need for larger sample sizes to confirm these preliminary findings and to explore the mechanisms underlying CSCR's association with psychological stress and choroidal dysfunction.



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sciforum-107606: Neurocognitive and Humoral Changes induced by EEG-Biofeedback: a Systematic Review of the Applicability and Therapeutic Effect in Patients with Schizophrenia Spectrum Disorders, Psychosis or Clinical High risks for Psychosis

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Introduction

Schizophrenia Spectrum Disorders are complex mental health conditions that significantly impact cognitive function and quality of life. While pharmacological and psychotherapeutic interventions are available, their effectiveness remains limited, particularly for negative symptoms and cognitive impairments. These limitations, alongside drug side effects and adherence difficulties, highlight the need for new treatments. Cognitive remediation strategies like EEG-biofeedback show promise by harnessing neuroplasticity. This systematic review aims to evaluate the neurocognitive and humoral changes induced by EEG-biofeedback and its therapeutic effects in patients with schizophrenia spectrum disorders.

Methods

Our review was conducted following PRISMA guidelines. Databases including EMBASE, ScienceDirect, Scopus, PsycINFO, and MEDLINE were searched for relevant studies: 15 studies, 10 RCTs and 5 Clinical trials were selected. Inclusion criteria encompassed studies involving patients with schizophrenia spectrum disorders, EEG-biofeedback interventions, and outcomes related to neurocognitive and humoral changes. The Cochrane Risk-of-Bias Tool for randomized trials (RoB 2) was used to assess the quality of included studies.

Results

The reviewed studies suggest that EEG-neurofeedback shows promise in addressing various aspects of schizophrenia spectrum disorders. Improvements were observed in processing speed, social functioning, working memory, and emotional regulation. Several studies reported successful modulation of brain activity in regions associated with auditory hallucinations. Neurofeedback training also led to increased functional connectivity between language networks and the default mode network. Some studies found improvements in brain-derived neurotrophic factor (BDNF) levels, self-efficacy, and clinical symptoms in schizophrenia patients.

Conclusions

Future research should focus on personalizing neurofeedback approaches and exploring their mechanisms of action in the context of schizophrenia pathophysiology.



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sciforum-107857: Molecular docking and ADMET prediction of compounds obtained from *Stephania dinklagei* roots as inhibitors of NMDA receptor

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Stephania dinklagei root is known in Nigeria for its medicinal properties, especially its role in the nervous system. N-methyl-D-aspartate receptor (NMDAR) has been linked to various neurological disorders. The potential of compounds obtained from *S. dinklagei* roots to inhibit the function of NMDAR is thus the focus of this *in silico* study. Liquid chromatography-mass spectrometry (LC-MS) was used to analyze compounds in *S. dinklagei* roots. Molecular docking against GluN2B NMDAR (PDB ID: 7SAD) was done using AutoDock Vina, while ADMET studies were carried out using SwissADME and ProTox 3.0 web servers. Memantine was used as the standard compound. Sixteen compounds were detected in the sub-fraction of *S. dinklagei* roots, with 75% having binding affinities > memantine (-5.3 kcal/mol). Geijerone, 7-(4,8-dimethylnona-3,7-dien-1-yl)-2,4',5,5',7',10'-hexahydroxy-2,2'-dimethyl-1,2,3,4,9',10'-hexahydro-[1,1'-bianthracene]-4,9',10'-trione (DHBT) and alpha,beta-Dihydroxanthohumol ($\alpha\beta$ D), exhibited the highest binding affinities: -9.5, -9.3 and -7.0 respectively. The three compounds interacted with the same amino acid residues as memantine. Geijerone and $\alpha\beta$ D had 0 Lipinski, Ghose, Veber and Egan violations. They also have a bioavailability score of 0.55, are both soluble, and have a high gastrointestinal (GI) absorption profile. The three compounds are not Pgp substrates, and only geijerone was predicted to be a blood-brain barrier (BBB) permeant. DHBT and geijerone do not inhibit cytochrome P450 (CYP) enzymes; however, $\alpha\beta$ D inhibits all except CYP2C19. LogKp values of geijerone and $\alpha\beta$ D, -5.26 and -5.01 cm/s respectively, are comparable to memantine (-5.06 cm/s). The compounds belong to toxicity class 3 – 5. DHBT and $\alpha\beta$ D were predicted to be immunotoxic, respectively carcinogenic and nephrotoxic. Geijerone had a better binding affinity, similar drug-likeness, and ADME properties as memantine, but with a lower toxicity profile, and can therefore be further explored as an inhibitor of NMDAR.



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sciforum-104003: Needle-guided scleral fixation IOL: easy technique for beginner surgeons

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To propose a very safe and efficient method for scleral fixation IOL applicable in all cases of aphakia and dislocated or subluxated lens and malpositioned IOL. This method is suitable for both experienced and inexperienced surgeons eliminating the need for a vitreoretinal surgeon, trocars or the risk of haptics rupture.

Methods: Fifteen patients, each with dislocated lens or subluxated lens, aphakia or malpositioned IOL in one eye, underwent transscleral needle-guided fixation of a PMMA single piece IOL. A long needle (e.g. CTC-6L, STC-6 or CIF-4) was inserted into a 24-gauge cannula. This assembly was passed from superotemporal sclerotomy (3 mm from the limbus) to superonasal sclerotomy (3 mm from the limbus). The needle was then loaded with double armed polypropylene 9-0 suture which passed through and emerged from the superotemporal incision, thus creating a single suture strand from nasal to temporal sides, each end carrying a needle -one straight and the other curved. The suture's extremities were knotted to the haptics of the single piece PMMA IOL loops and inserted into the AC through a 6 mm corneal incision, applying torsional forces in opposite directions, making the IOL less easily tiltable. Sutures were placed both on the sclera and cornea after the implant. **Results:** Visual acuity was of 0.1 Logmar in every patient on day one after the procedure. No IOL tilting was noted. Mild conjunctival hyperemia was present in 70% of the eyes. **Conclusion:** the needle-guided scleral fixation IOL is a highly safe and effective technique, even for a two-time surgery, in all cases of aphakia, dislocated/subluxated lens and malpositioned IOL. The pros of this technique are the safety of non tilting of the IOL, the absence of risk for subsequent vitrectomy due to IOL dislocation into the vitreous chamber and, its ease of reproducibility even for inexperienced surgeons.



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sciforum-101877: Peripheral venous simulator development for medical training

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The necessity to develop skills in medical training, from simple procedures such as sutures, venipunctures, and peripheral venous cannulations to complex surgeries, has driven innovation in the fabrication of medical simulators throughout history. These simulators are crafted using materials that mimic the physical and mechanical characteristics of human body parts, providing realistic training experiences. However, the costs associated with developing these simulators pose a significant challenge, especially for low-income areas. This work explores practical options for creating cost-effective and useful simulators by fabricating pieces that represent the forearm, a common site for venipunctures and peripheral venous cannulations. The fabrication process involved combining three types of polymers: PDMS, food-grade silicone, and Artesil shore 20 silicone, along with a Foley catheter to simulate the arm veins. The compatibility of these materials was thoroughly evaluated to produce valid prototypes, ensuring that the stress ratios closely matched the properties of human tissue. Preliminary evaluations of the simulators yielded promising results. They received an acceptability rating of 57.1% for excellent, 28.6% for good, and 14.3% for fair based on user experience. Medical students who tested the simulators found them effective for explaining the behavior of fluids in the body during venoclysis simulations. This feedback highlights the simulators' utility in providing hands-on training and enhancing the understanding of fluid dynamics in medical procedures.



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sciforum-103612: Precision Analysis of Prosthetic Abutment Couplings on Megagen® Dental Implants Using MicroCT

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Dental implants have revolutionized dental restoration, offering unparalleled functionality and aesthetics. However, the longevity and success of these implants are critically dependent on the precision of prosthetic abutment couplings. Micro-computed tomography (microCT) has emerged as a vital tool in assessing these parameters, providing detailed insights into the structural integrity and fit of dental components. This study aims to evaluate the precision of the couplings between prosthetic abutments and healing screws on Megagen® AnyOne® dental implants using microCT.

The investigation utilized the microCT technique with specific parameters: an optical axis of 502, an object-to-source distance of 226.60 mm, a camera-to-source distance of 266.50 mm, a source voltage of 50 kV, a source current of 800 μ A, and an image pixel size of 18.20 μ m. The samples analyzed included Megagen® AnyOne® implants with dimensions of 4x10 mm and 4x5 mm, tightened at 5-8 Ncm using a digital torque gauge. This study focused on identifying the presence of air gaps and the precision of the couplings through detailed three-dimensional reconstructions and radiographic evaluations.

The microCT analysis revealed no presence of air gaps or radiographic discrepancies in the couplings between the prosthetic abutments and the healing screws. The fixture dimensions were consistent with the expected standards, with a length of 9.347 mm and a radiographic width of 3.914 mm. The three-dimensional reconstructions confirmed the absence of communication between the external and internal environments of the implant connection, underscoring the precision and reliability of the Megagen® AnyOne® implants.

This study confirms the high precision and reliability of the Megagen® AnyOne® dental implants in the coupling of prosthetic abutments and healing screws. The absence of air gaps and the congruence of fixture dimensions with expected standards highlight the exceptional quality of these implants. Future research should focus on longitudinal studies to assess the long-term clinical outcomes and potential improvements in microCT technology to further enhance diagnostic capabilities.



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Session 2. Nanosciences, Chemistry and Materials Science

sciforum-104381: “Facile Chemo green synthesis of ZnO nanostructure from filtrate of Zinc acetate and aqueous leaf extract of *Psidium guajava* and *Azadirachta indica* : Degradation of Azo dyes under sunlight irradiation and Antimicrobial Potential”

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Background: Nanaocrystalline zinc oxide (ZnO NP) with a tunable morphology has been synthesised by means of a novel sol-gel method, and exhibits enhanced photophysical properties, high cytotoxicity, antibacterial, abated toxicity, and significant excitation energy. The presence of unreacted metabolites like carbohydrates, flavonoids, and gallic acid in the filtrate of the aqueous leaf extract of *Psidium guajava* (P) and *Azadirachta indica* (A) leaf aids in the green synthesis of ZnO NPs.

Methods: In the initial step, a 40 mL aqueous leaf extract from two plants is combined with 460 mL of 4.36 M zinc acetate and heated at 80 °C while stirring. A reddish-brown precipitate forms and is filtered, allowing the remaining filtrate to be used for the chemo-green synthesis of ZnO NPs. Then, 20 mL of 1 M NaOH is separately added dropwise in 480 mL of the filtrate of **P** plants and **A** plants, with constant stirring for 20 minutes at room temperature and then stirring at 80 °C for 6 hours. The resulting ZnO NPs are filtered, washed with ethanol, subjected to calcination at 4500C for 2 hours and characterised by XRD, DRS, and Zeta potential for crystalline, optical, and surface charge. For photocatalytic testing, a 100 mL solution of reactive blue-171 at 10 ppm is stirred, followed by exposure to sunlight. Additionally, the antimicrobial efficacy against Gram-negative *Escherichia coli* is evaluated.

Results and Conclusion:

Synthesised ZnO NPs from **P** and **A** have direct band gap energies of 4.72 and 4.611 eV and negative zeta potentials of 22.4 and 23.4 mV, and lead to 89.2% and 96.4% dye degradation in 140 minutes, respectively. The antibacterial activity of A is superior to that of P. This study suggests that the repurposing of waste filtrate by the green method for the high-yield synthesis of ZnO NPs with scant use of an alkali fosters sustainability and alleviates economic strains.



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***sciforum-103396: In situ* modifications of porphyrin-conjugated magnetic nanoparticles for photodynamic inactivation of pathogens**

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The spread of infectious diseases is a consequence of environmental contamination due to the presence of pathogenic agents in aqueous media. Therefore, it is of a vital importance the development of an economical and eco-friendly method to eradicate these microorganisms. The use of photodynamic inactivation (PDI) with photosensitizers conjugated to magnetic nanoparticles (MNPs) has emerged as a successful approach for the rapid elimination of microorganisms. For this purpose, MNPs of Fe₃O₄ coated with silica and terminal amine groups were synthesized. After that, 5,10,15,20-tetrakis(pentafluorophenyl)porphyrin (TPPF₂₀) was covalently immobilized on the MNPs by nucleophilic aromatic substitution reaction. Then, the remaining pentafluorophenyl groups of attached to MNPs were substituted by polyethylenimine (PEI) or spermine (SP). Absorption and fluorescence emission spectra of these conjugates showed the typical bands of tetrapyrrolic macrocycles in water. On the other hand, photodynamic activity investigations indicated that these MNPs generated singlet molecular oxygen and superoxide anion radical in solution. In addition, PDI studies were carried out with *Staphylococcus aureus* and *Escherichia coli*. These MNPs were able to eradicate microorganisms (>6 log decrease) after 30 min of irradiation with white light. Therefore, the basic amine groups can be used to generate positive charges at physiological pH, which improve the interaction with the bacteria. Furthermore, this procedure facilitates the recycling and reuse of these MNPs after treatments using a magnetic field. These

results indicate that conjugates of TPPF₂₀ to MNPs are interesting photodynamic materials to eliminate pathogens.



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sciforum-106415: Preparation and characterization of vertical graphene-based nanocomposites for electrochemical applications

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Graphene or carbon nanowalls, graphene sheets, and graphene nanoflakes are other names for vertical graphene (VG), a three-dimensional form of graphene. Compared to conventional horizontally oriented or randomly arranged graphene, the interest in vertically oriented graphene can be attributed to its unique geometry and open three-dimensional lattice, which allows easier access to the graphene edges, higher surface-to-volume ratio, high electrochemical activity, and electrical conductivity. The electrochemical properties of VG can be improved by incorporating nanoparticles that can change the major type of charge carriers, increase the specific surface and prevent the aggregation of graphene sheets. In this paper, we established a process for synthesising VG-based nanocomposites by treating graphene in an acid solution and then decorating the sheets with gold nanoparticles. The vertical graphene obtained by the chemical vapour deposition process on the Si/SiO₂ substrate is subjected to a treatment with H₂SO₄ and HNO₃ to improve the wetting capacity. The anchoring of the metallic nanoparticles is carried out through an ex-situ process, which involves 2 stages, in the first part the synthesis of the metallic nanoparticles is performed, and in the second step, the GV substrate is immersed in the gold NPs solution. Gold nanoparticles are obtained using chloroauric acid, as a precursor, and trisodium citrate, as both reducing agent and electrostatic stabilizer of the nanoparticles to avoid agglomeration. Using SEM microscopy, the shape, size, and distribution of metal nanoparticles inside the graphene were evaluated. Spectroscopy was used for the structural analysis, and goniometric studies revealed the wetting and percolation capacity of the obtained materials. The application capacity was demonstrated by cyclic voltammetry.

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sciforum-106953: Effect of the manufacturing process on the electromagnetic interference shielding properties of graphene nanoplatelet/epoxy composites

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In this work, we studied the electrical and thermal properties of graphene nanoplatelet (GNP)/epoxy nanocomposites in terms of different variables, such as GNP type or dispersion time. The relationship between these parameters and the electrical and thermal properties of the samples was analyzed, focusing on samples over the percolation threshold (which is around 7 %wt). The best results were observed with 10–12% loading and a higher surface area, as the optimal electrical conductivity and an increase on the shielding effectiveness were achieved in the GHz range. Several characterization techniques, such as Raman spectroscopy and X-ray diffraction, were employed to analyze the GNPs after the sonication process, providing valuable information about the aspect ratio of the GNPs. The electromagnetic interference shielding (EMI) was studied between 100 MHz and 4 GHz, showing an increase in value with increasing GNP content, achieving a maximum of nearly 5 dB at 2 GHz. The influence of sonication on the results was analyzed, as sonication affects the morphological characteristics of nanoplatelets, introducing defects and modifying their aspect ratio. This shows the importance of the proper selection of sonication time to achieve the best dispersion state of the reinforcement within the epoxy matrix to achieve the maximum electrical conductivity and, thus, the optimal shielding performance.



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sciforum-103826: A qualitative characterization study of peptide complexes isolated from the epidermal mucus of the *Clarias gariepinus*

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Regulatory peptides are widely used as immunomodulators, neuroprotectors, and neurometabolicstimulators. This work is devoted to the isolation of peptide complexes from the epidermal secretion of ascaleless fish species and the study of these complexes properties. It has been suggested that suchpeptides can suppress inflammation and promote the regeneration of human integumentary tissue.The skin secretion of the African catfish (*Clarias gariepinus*) was taken as a source of low-molecularpeptides. Peptide isolation was carried out according to the following scheme: acetic acid extraction inthe presence of a biogenic salt ($MgCl_2$, $CaCl_2$, $ZnCl_2$, $MgSO_4$, $CaSO_4$); ultrasonic cavitation treatment;removal of major proteins by filtration; precipitation of low-molecular weight peptides using acetone.To qualitatively check the resulting product, IR spectroscopy and chromatomass spectrometry wereused. Using these methods, it was possible to prove that the isolated product is a complex containingtens of thousands of low molecular weight peptides. To confirm the antioxidant properties of theproduct, the autoxidation of adrenaline in an alkaline medium was used. Antioxidant properties aredecisive in wound healing preparations of peptide origin. It was found that the resulting peptidepreparation is capable of inhibiting the oxidation reaction of a 1% solution of adrenaline in a buffersolution, which clearly indicates its antioxidant properties. It has been shown that the use of $CaCl_2$ makes it possible to isolate the peptide fraction with the highest antioxidant activity.



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sciforum-104534: Advances in implementation of metal oxide nanoparticles for urban water pollution treatment

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Urban water bodies are facing a growing crisis due to contamination from a diverse array of pollutants, encompassing heavy metals, oil and grease, organic and inorganic chemicals, industrial effluents, and pathogenic microorganisms. This study focuses on the burgeoning field of utilizing metal oxide nanoparticles (MONs) as a potential solution to this pressing environmental challenge. The distinctive physicochemical properties of MONs, including their large surface area, catalytic activity, and photocatalytic ability, position them as promising candidates for water purification technologies. This study also comprehensively discusses the sources of urban water pollution and the specific challenges posed by different types of contaminants. A critical evaluation of MONs' efficacy in removing heavy metals, oil and grease, organic and inorganic chemicals, and industrial pollutants is presented, with a focus on the underlying mechanisms such as adsorption, photocatalysis, and redox reactions. Furthermore, the potential of MONs to neutralize pathogens and microbial contaminants is investigated. While MONs exhibit significant advantages, this study acknowledges the challenges associated with nanoparticle stability, recovery, and potential environmental repercussions. To fully realize the potential of MONs in water treatment, sustained research is imperative to refine treatment processes, develop economically viable strategies, and ensure the long-term sustainability of these technologies in addressing urban water pollution.



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sciforum-106519: Antioxidant activity of ablated CeO₂ nanoparticles with narrow size distribution

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Cerium dioxide nanoparticles exhibit antioxidant properties by neutralizing free radicals and ROS [1]. In the process of laser ablation, it is possible to obtain cerium dioxide nanoparticles with surface structural defects that determine their antioxidant properties [2]. However, since the ablation method produces particles in a wide size range, it is of interest to separate nanodispersed solutions of ablated cerium dioxide particles into narrow-sized groups to study the dependence of the antioxidant properties of nanoparticles on their sizes.

Seven samples of nanodispersed aqueous solutions of cerium dioxide particles with different average sizes were obtained by sequential centrifugation. Average sizes of homogeneous spheres of ablated cerium dioxide nanoparticles in solutions were determined using SAXS. The efficiency of their antioxidant properties in the process of photocatalytic degradation of methylene blue in the presence of TiO₂ photocatalyst particles was determined using spectrophotometry.

For the solution samples, the average size of the homogeneous sphere varied from 30±0.5 nm to 41±0.5 nm. The results of the experiments showed the samples with the smallest sizes exhibit pronounced antioxidant properties. This is due to the high concentration of structural defects on the surface of the nanoparticles and the large area of their specific surface. With an increase in the particle size, antioxidant activity was also observed, but to a lesser extent, which is due to the high crystallinity of the particles and a decrease in the width of the forbidden zone.

Thus, in this work, the production of systems of nanodispersed solutions of ablated cerium dioxide nanoparticles with a narrow size distribution, characterized by different average sizes, is demonstrated. The influence of the size factor on the antioxidant properties of ablated cerium dioxide nanoparticles in a photocatalytic reaction is studied.



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sciforum-107869: Development and optimization of geopolymer concrete with different supplementary cementitious materials.

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Sustainable construction materials are developed using alternative cementitious materials. Concrete durability is aligned with longevity of structures, especially when exposed to aggressive environments. This study explores the effects of partial replacement of cement with supplementary cementitious materials (SCMs) like silica fume (SF), metakaolin (MK), and fly ash (FA) on the durability and strength of concrete exposed to nitric acid solution. Concrete cubes were developed varying percentages of SF, MK, and FA, and were subjected to water curing. Developed samples were exposed to Nitric acid to assess the performance of material against harsh environment. The study includes performance analysis of mechanical properties through compressive strength tests, rebound hammer tests, as well as durability assessments using the volume of permeable voids (VPV) and mass loss measurements. The results indicate that the inclusion of SCMs significantly enhances the resistance of concrete to nitric acid attack, reducing both mass loss and strength degradation. Optimal performance was observed with 10% SF showing 52.22 MPa strength, which provided superior durability and maintained structural integrity under acidic conditions. This study has been conducted to developed concrete materials for Industrial plants, wastewater treatment plants and infrastructures exposed to chemically challenging environment like acidic rain and aggressive chemical exposure. This study is aligned with achievement of sustainable goals regarding innovation for industry and sustainable development of cities and communities.



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sciforum-104454: Development of a New Spectrophotometric Visible (VIS) Analysis Method of Loratadine in Pharmaceutical Tablets

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Loratadine is an effective antihistamine, or anti-H1 histamine receptor inhibitor, frequently used to relieve the major symptoms of hay fever and hives of the skin. It is a tricyclic H1 inverse agonist that is used to treat various allergies, like allergic rhinitis, nasal congestion and chronic idiopathic urticaria. The main purpose of this research was to find and develop a new spectrophotometric method in the visible (VIS) range for the quantitative analysis of Loratadine from various samples, including pharmaceuticals, and to exactly compare the final experimental obtained result with the officially stated amount of Loratadine reported on the tablet. Following the quantitative color reaction with alpha naphthylamine 0.2% from an alkalized alcoholic solution, in the presence of sodium nitrite 4-5% and hydrochloric acid 10-15% solution, an intense bright orange azo dye with a reddish shade quantitatively obtained was analyzed at its maximum absorption wavelength $\lambda = 490$ nm. The amount of pure Loratadine in the pharmaceutical was found to be 9,777 mg of pure active substance / film-coated tablet, very close to the official stated reference value of 10 mg, corresponding to 97.776 % of pure Loratadine. The average percentage deviation was (+) 2.224 %, below the maximum allowed average percentage deviation (± 7.5 %) imposed by the rules of the Romanian, European and International Pharmacopoeias. The proposed method was linear over the entire standard concentration range of 0,75 $\mu\text{g/mL}$ - 11.25 $\mu\text{g/mL}$. The linear regression coefficient ($R^2 = 0.9993$, $R^2 \geq 0.9990$) and the correlation coefficient ($R = 0.9996$, $R > 0.9990$) were within the normal range of values. The standard error of the regression line was very low, within the normal limits: $\text{SE} = 0.007078$, $\text{SE} 1$. The applied method was subjected to a complete statistical validation process. All statistical parameters were found to be within the normal accepted values.



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sciforum-106179: Effect of soil mineralogy on the performance of Rice husk ash and wood ash (RHAWA) as Agrowaste-based alkali-activated Binders/modifiers in soil stabilisation

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Soil stabilisation is crucial for enhancing the strength and bearing capacity of earth roads, particularly in regions where soils lose stiffness when saturated with moisture. Traditional stabilisers like Portland cement have been used, but emerging technologies such as alkali activation offer promising alternatives. However, the high energy requirements of alkali activators raise concerns about their environmental impact. This study investigates the feasibility of using agro/industrial wastes as alkali activator replacements for soil stabilisation and the effect of mineralogy on the performance of the binders. Materials from various regions were sourced, including wood ash and rice husk ash from Fursa rice mill, Kano, and kaolin from Bokkos, Plateau State in Nigeria. Soil samples from Abuja were also collected. Characterisation of source materials determined geotechnical properties and mineralogical/elemental oxide compositions. Initial trials determined optimal mix ratios for developing waterproofing binders. Optimised mixes were then introduced into soils at varying proportions (0-15% by dry weight) at moisture contents corresponding to the optimum moisture content of respective soils. Unconfined compressive strength tests were conducted after 24 hours and 7 days of curing at room temperature, both in dry and soaked conditions. Two-way ANOVA analysis revealed that the mineralogical composition of soils significantly influenced the strength and density of treated soils at a 5% confidence level. Additionally, alkali-activated modifiers significantly improved soil strength, with curing time showing minimal effect on soil behaviour. These findings underscore the potential of utilising waste materials for developing sustainable soil stabilisation solutions, aligning with the global transition toward a circular economy as well as showing the significance of mineralogy on the performance of the binder.



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sciforum-103562: Experiment design for copper corrosion inhibition using an expired drug

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This study investigates the use of a liquid pharmaceutical drug as a corrosion inhibitor for copper in 1M perchloric acid, aiming to explore environmentally friendly corrosion protection solutions.

Response Surface Methodology (RSM) was employed to optimize and model the inhibition efficiency based on key experimental parameters: drug concentration (0.1% to 0.5%), temperature (20°C to 60°C), and immersion time (0.5 to 1.5 hours).

A quadratic model was developed to predict inhibition efficiency. Upon careful examination of the main effect coefficient plot, it was observed that a negative sign in the coefficients signifies an antagonistic effect of the factors on inhibition efficiency, whereas a positive sign indicates a synergistic effect, enhancing the efficiency of the inhibitor. The optimization process identified conditions that yielded the highest inhibition efficiency (99.71%), specifically at a drug concentration of 0.49%, a temperature of 20.71°C, and an immersion time of 1 hour. The experimental design was validated by a high coefficient of determination ($R^2 = 0.994$), an adjusted R^2 of 0.986, and a predictive Q^2 value of 0.945, all of which indicate strong model reliability.

This study highlights the practicality of repurposing pharmaceutical compounds for corrosion inhibition, thereby contributing to green chemistry by promoting the use of environmentally benign substances. The successful application of RSM underscores its utility in optimizing corrosion inhibition processes. The findings encourage further exploration of pharmaceutical inhibitors in various corrosive environments, suggesting potential advancements in sustainable corrosion protection strategies.



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sciforum-103588: In Silico Evaluation of Gold and Silver Nanoparticles' Efficacy Against Five COVID-19 Variants

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The emergence and rapid spread of SARS-CoV-2 variants have underscored the urgent need for innovative antiviral strategies. This study investigates the potential of gold and silver nanoparticles as effective agents against COVID-19 variants, including Alpha, Beta, Gamma, Delta, and Omicron. Nanoparticles possess unique physicochemical properties that enable them to interact with viral particles and disrupt crucial viral functions, making them promising candidates for antiviral therapy. Through advanced computational modeling, integrating techniques such as molecular dynamics simulations and quantum mechanical calculations, we explore the interaction dynamics between nanoparticles and key viral spike glycoprotein specific to each variant, which plays a pivotal role in host cell entry. Our analysis elucidates the mechanisms by which gold and silver nanoparticles interact with variant-specific targets, docking analysis underscores their notable affinity towards all five ACE2-spike receptor variants. Notably, the binding affinities range between 0.18 and 0.27 Kcal/mol, indicative of strong interactions. Across the complexes, AuNPs generally exhibit a slightly higher affinity compared to AgNPs. Furthermore, we investigate the physicochemical properties of nanoparticles, such as size, shape, and surface functionalization, that influence their antiviral efficacy against different variants. Our findings provide valuable insights into the design and optimization of nanoparticle-based therapeutics for combating the evolving landscape of COVID-19 variants.



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sciforum-088318: Novel $\text{Zn}_2(\text{V}, \text{Nb}, \text{Ta})\text{N}_3$ Monolayers for Application in Tandem Solar Cells

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The discovery of novel nanomaterials with outstanding functionality remains paramount for continuous technological advancements. Recently, significant attention has been paid to a family of zinc-based ternary nitrides¹. For instance, a comprehensive computational study demonstrated hundreds of new (meta)stable ternary nitrides².

Using ab initio modeling simulations, novel ternary nitride $\text{Zn}_2(\text{V}, \text{Nb}, \text{Ta})\text{N}_3$ monolayers are predicted. A mechanism for the formation of the $\text{Zn}_2(\text{V}, \text{Nb}, \text{Ta})\text{N}_3$ monolayers is evaluated using ab initio molecular dynamics to facilitate their the chemical vapor deposition.

The predicted $\text{Zn}_2(\text{V}, \text{Nb}, \text{Ta})\text{N}_3$ monolayers reflect light in the far-infrared and infrared regions from 0.1 to 1.65 eV and absorb light in the visible range. The maximum absorption values reach 16.06%, 17.46%, and 17.72% for the Zn_2VN_3 , Zn_2NbN_3 , and Zn_2TaN_3 monolayers, respectively. Moreover, the Zn_2VN_3 monolayer possesses the highest strength and elasticity. In addition, the Zn_2VN_3 monolayer is the most stable in moist environments and is less reactive towards atmospheric N-containing gas molecules. It is also found that there is a local surface dipole at the interface between the $\text{Zn}_2(\text{V}, \text{Nb}, \text{Ta})\text{N}_3$ monolayers and the NH_3 , NO, and NO_2 molecules, which affects their functionality.

In conclusion, the Zn_2VN_3 monolayer is the most promising for application in solar energy devices, such as for blocking layers in tandem solar cells. The discovered high sensitivity towards NH_3 , NO, and NO_2 molecules and reversibility of the Zn_2TaN_3 monolayers make it promising for application in molecular sensing.

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sciforum-093522: Stabilization Mechanism of a Self-synthesized Nanobiosensor, DiR Accommodated Solid Lipid Nanoparticles

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Introduction

Nanobiosensors, i.e., probes encapsulated in nanoparticles, have been widely employed in disease diagnosis and pharmacokinetic analysis. In our published work, a probe with a dialkylcarbocyanines skeleton (generally known as DiR) was incorporated into solid lipid nanoparticles (SLNs) to produce DiR-SLN, which was intended for biological fate tracking after pulmonary delivery. As shown by the previous results, the self-synthesized DiR-SLN possessed great chemical and physical stability during storage. Of note is that the stabilization mechanism of such a system remained unclear. Based on a preliminary study and literature survey, we hypothesized that the strong interaction between DiR molecules and SLN carrier materials guaranteed great stability. In order to validate this hypothesis, we examined the interaction between DiR and the main components of SLN, viz. cetyl palmitate (CP) and Tween 80 (T80) by the isothermal titration calorimetry (ITC) technique.

Methods

ITC was a technology commonly used in biochemistry to unravel the interaction pattern between various molecules. In the present study, titrations of DiR towards CP and DiR towards T80 were performed, in a cosolvent of 98% acetone–water (v/v). The tests were conducted in triplicates.

Results

It was shown that both DiR-CP and DiR-T80 titrations exhibited negative peaks (peak value -2 and -4 $\mu\text{cal/s}$, respectively), suggesting exothermal interaction modes. After integration processing, the change in enthalpy (ΔH) was calculated to be approximately -5 and -20 kcal/mol for DiR-CP and DiR-T80, respectively. Considering the exothermal nature and the ΔH values, it was inferred that weak (in DiR-CP) and moderate (in DiR-T80) hydrogen bonds were generated.

Conclusions

The hydrogen bonds between cargo and carrier might be a critical contributor to system stability. Our study provided a potential approach to analyze the stabilization mechanism of nanobiosensors, which could pave the way for the future studies.



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sciforum-106655: Star- and comb-shaped betulin-based polyanhydrides with anticancer activity—synthesis and characterization

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Betulin exhibits a broad spectrum of biological relevance, including anticancer activity. Due to this, betulin and its derivatives, e.g. betulin disuccinate (DBB), can be used as new potential therapeutic agents. The presence of two carboxyl groups in DBB allows for the preparation of polyanhydrides.

The aim of this work was to obtain betulin-based highly branched polyanhydrides with star- or comb-shaped architectures. Branched polymers offer significantly different physical properties from linear polymers and can provide several advantages for drug delivery applications.

In this study, we develop novel highly branched polyanhydrides with different DBB contents and different architectures through the two-step melt polycondensation of DBB and polycarboxylic derivatives of succinic acid oligomers (OSAGE-COOH and PSAGE-COOH). The content of DBB in the polymers ranged from 70 to 95 wt %. The use of OSAGE-COOH as a branching agent allowed us to obtain star-shaped polymers, while the use of PSAGE-COOH resulted in comb-like polymers. The protein-staining sulforhodamine B assay, developed by the National Cancer Institute for in vitro antitumor screening, was employed in this study for the determination of the cytotoxic activity of the polymers.

The physicochemical properties of the polymers varied depending on the content and structure of DBB. All the obtained polymers released DBB as a result of hydrolysis under physiological conditions and exhibited cytostatic activity toward cancer cell lines while being non-toxic to normal cells. The obtained results offer a promising area for further research into these copolymers' use in medicine.

Branched betulin-based polyanhydrides exhibit anti-cancer activity; thus, they can be used as a polymeric prodrug. Due to their biodegradability and non-toxicity, they are also ideal candidates for carriers of other biologically active substances.



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sciforum-102703: The Synthesis of Silver Nanoparticles by Marine Brown Algae *Padina commersonii*: The Characterization and Evaluation of their Antimicrobial Potential.

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Drug-loaded nanoparticles serve as carriers for targeted therapies, with silver nanoparticles being particularly noted for their conductivity, stability, and safety in treating diseases. *Padina commersonii*, an edible brown macroalgae found along Sri Lanka's coastal beaches, is eco-friendly. The bioactive compounds in *Padina commersonii* can reduce metal ions to form nanoparticles, acting as stabilizers and capping agents. This research aims to green-synthesize silver nanoparticles using *Padina commersonii*, characterize the nanoparticles, and evaluate their in vitro antioxidant efficacy. Silver nanoparticles were synthesized by mixing crude methanol extract of *Padina commersonii* with silver nitrate. Characterization of the synthesized nanoparticles was conducted using UV-Vis spectroscopy, Dynamic Light Scattering (DLS), Zeta potential analysis, Scanning Electron Microscopy (SEM), Energy Dispersive X-ray (EDX) analysis, X-ray Diffraction (XRD), FTIR spectroscopy, and Raman spectroscopy. Antimicrobial activities were evaluated against bacterial and fungal strains via the Agar well diffusion method. A colour change from pale yellow to reddish-brown within 48 hours indicated nanoparticle formation. UV-Vis spectrophotometry revealed a surface plasmon resonance peak at 424 nm, confirming silver nanoparticles. DLS analysis showed an average size of 79.34 nm, with zeta potential at -21.5 mV indicating stability. SEM images depicted spherical nanoparticles with smooth surfaces and no aggregation. EDX analysis confirmed 19.5% silver content by weight, and XRD analysis showed a face-centered cubic structure. FTIR and Raman spectroscopy identified proteins, phenolic compounds, and amines as capping agents, with polyphenolic compounds and flavonoids as reducing agents. The antimicrobial potential of silver nanoparticles synthesized using *Padina commersonii* against bacterial strains *Staphylococcus aureus* (12.77 ± 0.58 mm), *Escherichia coli* (15.27 ± 0.58 mm), and fungal strains *Aspergillus niger* (18.10 ± 0.15 mm) and *Candida albicans* (17.43 ± 0.57 mm) was greater than that of the crude extract of *Padina sp.* (*S. aureus* = 11.17 ± 0.29 mm, *E. coli* = 10.50 ± 0.50 mm, *A. niger* = 12.66 ± 0.10 mm, *C. albicans* = 15.66 ± 0.10 mm). These findings highlight the potential of eco-friendly synthesized silver nanoparticles as a therapeutic approach for treating microbial infections.



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sciforum-105484: Visible (VIS) Spectrophotometric Analysis of Phenobarbital from Pharmaceuticals through a Quantitative Coupling Reaction with diazonium salt of Beta-Naphthylamine

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Phenobarbital, also known as Luminal, is a barbituric acid derivative that possesses an intense hypnotic and sedative effect. It also has a secondary important anti-convulsant effect. The main purpose of this research consisted of the development and optimization of a new, simple, rapid, and accurate spectrophotometric method in the visible range (VIS) for quantitative analysis of Phenobarbital from various different pharmaceutical samples. Beta-naphthylamine from 0.1 % alcoholic solution underwent a complete diazotization reaction in the presence of sodium nitrite NaNO_2 , 5%, and hydrochloric acid HCl, 15%-20%, for half an hour in cold conditions (0-5°C). The diazonium salt of beta-naphthylamine formed was then quantitatively coupled with Phenobarbital from a 5% sodium hydroxide NaOH solution, which led to the synthesis of a bright red-orange dye providing a prominent maximum absorption wavelength at $\lambda = 487 \text{ nm}$. This azo dye was formed in equivalent proportions to the Phenobarbital from the sample and was spectrophotometrically determined. Through spectrophotometric determination of the bright red-orange azo dye at $\lambda = 487 \text{ nm}$, the content expressed in milligrams of pure Phenobarbital from the tablets was effectively calculated. The pure Phenobarbital content calculated was found to be 97.104 mg, very close to the official amount of 100 mg stated by the pharmaceutical company. This pure amount found corresponded to a 97.104 mg % content. The average percentage deviation from the official reference value (100 mg) of the 97.104 mg Phenobarbital content calculated was only (+) 2.896 %, located below the maximum allowed limit of $\pm 5\%$ imposed by the European Pharmacopeia and by the Romanian Pharmacopoeia's official rules. Finally, the statistical validation procedure consisted of a linearity analysis and detection limit (LOD) and quantitation limit (LOQ) calculations, as the first stages. The stability of the prepared solutions, the system's precision, the intra-day and inter-day precision of the method, and the accuracy of the method were also within the normal range of values.



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sciforum-107769: A Computational Approach to Thiosemicarbazone Metal Complexes: Structure, Reactivity, and Biomedical applications

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Thiosemicarbazones are recognized for their flexibility in coordination and various applications in areas such as medicinal chemistry, catalysis, and material science. Thiosemicarbazone metal complexes are a significant area of study due to their intriguing properties and applications across multiple scientific fields. By using density functional theory (DFT) and molecular docking methods, researchers conduct computational studies to elucidate the structural, electronic, and reactivity characteristics of these complexes. These investigations not only aid in understanding experimental data but also guide synthetic strategies by offering predictive insights into the structural features of the complexes. Additionally, these computational approaches allow scientists to analyze electronic structures and spectroscopic properties, which is essential for elucidating reactivity patterns and establishing structure–activity relationships (SARs). In biological contexts, these studies provide insights into how these complexes interact with biological targets, enhancing our understanding of their mechanisms of action and informing the design of therapeutic agents that exhibit improved efficacy and decreased toxicity. Computational studies bridge the gap between experimental research and theoretical understanding, enabling scientists to predict and optimize the behavior of metal complexes in various chemical and biological systems. In this study, we discuss the computational insights of thiosemicarbazone metal complexes, exploring their structural properties, reactivity, and biomedical applications.



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sciforum-103360: A kinetics and mechanistic study of two 1,3-dipolar cycloaddition reaction types

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The Huisgen reaction, also known as 1,3-dipolar cycloaddition, has become an indispensable tool in modern organic chemistry. This type of reactions is now widely employed for the preparation of heterocycles and is also involved in many applications for the synthesis of natural products and biologically active compounds. The success of cycloaddition reactions relies on their potential to provide access to four-, five-, and six-membered rings with excellent stereocontrol and yield. For instance, the Diels–Alder reaction is a [4+2] cycloaddition that yields a functionalized six-membered ring product. Generally, it is well known that cycloaddition reactions are commonly characterized by a concerted mechanism, and thus, the atoms on the dienophile or the diene maintain their orientation in the product. Additionally, 1,3-dipolar reactions have also been theoretically investigated over the last few decades by theoretical chemists in order to explain their kinetics mechanism and study their yields, regioselectivity, and stereochemistry with available theories and approaches. The analogy to the electronically equivalent Diels–Alder reactions was evident. Back in 1960, the concerted reaction mechanism of cycloadditions was proven by both experiment and theory, and it was found to be a good explanation for most [3+2] cycloadditions. In this study, the most popular density functional theory (DFT) B3LYP method was used to characterize two 1,3-dipolar cycloaddition reactions, i.e., the regioselectivity using conceptual DFT, such as Fukui and Parr functions, and the exploration of reaction mechanisms via the elaboration of the energetic profile.



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sciforum-106494: A low-cost and portable biosensor array for the simultaneous multi-analyte monitoring employed in health and athletic performance exploiting a multi-channel surface plasmon resonance platform based on plastic optical fibers

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Hormones are crucial in regulating physical and mental health and athletic sports performance. In particular, cortisol, estradiol, and testosterone monitoring can provide insights into their effects on mood, stress responses, and athletic performance. Increasing levels of these hormones are linked to increased anxiety and depression, and measurements of their fluctuations can provide predictions of sports performance. Both sex hormones and cortisol significantly modulate stress responses, with distinct effects observed in men and women and in individuals undergoing hormone treatments. These insights underscore the importance of hormone monitoring for optimising mental health and athletic outcomes. This work proposes a compact and low-cost multi-channel surface plasmon resonance (SPR) platform based on plastic optical fibers (POFs) combined with several specific bio-receptor layers as a point-of-care measurement tool. This multi-channel SPR-based tool is based on optical fiber components for precise, label-free, and high-throughput detection without complex and expensive instrumentation. The multi-channel SPR-POF tool is applied to simultaneous multi-analyte detection of cortisol, estradiol, and testosterone in saliva. The plasmonic POFs' sensitive surfaces are functionalised with different bio-receptors, such as the Glucocorticoid Receptor (GR) and the Estrogen Receptor (ER). This compact and cost-effective multi-channel SPR-based point-of-care tool could be of interest for the simultaneous detection of several biomarkers in saliva for health and sports purposes.



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sciforum-107289: A Statistical Study on Antibiofilm Activities of nanosized metal oxide particles: investigating the relationship with nanoparticle size.

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Biofilm formation is a bacterial phenotype by which bacteria can make antibiotic resistance. The extracellular polymeric substances (EPS) matrix of biofilm protects bacteria against environmental stresses, including antibiotics, immunological reactions, and disinfectants. The inhibition of antibiotic resistance is now a concern in medical science. In nanotechnology area nanoparticles are showing promising effect in inhibiting biofilm formation. *Pseudomonas aeruginosa*, *Streptococcus pneumoniae*, *Listeria monocytogenes*, and *Escherichia coli* are some of the bacteria that are susceptible to the powerful antibacterial and antibiofilm activities that are exhibited by several nanoparticles. These nanoparticles can generate reactive oxygen species (ROS) and release ions, which make them effective for inhibiting biofilm formation. Some nanoparticles bind with bacterial membrane or bacterial protein to remove antibiotic resistance and to make them possible in antibiofilm activities. The effect of nanoparticles in antibiofilm activity may depend on size. Because generating reactive oxygen species (ROS) and releasing ions property is dependent on size. This statistical study will show the utilization of nanoparticles in inhibiting antibiotic resistance by inhibiting quorum sensing and by inhibiting biofilm formation will depend on their size. We will demonstrate the effect that the sizes of the NPs have on the antibiofilm activity through our investigation. In this instance, we obtained information needed for data analysis from a variety of research articles. The descriptive analysis and cross-sectional study are all components of our analysis, which involves employing those data. The results of this investigation will indicate that size influences the antibiofilm activity.



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sciforum-107297: A Statistical study on nanoparticle utilization to reduce swarming motility in Gram-negative bacteria: exploring the effect of the size and concentration of the nanoparticles

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Swarming motility (SM) is a term that describes the rapid movement of bacteria across a surface with the assistance of their flagellar rotation. Flagellar motility has been discovered to drive transitory cell–surface interactions and overpower the electrostatic repulsive forces at these interfaces. As a result, it is necessary for bacterial self-aggregation and irreversible surface adherence, both of which are necessary for the creation of antibiotic resistance in bacteria. In bacteria such as *Pseudomonas aeruginosa*, *Escherichia coli*, and *Proteus mirabilis*, SM is a crucial pathogenicity factor that allows them to acquire resistance to several antibiotics. As the prevalence of antibiotic resistance has increased, researchers have begun to investigate alternate approaches to inhibiting the motility of bacteria. One such approach is the utilization of nanoparticles (NPs). Within the objectives of this work, the size-dependent impacts of nanoparticles such as copper oxide (CuO), zinc oxide (ZnO), gold nanoparticles (AuNPs) and chitosan nanoparticles (CS-NPs) on the prevention of bacterial swarming are investigated. These findings highlight the significance of nanoparticle size and concentration in the process of modifying motility in bacterial swarming. The results of this statistical analysis demonstrate that the effectiveness of nanoparticles in preventing antibiotic resistance by suppressing SM is contingent on the size of the nanoparticles and the concentration that is employed. The information that we required for the data analysis was acquired from several different research articles in this instance. Our study method included a descriptive analysis and cross-sectional study of these data. Through our inquiry, we illustrate how NPs' anti-swarming activity is affected by their size and concentration.



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sciforum-107319: A Systematic Review of Conductive Polymers for Advanced Sensor Technologies: Synthesis, Developments, and Applications

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Pamantasan ng Lungsod ng Maynila

Conductive polymers (CPs) are a type of organic materials that combine the flexibility and processability of polymers with the electrical properties of inorganic semiconductors, making them highly suitable for sensor development. These materials, including polyaniline, polypyrrole, polythiophene, and PEDOT, exhibit unique electrical, optical, and chemical properties, enabling their use in the design of highly sensitive and selective sensors for a broad range of environmental, industrial, and biomedical applications. The conductivity of CPs is derived from their conjugated structure, which can be “tuned” through doping and functionalization to optimize the performance of various sensing materials. This systematic review provides a comprehensive examination of the synthesis techniques, conductive mechanisms, and structural modifications that make CPs effective in chemical, gas, and biosensors. It discusses how CPs, which have significant advantages in terms of selectivity and responsiveness, enable real-time, high-precision detection of chemical and biological analytes. The paper also categorizes the types of sensors made with CPs, including chemical sensors for pollutant detection, gas sensors for CO₂, CO, and NH₃ sensing, and biosensors for medical diagnostics like glucose monitoring. In addition, this systematic review addresses important issues such as enhancing sensor sensitivity, selectivity, and stability over time, all of which are significant in providing dependable performance in practical applications. This systematic review highlights the significance of conductive polymers in developing sensor technologies and promoting innovation in fields ranging from environmental monitoring to biomedical diagnostics by addressing current advancements and identifying future research directions.



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sciforum-105855: Adhesion of PJM-printed MED610 objects on textile substrates

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Three-dimensional printing on textile fabrics was first suggested around 10 years ago, leading to an increasing amount of research on this topic. While first approaches aimed at offering new design possibilities, the mechanical properties that can be achieved by these polymer/textile composites are more the focus of recent investigations. For such technical applications, adhesion between both parts of the composite is crucial. While most studies have concentrated on fused deposition modeling (FDM) on textile fabrics so far, the adhesion of these polymers on textiles is still problematic. For this reason, recently, resin-based 3D printing on textile fabrics has been investigated. The possibility to print on textiles by stereolithography (SLA) was already shown a few years ago and has been further investigated since. PolyJet modeling (PJM) was reported as another method for direct printing on textiles only recently. This presentation shows the first study of PJM printing on different fabrics with the medical resin MED610. While a high textile surface roughness increases the printed material's adhesion, high hydrophobicity reduces it. In addition, first experiments on the impact of different textile substrates on the porosity of the MED610 surface are reported, which may support the tailoring of the porosity for the composites' potential use in tissue engineering and similar biotechnological applications.



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sciforum-105852: Adsorption of Nickel (II) From Aqueous Solution Using Cellulose Nanocrystals Hydrogel, Employingcentral Composite Design

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Cellulose nanocrystals (CNCs) were modified to work as an adsorbent in order to remove nickel (II) from an aqueous solution. The structure and properties of CNCs were characterised using FTIR and SEM. Statistics show that the response surface model approach performs well. Four operational variables were studied: The initial concentration of the Nickel (II) solution in mg/L, the pH, the contact period in minutes, and the adsorbent dose in mg/100 mL. The removal percentage (%) indicated the result. After 60 minutes of contact time, a beginning concentration of 50 mg/L, an adsorbent dose of 15 mg, and an initial pH of 2, the adsorption capacity was 300 mg/g. FTIR examination revealed the following functional groups: hydroxyl groups (OH), which peaked around $3300\text{--}3500\text{ cm}^{-1}$, and carboxyl groups (COOH), which peaked around 1700 cm^{-1} . The AAS was used to determine the remaining concentration in the solutions. With maximum removal capacities of 80–98% at initial concentrations of 175–250 mg/L, the results demonstrated that the modified CNCs hydrogel exhibited high Nickel(II) removal efficiencies. It was found that the adsorption process was massively affected by pH. The adsorption capacity is generally larger at lower pH values because protons are more readily available and can compete with nickel ions for adsorption sites. The elimination of Ni(II) ions from the solution is most effective when the pH is kept between 2–5.



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sciforum-106374: Advancing skin cancer treatment through dual drug loading into liposome-derived nanosystems

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As a complex disease, skin cancer is a major public health challenge. Recent advances in nano-delivery systems have broadened the possibilities for the development of chemotherapy and immunotherapy. Furthermore, nanovesicles offer a precise, targeted, and effective approach for delivering therapeutic molecules.

The goal of the researchers in this field is to improve the effectiveness of therapy, safeguarding active compounds from degradation, and minimizing side effects. The implementation of the advanced formulations in clinical practice has been slow, mainly due to the difficulty in managing skin cancer therapeutically.

This evaluation investigated how dual-loaded liposomes and similar nanosystems, administered through various routes, can enhance the effectiveness of skin cancer treatment. The characterization of the developed formulations considered factors such as the average particle size, polydispersity index, and zeta potential of the co-loaded nanosystems, along with the encapsulation efficiency of the molecules and the drug release profile. Furthermore, the dual-loaded nanosystems were also evaluated through in vitro and in vivo studies. The use of nanosystems was suggested, featuring characteristics like biocompatibility, the ability to encapsulate both lipophilic and hydrophilic drugs, and enhanced retention and permeability effects. Additionally, liposomal formulations increased the efficacy and safety of drug delivery. The nanosystems enabled simultaneous delivery of drugs, potentially leading to better results by lessening side effects and enhancing synergy.

Therefore, the significant potential of co-delivery nanosystems was shown as a very promising approach to improve skin cancer treatment, emphasizing the synergistic impact.



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sciforum-106492: An innovative POF-based device for real-time monitoring of binding processes at ultra-low concentrations via a plasmonic sensor combined with a microcuvette chip

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Surface plasmonic sensors are widely utilized in bioanalytical and diagnostic laboratories to track interactions between analytes and receptors.¹ The primary advantage of plasmonic technology over traditional diagnostic methods is the possibility of label-free monitoring of binding events in real time. However, the expensive chip and the laborious surface chemistries required for functionalization are notable drawbacks.

In this study, a novel sensing approach is introduced to detect receptor-target interactions at extremely low concentrations without any kind of sensing surface functionalization. The biosensor operates using a sensitive chip based on a microcuvette device fabricated by drilling the core of a multimode polymer optical fibre (POF) with nanoholes. This is connected in series with a surface plasmon resonance (SPR) D-shaped POF probe, and the detection is performed using a broad-spectrum halogen lamp and a spectrometer. The microhole is filled with a solution containing specific receptors that selectively capture the target molecules from samples placed on top of the filled nanohole. Any changes over time due to analyte-receptor binding alter the mode profile of the light propagating through the POF core, affecting the plasmonic interactions and resulting in a time-dependent shift in the resonance wavelength.²

In particular, The interactions of estradiol and cortisol, with their respective receptors (Estrogen Receptor³ and Glucocorticoid Receptor⁴) were tested as proof of concept.² The resonance wavelength shift was monitored over time to trace the interactions between the receptor-target pairs at attomolar concentration.²

This advanced sensing approach acts as a new class of laboratory instruments offering distinctive capabilities in ultra-high sensitivity and affordability.

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sciforum-107656: Analysis of Performance of Flexible Polymer Nano-Sized Layered Humidity Sensor

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Creating inexpensive sensors that are easy to use is the goal of many authors and researches. Materials for implementation in similar types of devices as a sensitive medium are increasingly in demand. This medium in optical sensors needs to fulfill certain specifications: it needs to be compatible with various substrates, have an appropriate refractive index, be alterable in thickness, etc.

In the present study, the influence of deformations of a flexible substrate on an active amphiphilic PVA-Ac copolymer with a 24%-acetal-content sensing layer in a thin-film humidity sensor was studied. To improve the optical contrast, metallization of the PET substrate was used, which also aimed to increase the sensitivity. After a series of up to 1000 bends, certain characteristics of the sensor were studied: hysteresis, sensitivity, the change in the transmission coefficient, etc. The initial active layer was deposited using the spin-coating method, which is fast and easy and ensures the repeatability of the results. By using 3D profilometry, the quality of PVA-based active media thin films containing additional acetal groups was observed. It was demonstrated that the deformations had no negative effects on the sensor thin-film systems and, in fact, increased their sensitivity by more than 40%. We then present a discussion of the potential causes for this, including a decrease in the adhesion between the transparent metallized substrate and the sensing medium.



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sciforum-102616: Analyzing the Thermal Behavior and Phase Transitions of ZnSnO_3 Prepared via Chemical Precipitation

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This study investigates the synthesis and phase transition behavior of ZnSnO_3 nanoparticles prepared via chemical precipitation. To understand their properties, the nanoparticles were characterized using several techniques: thermogravimetric analysis (TGA), X-ray diffraction (XRD), UV-visible spectroscopy, and Fourier transform infrared spectroscopy (FTIR). TGA measured the weight changes of the nanoparticles as they were heated from 200°C to 600°C, revealing their thermal stability and decomposition patterns. Initially, at 200°C, the nanoparticles showed minimal weight loss, indicating they were stable. As the temperature increased to 300°C, a noticeable weight reduction occurred, likely due to the removal of residual organic materials and the onset of structural transformations. Between 400°C and 500°C, significant weight loss was observed, corresponding to major phase transitions and the release of volatile components. By 600°C, the nanoparticles exhibited enhanced thermal stability with only minor additional weight loss, suggesting the formation of a stable Zn_2SnO_4 phase. XRD analysis confirmed the evolution of the crystalline structure, showing a transition from cubic ZnSnO_3 to orthorhombic Zn_2SnO_4 as the temperature increased. UV-visible spectroscopy revealed changes in the bandgap energy associated with these phase transitions, which is important for understanding the material's optical and electronic properties. FTIR spectra confirmed the presence of specific functional groups, providing insights into the chemical bonds within the nanoparticles. These findings offer critical insights into the thermal behavior and phase transitions of ZnSnO_3 nanoparticles. Understanding these properties is essential for tailoring the material for various applications, including advanced materials, catalysis, and electronic devices. Moreover, the study provides valuable guidance for optimizing synthesis conditions to achieve the desired material properties, enhancing their performance in technological applications. By elucidating the phase transitions and thermal stability of ZnSnO_3 nanoparticles, this research contributes to the development of materials with specific and enhanced properties for diverse scientific and industrial uses.



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sciforum-103778: Anodic Response of Ferricyanide on a Mechanochemically Enhanced Graphite Electrode With Alumina for Enhanced Energy Storage

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Mechanochemical synthesis has emerged as a pivotal approach in sustainable chemistry. The synthesis method involves using mechanical energy to drive chemical reactions, often eliminating the need for solvents and reducing waste generation. This method enhances reaction efficiency and minimizes environmental impact by utilizing less hazardous materials and energy. The importance of mechanochemical synthesis is underscored by its contributions to SDG 12 (Responsible Consumption and Production) by promoting sustainable industrial processes and reducing the carbon footprint associated with traditional chemical manufacturing. This study investigates the anodic response of ferricyanide on a mechanochemically enhanced graphite electrode modified with aluminum oxide (Al_2O_3). The enhanced graphite electrode was characterized using Fourier Transform Infrared Spectroscopy (FTIR), Scanning Electron Microscopy (SEM), and X-ray Diffraction (XRD). FTIR analysis revealed the presence of functional active sites that facilitate electrochemical reactions. SEM images demonstrated a smoothened surface morphology of the graphite post- Al_2O_3 incorporation, indicating an increase in surface area conducive to enhanced electrochemical activity. XRD patterns confirmed the formation of new compounds resulting from the mechanochemical synthesis of graphite and Al_2O_3 , suggesting structural modifications that contribute to improved conductivity. Cyclic voltammetry experiments showed a significant enhancement in the anodic response of ferricyanide on the modified electrode, with increased peak currents observed at elevated scan rates. The study findings suggest that mechanochemical treatment not only alters the physical properties of graphite but also optimizes its electrochemical performance, positioning it as a promising candidate for future energy storage applications. Overall, the results underscore the potential of mechanochemical methods to enhance electrode materials for improved energy efficiency in electrochemical systems.



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sciforum-101922: Antioxidant properties and release of phenolic compounds from hydrogels as wound dressings

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Hydrogels are gaining attention in drug delivery systems due to their large surface area and absorption capacity, which enhance interaction with surrounding media. This study focuses on the release of tannic acid (TA) from alginate hydrogels and reduced graphene oxide (rGO) in a phosphate-buffered saline (PBS) solution at 37°C and pH 7.4, simulating physiological conditions similar to those found in wounds. The release profiles reveal two distinct patterns: hydrogels with 9% reduced graphene oxide (rGO) release TA rapidly, reaching equilibrium within 80 minutes. This quick release may result from poorly adhered TA transitioning into the medium, which aligns with previous findings on alginate/chitosan/tannic acid hydrogels. Conversely, hydrogels containing 4.5% rGO exhibited a controlled, sustained release throughout the experiment, with the highest TA release noted at 21.3% and 26.4% for Alg/rGO_{4.5}/TA₉ and Alg/rGO₉/TA₉, respectively. Furthermore, the antioxidant capacity of the hydrogels was evaluated using the DPPH method, which assesses their electron donation capability. The results indicated that only the TA functionalized hydrogels exhibited antioxidant properties, with notable improvement over time, particularly in the Alg/rGO₉/TA₉ material, which reached 15% antioxidant capacity. Comparatively, prior studies showed higher antioxidant capacities due to differences in experimental conditions. Overall, the findings emphasize the potential of these hydrogels as effective agents in reducing reactive oxygen species levels, thereby promoting wound healing.



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sciforum-099942: Application of computer modeling to the study of nimesulide inclusion complexes with β - and γ -cyclodextrin

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The encapsulation of low-soluble pharmaceutical agents in the β - and γ -cyclodextrin cavity (β -CD, γ -CD) successfully solves the current issues related to bioavailability and dose reduction of a variety of anti-inflammatory drugs. This study is focused on nimesulide (Nim), a nonsteroidal anti-inflammatory drug (NSAID).

The molecular complexation of nim/ β -CD and nim/ γ -CD was modelled via the Gaussian 09W computer program using the B3LYP method for DFT calculation. Molecular dynamics simulations of the complexes were performed via the NAMD2 software.

The set of conformations, characterized by lowest potential energy was obtained by Gaussian 09W for the nim/ β -CD and nim/ γ -CD molecular systems. The results of calculations indicated a low probability of complexation under the standard conditions. Nimesulide molecule exhibits a steric hindrance, leading to instability of the nim/ β -CD complex with minimal bond distances of 1.92Å. At the same time, nim/ γ -CD complex shares a higher stability due to the larger dimensions of the carrier molecule. Conformational analysis indicated a deep minima in the product area of the plot, demonstrating stability of the nim/ γ -CD system.

The stability of the nim/ β -CD complex was studied using molecular dynamics approaches. The simulation with length of 5 ns was performed via the NAMD2 computer program using the CHARMM36 forcefield. The further analysis including visualization and data plotting was completed by the VMD software (V1.9.4). The idea of hydrophobic-hydrophilic interactions between molecules was confirmed by the obtained data. In addition, lack of dissociation of nim/ β -CD complex was observed during the entire period of simulation. Stability of complex was also proved by RMSD trajectories analysis, as the corresponding curves were not drastically deviated.

Obtained data support the idea of complexation and relative stability of complexes. The approaches of computational chemistry in study of supramolecules provide deep insights into complexation and make it possible to evaluate affinity.



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sciforum-103805: Approach to the synthesis of new bis(6-hydroxypyrimidin-4(3H)-ones) with an aromatic bridging fragment

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Introduction. Among the 5-substituted-6-hydroxy-2,3-diarylpyrimidine-4(3H)-ones derivatives, there are compounds with reported anti-inflammatory activities and analgesic activity. It is known that the pharmacological activity can vary depending on how many pyrimidine rings there are in the molecule. Various reports in the patent and scientific literature have revealed that bis(pyrimidine) derivatives exhibit antitumor and antimicrobial activity. Therefore, the aim of our work was the synthesis of new derivatives of bis(6-hydroxypyrimidin-4(3H)-one) with aromatic linker – 2,2'-(1,4-phenylene)bis(6-hydroxy-5-methyl-3-phenylpyrimidin-4(3H)-one) (**1**) and 3,3'-(1,4-phenylene)bis(6-hydroxy-5-methyl-2-phenylpyrimidin-4(3H)-one) (**2**). Proof of structure and assessment of the biological activity were conducted through in silico analysis. **Methods.** Compounds **1** and **2** were obtained as a result of the interaction between methylmalonyldichloride and the corresponding carboximidamide in boiling benzene medium for 17 h. The structure of the obtained compounds was reliably proven by ¹H and ¹³C NMR spectroscopy data. Prediction of biological activity spectra was carried out using web resources: GUSAR, PASS Online, AntiHIV-Pred и CLC Pred. **Results and Conclusions.** 2,2'-(1,4-phenylene)bis(6-hydroxy-5-methyl-3-phenylpyrimidin-4(3H)-one) and 3,3'-(1,4-phenylene)bis(6-hydroxy-5-methyl-2-phenylpyrimidin-4(3H)-one) were obtained in 36 % и 42 % yields, accordingly. The structure of the obtained compounds was reliably proven by ¹H and ¹³C NMR spectroscopy data. The biological activity of the synthesized compounds was evaluated in silico, specifically, the acute toxicity and spectrum of pharmacological properties. According to the results of screening, compounds **1** and **2** potentially exhibit antitumor activity against cisplatin-resistant ovarian carcinoma and diffuse large B-cell lymphoma-activated B-cell type, antiviral activity against Dengue virus type 2 and SARS-CoV-2 with a high probability. Also, they can effectively inhibit reverse transcriptase (HIV-1). The predicted values of acute toxicity in rats (LD₅₀) with the intravenous route of administration for compounds **1** and **2** were 314 mg/kg and 309 mg/kg, accordingly, with the oral routes of administration at 1525 mg/kg and 1611 mg/kg, accordingly.



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sciforum-102899: Aqueous dispersions of nanodroplets containing essential oil components mixtures

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This work is aimed is to formulate, characterize and evaluate different aqueous formulations based on emulsions with a relatively simple composition. In particular, this study focuses on a pseudo-ternary system water-oil-stabilizing agent (Pluronic F-127), where the oily phase is constituted by a mixture of two components of essential oils, eugenol and thymol, in different proportions. The choice of this type of systems lies in the multiple beneficial properties of some essential oil components. However, their low solubility in water makes it necessary to look for strategies for their transport and controlled release, being emulsions ideal platforms to exploit the use of these bioactive compounds by encapsulation. For this purpose, in this work, the determination of compositions leading to stable formulations is explored. This implies studying formulations where both the total oil fraction and the composition of the oily phase are varied. In this way, it will be possible to find the compositional regions of stability and instability of the system, i.e., to obtain a compositional map or phase diagram. On the other hand, a characterization of stable formulations will be performed due to the impact of the characteristic of the formulations for their possible practical applications. This characterization included the study of the distribution of the oil or the droplet size of the emulsions, but also some specific details related to the potential applications of these systems.



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sciforum-103986: Biowaste-mediated green synthesis of well-defined silver nanoparticles and nanocomposites for biomedical and environmental applications: Waste-to-Wealth Approach.

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Introduction

Utilizing organic biowaste to produce nanoparticles has become of great interest in the field of nanotechnology. Nanomaterials produced through this green route are non-toxic, and the process is environmentally friendly. In this project, we synthesized stable and well-defined silver nanoparticles and nanocomposite films using organic biowaste such as banana peels, chikoo peels, and lemon peels. The synthesis methodology and their application as antibacterial and catalytic agents were investigated.

Method

The formation of silver nanoparticles was achieved using biowaste extracts as reducing and stabilizing agents. Sodium alginate–polyvinyl alcohol–silver nanocomposites were prepared by crosslinking using glutaraldehyde. All the materials were characterized by UV-Vis spectroscopy and electron microscopy. Their antibacterial properties were assessed against *Staphylococcus epidermidis*, *Staphylococcus aureus*, and *Escherichia coli*.

Results

The color change to black with the addition of NaOH indicated the formation of silver nanoparticles. The nanoparticles exhibited a strong plasmon resonance (SPR) peak at around 400 nm, confirming their presence. The peak was sharp and narrow, indicating low polydispersity. The nanocomposite films were effective against the bacteria tested, especially *Staphylococcus epidermidis*.

Conclusion:

The green synthesis of silver nanoparticles using biowaste yielded promising results, such as the creation of flexible films. The re-use and application of the nanocomposite films in the proliferation of fibroblast cells are currently in progress.



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sciforum-104372: Chromatographic behaviour of arylidene 2-thiohydantoin derivatives in an acetonitrile and F5 column

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Hydantoins are a class of five-membered heterocyclic compounds with a cyclic ureide structure, and thiohydantoins represent their sulphur analogues, where a sulphur atom replaces one or both carbonyl group oxygens. Anticancer, antimicrobial, anticonvulsant and anti-inflammatory are some of many biological activities that hydantoins possess and are the reason why this class of compounds has been and continues to be the topic of research in medicinal chemistry. Some hydantoins have found use as clinically approved commercially available drugs, while many others have found applications in various branches of industry. As determination of the chromatographic parameters is an important step in drug discovery, the aim of this study was to examine the retention behaviour of 13 arylidene 2-thiohydantoin derivatives using the HPLC technique. Also, the potential in terms of the hydrophobicity index φ_0 was examined to approximate the lipophilicity of the analysed compounds. The HPLC analysis was performed using an F5 column. The mobile phase was a binary mixture of the solvents acetonitrile and water (ACN-W). The retention behaviour of the compounds was observed using various proportions of acetonitrile (φ), starting with 20% and increasing it in increments of 5% to a final amount of 50% acetonitrile in the mobile phase. The retention coefficients $\log k$ were calculated using the retention times and death times collected from all of the chromatograms. Furthermore, $\log k$ was fitted to φ . The fittings were linear within an R^2 (coefficient of determination) range of 0.98265–0.99998. The hydrophobicity index φ_0 of all of the examined compounds was calculated by dividing the intercept ($\log k_0$) by the slope (S) of the obtained linearities. To approximate the lipophilicity, φ_0 has to show a correlation with the generally accepted lipophilicity coefficient $\log P$. The fitting of φ_0 and $\log P$ was linear, with an R^2 value of 0.8416. The obtained results indicate that the hydrophobicity index φ_0 has the potential to be used to approximate the lipophilicity of the examined arylidene 2-thiohydantoin derivatives.



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sciforum-106712: Comparison the separation of four selected immunosuppressants in different thin-layer chromatographic conditions

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Introduction Thin-layer chromatography (TLC) is a useful tool that enables the separation of the components of a mixture for qualitative and quantitative analysis. The aim of this study was to find the conditions for separation of four immunosuppressants, such as everolimus, zotarolimus, tacrolimus and temsirolimus.

Methods TLC was performed on 10 x10 cm plates precoated with silica gel 60F₂₅₄, silica gel 60 with kieselguhr 254 and silica gel RP-18F₂₅₄. Five microliters of ethanol solution (1 µg/µL) of each drug was applied to the plate using micropipettes. The chromatograms were developed by using mobile phases composed of toluene/acetonitrile/acetic acid (6:4:0.1 v/v/v; F1), chloroform/toluene/methanol/glacial acetic acid (4:4:2:0.1 v/v/v/v; F2), propan-2-ol/water (4:1 v/v; F3), acetonitrile/methanol/propan-2-ol (4:3:3 v/v/v; F4), ethanol/water (4:1 v/v; F5), acetonitrile/water (4:1 v/v; F6) and methanol/water/formic acid (36:14:0.1 v/v/v; F7). Chromatograms showing spots with a diameter of 5-7 mm were visualized at 254 nm.

Results TLC analyses showed the influence of the applied mobile and stationary phases on the values of the retardation factor (R_f) and separation parameters of the pairs of examined compounds. The highest R_f values (close to 0.99) for studied compounds, not allowed for their separation were obtained with phase F7 and RP18F₂₅₄ plates. The optimization of separation conditions indicates that the best separation was achieved with the mobile phase F4 and RP18F₂₅₄ plates. Under these conditions, the highest separation factors for the three studied pairs, namely ΔR_f : 0.06-0.25; R_S : 1.08-1.36, α : 1.37-8.14 and R_f^{α} : 1.08-3.00, were obtained.

Conclusions The optimized TLC conditions consisting of mobile phase F4 and RP18F₂₅₄ plates may be applicable to the quality control of drugs under study. The developed method is fast and economic. It allows for the analysis of four tested compounds simultaneously.



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sciforum-106152: Composites Based on In_2O_3 and Nafion for Possible Applications in Electrochemical Devices

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The embedding of metal oxide nanoparticles into polymeric matrices creates composite materials with interesting physicochemical properties and potential applications in various fields, such as environmental and food monitoring, optical devices, and biosensors.

In the present paper, In_2O_3 -based composites were prepared by an ex situ method, where In_2O_3 nanostructures were dispersed into a nafion matrix through an ultrasound mixing process under rigorous control of the process parameters (time, temperature, ultrasound intensity, frequency, etc). The morphological and structural behaviors of the composites were evaluated using Fourier transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM), and X-ray diffraction (XRD), and the surface-wetting capacity was determined by contact angle (CA) measurements. Morphological analysis showed that the In_2O_3 nanoparticles were uniformly distributed in the nafion matrix, with a slight tendency to agglomerate. The structural investigation revealed a slight shift in the characteristic In_2O_3 peaks, indicating a good interaction between the main phase characteristics of the composite. Nafion exhibits high hydrophobicity properties, and by adding In_2O_3 to the matrix, a decrease in the contact angle at approximately 91° was observed while maintaining hydrophobicity. The electrochemical performance of the composites was evaluated by cyclic voltammetry. This study provides new insights into composite materials and highlights their performance in the development of biosensors, focusing on the properties of composite films.

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sciforum-104189: Computational Analysis of Diverse Hole Transport Materials for Enhanced Efficiency in Perovskite Solar Cells

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Hole transport materials stabilize and boost perovskite solar cell efficiency. In depth, understanding of the structure-property relationship will help in the rational design of efficient HTM for PSCs. In the present work, we have theoretically designed five efficient hole transport molecules based on triphenylamine as acceptor units. Their architecture is based on donor-acceptor-donor style using various core molecules e.g. thiophene, benzotrithiophene (BTT), benzo-2,1,3-thiadiazole (BT). Various p-linkers such as 3,4-ethylenedioxythiophene (EDOT), benzothiadiazole and thiophene are used for connecting both ends. Optical properties, electronic properties, hole transport behaviour, and photovoltaic properties are computed for the designed molecules based on DFT and TD-DFT methods on the basis of B3LYP hybrid functional. The geometries, ESP distribution, dipole moment, reorganization energies, UV-spectrum, and frontier molecular orbitals (FMOs) were discussed to study the electronic properties of the designed molecules. And the hole electron distribution, absorption spectra, Light harvesting Efficiency (LHE), alignment of the density of states along with transition density matrix, binding, and excitation energy were discussed to study the optical properties. This investigation provides an understanding of how the structure and properties of these molecules are related and how they can be modified to obtain desirable properties. This work will help design novel, efficient HTM molecules in the future by computational modelling and later leading to the fabrication of PSC devices with these types of HTMs.



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sciforum-106929: Computational Drug Likeness Studies of Selected Thiosemicarbazones: A Sustainable Approach to Drug Design

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The intake of drugs, their absorption in the body, their removal, and various side effects are factors that should be considered in drug design. Here, *in silico* tools act as virtual shortcuts assisting in the prediction of several important physicochemical properties like molecular weight, polar surface area (PSA), molecular flexibility, etc., to evaluate probable drug leads as potential drug candidates. Moreover, these tools also play an important role in the prediction of the bioactivity score of a probable drug lead against various human receptors. This paper presents a virtual combinatorial library of selected thiosemicarbazone ligands and their metal complexes. Different properties, like physicochemical properties, bioactivity score, and absorption, distribution, metabolism, excretion, and toxicity (ADMET) parameters were assessed. The structures of ligands and complexes were drawn and downloaded in PDB format using ChemDraw Ultra 12.0. Physicochemical parameters were calculated using online software, viz., Molinspiration and SwissADME, and ADMET properties were calculated using admetSAR (2.0). Molecular docking was performed using PyRx Python Prescription 0.8. with two proteins, namely Transforming Growth Factor Beta (Tgf- β) and Janus Kinase. Transforming Growth Factor Beta (Tgf- β) and Janus Kinase are some of the cytokines involved in cell development, proliferation, and death. Salicylaldehyde thiosemicarbazone, acenaphthenequinone thiosemicarbazone, and 2-chloronicotinic thiosemicarbazone and their virtually designed complexes exhibited appreciable *in silico* results. Most of the ligands and complexes had good bioactivity values against all the biological targets.



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sciforum-103947: Copper (II) Adsorption On Activated Carbon From Moringa Waste Using Artificial Neural Network Modelling In A Continuous System

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Novel materials or techniques for treating wastewater are needed since the presence of developing pollutants in it presents a worldwide environmental issue. This investigation concentrated on turning moringa waste into activated carbon and using it to copper (II) adsorption. Analysis using thermogravimetric revealed the activated carbon's thermal degradation characteristics. BET analysis showed that it had mesoporous properties with increased surface area and pore volumes. The impacts of operating factors including pH, bed depth, concentration, and flow rate were examined using the column approach. The results of the experiment demonstrated that the adsorption capacity rose with input concentration and bed depth and declined with increasing flow rate. The ideal values were discovered to be 40 mg/L for concentration, 5 cm for bed height, and 6 for pH. 30% of the data were used for validation and testing when the ANN technique was developed, with the remaining 70% being used for training. The training dataset's R^2 , MSE, ARE, and RMSE were 0.996, 0.011, 0.048, and 0.021. The curves were analyzed using ANN, and the results revealed that the best ANN architecture for representing the experimental data is consisting of [3 8 1] with the BR algorithm. These findings demonstrate the material's potential to serve as a viable adsorption material for the focused elimination of contaminants, increasing both the application of machine learning in sorption studies as well as the remediation of novel pollutants.



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sciforum-107819: Coupling biological detection to liquid chromatography is an effective tool in Organic Chemistry and Pharmacology.

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Introduction.

Liquid chromatography (LC) is widely used technique for separation, isolating and purification of chemical compounds present in mixtures. The direct coupling biological detection to liquid chromatography may to facilities the chemical and biological characterization of active compounds.

Methods.

In previous years, it was optimized a system that combined the advantages of LC separation with classical systems for analyzing pharmacological activity in isolated perfused or perfused organs.¹ Thus, It was studied a hydro-ethanolic extract of *Stevia rebaudiana* Bertoni (Asteraceae) through a method based on medium pressure liquid chromatography separation (MPLC) coupled directly to living superfused organ cascade as a quadruple biosensor.¹

In this poster communication, potential uses and perspectives in Organic chemistry and Pharmacology of this directly coupling biological detection to MPLC system are present.

Results.

Rebaudioside N, a minor natural product produced from *Stevia rebaudiana* Bertoni, was identified as the compound responsible for the contractile activity detected in an active fraction of the hydro-ethanolic initial extract.¹ The isolated rebaudioside N contracted the smooth muscle present in portions of the rat ileum. This stevioside was structurally identified by mass spectrometry.¹

In the pharmacological characterization process of new active compounds, this type of methodology reduced the investigation time, number of animals slaughtered, use of organic solvents, and associated expenses.¹

Conclusions.

This direct combination of liquid chromatography with perfusion system will allow isolating and pre-characterization bioactive compounds present in mixtures derived from extracts of natural origin or chemical synthesis (for example, combinatorial chemistry).

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sciforum-103953: Cu – Electrodeposited Catalysts for the Sustainable Electrochemical Reaction of Nitrate to Ammonia

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The electrochemical nitrogen reduction to ammonia (NRR) is a green and alternative to the Haber-Bosch process. The reaction is carried out at room temperature and pressure, but has low efficiency due to the difficulties associated with breaking the nitrogen triple bond. It is possible to replace the traditional reaction with a nitrate reduction reaction (NO₃RR). In addition, the electrochemical nitrate reduction (NO₃⁻) to ammonia (NH₃) is an urgent and important task from the point of view of economics and environmental protection. The unique electronic structure and large reserves of transition metals have made transition metal-based catalysts widely studied in the field of electrochemical conversion of NO₃⁻ to NH₃. Copper-based catalysts have a special electronic structure and exhibit the highest activity and selectivity among single-component metal catalysts for the NO₃RR electrochemical reaction. The unique electronic configuration of copper on the surface promotes adsorption and electron transfer of nitrate ions, which can effectively inhibit HER (hydrogen evolution reaction) and promote the processes of initial conversion of NO₃⁻ to NH₃. In this study, the catalytic efficiency of copper electrodeposited catalysts in the NO₃RR reaction was studied. The conversion of NO₃⁻ to NH₃ involves a complex transfer of eight electrons and many intermediates. The reaction was carried out at a controlled potential, which was previously established using the method of linear voltammetry. The catalysts were represented by copper and graphite substrates with electrodeposited copper particles on the surface. It is shown that the catalysts have a certain catalytic activity. Calculations of Faradaic efficiency showed values to 29%. All electrocatalysts have been characterized by SEM, EDX and other modern methods. The study is a composite, but at the same time complete, part of the work focused on the synthesis of new catalysts for NO₃RR and NRR.



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sciforum-104143: Development of an Affordable Graphite-Based Conductive Ink for Printed Electronics

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Printed electronics (PE) are rapidly growing, especially in wearable sensors, smart textiles, and IoT devices. Conductive inks, essential for the fabrication of PE, must be highly conductive, cost-effective, biocompatible, easy to prepare, and less viscous. Conductive inks comprise of a conducting material (metals like silver, gold, copper, or carbon-based alternatives like graphite, graphene, and carbon nanotubes), a binder, and a solvent. In this work, a water-based graphite conductive ink is developed using graphite as a conductive material, corn starch powder (non-toxic and biodegradable) as a binder, and distilled water as a solvent. Firstly, corn starch powder is added to distilled water which is heated up to 100 °C and stirred continuously until a homogeneous gel-like mixture is formed. After cooling the mixture, graphite powder is added to it, and stirred for an hour at 450 rpm to obtain the ink. To check the conductivity, the ink is brush-painted on a paper substrate with a dimension of 20 mm x 10 mm and the result shows a low ohmic resistance of ~ 560 Ω , confirming the highly conductive nature of the ink. Additionally, thermogravimetric analysis (TGA) is performed on the prepared ink to evaluate its thermal stability, and a very strong X-ray diffraction (XRD) peak obtained at $2\theta = 26.5426^\circ$, a small peak at $2\theta = 54.6145^\circ$, along with a few other small peaks, confirms the presence of graphite with corn starch. Thus, this conductive ink can be used for PE owing to its affordability, biocompatibility, and ease of preparation.



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sciforum-105281: Development of Anticancer Silver-Incorporated PVDF Nanofibrous Scaffold

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In this study, we present the fabrication of electrospun scaffolds consisting of polyvinylidene fluoride (PVDF) incorporated with silver nanoparticles (AgNPs) and investigate their potential anticancer properties. Using the electrospinning technique utilizing in-house built electrospinning device, we successfully produced nanofibrous scaffolds incorporating AgNPs through a simple and cost-effective method. Dissolution of 21% of PVDF was achieved in a combination of organic solvents acetone and dimethylformamide (Ac:DMF, volume ratio 1:3).

Anticancer efficacy was evaluated through in vitro cytotoxicity assay using MDA-MB-231 breast carcinoma and healthy MRC-5 fibroblast cell lines, yielding promising results that highlight the potential of silver-incorporated PVDF scaffolds for anticancer applications in tissue engineering. Different concentrations of silver nitrate (AgNO₃) (0.1%, 0.3%, and 0.5%) were incorporated into the PVDF nanofibrous scaffolds and evaluated by the MTT assay. Notably, the most significant anticancer effect on MDA-MB-231 cancer cells was observed at a concentration of 0.1%, without causing cytotoxic effects on MRC-5 cells, while 0.5% exhibited cytotoxic effects on both cell lines.

The data suggest that even slightly higher concentrations of AgNPs can affect the viability of both cell lines. Thus, careful selection of silver nitrate concentration promises to achieve prominent results in in vitro and in vivo biological activities. Future research will focus on further exploring these findings.



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sciforum-103983: Development of Flexible and Biocompatible Gelatin-Chitosan-based Hydrogels containing various types of Honey for Wound Dressing Application

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Introduction

An optimal wound dressing should facilitate gaseous exchange, absorb excess exudate, establish a moist wound-healing environment, and be easily removed without causing damage to the wound. It should also be nontoxic, biocompatible, and antimicrobial. The leading causes of these performances are the material's functional properties and the microenvironment that was established. It seems that no single substance can fulfill all the demands for every phase of the healing process of wounds. In this project we have developed hydrogels based on gelatin and chitosan containing honey for wound healing applications, as honey is known to have antibacterial properties. Preliminarily we have studied the effect of various types of honey containing hydrogels as antibacterial materials. The preliminary results are presented in this study.

Method

Hydrogel films based on gelatin and chitosan containing various types of honey were prepared by solvent casting method. The antibacterial properties of the material were tested using the incubation method. The surface morphology was studied by electron microscopy and swelling in water was measured gravimetrically.

Results

The hydrogel in water exhibited excellent swelling with high equilibrium water content and excellent mechanical properties. In the presence of bacteria, the hydrogels degraded slowly due to disintegration of collagen matrix by the bacteria. Interestingly, the hydrogels containing Manuka honey exhibited good antibacterial properties.

Conclusion and work-in-progress

Based on the formulation containing manuka honey, cell-growth on the hydrogel is currently in progress.



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sciforum-104134: Development of Multilayer MoS₂ for photocatalytic applications

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Molybdenum disulfide (MoS₂) has been regarded as a promising material for solving the current fossil fuel shortage and environmental problems due to its remarkable semiconducting and photocatalytic properties. However, monolayer MoS₂ has attracted most of the scientific interest, leaving its multilayer counterpart neglected. Multilayer or bulk MoS₂ has its own advantages, e.g., low cost and restricted recombination of photoexcited electrons and holes due to its indirect band. The major barrier for its application is the large proportions of inert basal planes. Given this, activating the inert sites of multilayer MoS₂ would develop a practical candidate for the photocatalyst family. Efforts have been devoted to introducing S vacancies through various sophisticated techniques; however, most of these are not applicable in real-life applications.

In our recent work, we proposed a nanofabrication strategy to join transition metal nanoparticles to MoS₂ via silver buffer layers [1,2]. Typically, nickel nanoparticles up to 200 nm could be chemically attached to both the edges and basal planes of multilayer MoS₂ through this method, leading to activated MoS₂ with greatly enhanced photocatalytic hydrogen evolution efficiency. Further investigation has also revealed its feasibility for photodegradation of organic pollutants in natural water. Therefore, hydrogen production and water purification could be achieved simultaneously. Based on high-resolution XPS analysis, we believe that the successful nickel doping and high photocatalytic performance can be attributed to the effective bonding between Ni and MoS₂, which serves as an expressway for electrons crossing between the semiconducting side and the active metallic sites.

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sciforum-104400: Dielectric and Catalytic Behavior of V₂O₅-Rich Glass-Ceramics Synthesized by Controlled Heat-Treatment-Induced Crystallization

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The need for innovative, sustainable materials for electrochemical devices and catalysts highlights V₂O₅-based materials as particularly promising. They can serve as cathodes for Li-ion, Na-ion, and all-solid-state batteries due to their high safety, energy density, and long life cycles. Additionally, they function as catalysts in oxidation reactions, especially fatty acid decarboxylation, which is crucial for biodiesel production—a renewable, lower-toxicity alternative to petroleum diesel that reduces greenhouse gas emissions and addresses environmental challenges. V₂O₅-rich glasses and glass-ceramics (GCs) stand out due to their dense, uniform microstructures and exceptional mechanical, thermal, electrical, dielectric, and catalytic properties. Furthermore, GCs are particularly interesting because they offer unique control over composition, crystallographic structure, and microstructure, including the type and quantity of crystalline phases within the residual glassy phase, all of which can be finely adjusted through heat-treatment conditions such as temperature and duration. In light of these factors, this study examines how controlled crystallization of V₂O₅-rich parent glass affects the structural, dielectric, and catalytic properties. The composition of prepared samples is analyzed using powder X-ray diffraction (PXRD), while their (micro)structural properties are characterized by scanning electron microscopy and energy-dispersive X-ray spectroscopy (SEM-EDS) and infrared attenuated total reflectance spectroscopy (IR-ATR). Dielectric properties are investigated via solid-state impedance spectroscopy (SS-IS) across a broad frequency range (0.01 Hz to 1 MHz) and temperature range (−90 °C to 210 °C). Additionally, catalytic activity in fatty acid decarboxylation is evaluated using thermogravimetric analysis and differential scanning calorimetry (TG/DSC). The results demonstrate significant improvements in both dielectric and catalytic performance, highlighting the versatile potential of V₂O₅-rich glass-ceramics for advanced electronic applications and sustainable biodiesel production.

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sciforum-101410: Dielectrophoretic Deposition of Single-Walled Carbon Nanotubes on Silicon/Silicon Dioxide Substrates Using Interdigitated Gold Electrodes

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Finite Element Method (FEM) simulations offer a powerful tool for investigating the process of dielectrophoresis (DEP) to deposit single-walled carbon nanotubes (SWCNTs) on a silicon/silicon dioxide substrate using interdigitated gold electrodes. This study focuses on the precise control and manipulation of SWCNTs by applying the non-uniform electric fields generated by these electrodes. Using FEM, we simulate the electric field distribution and the resulting dielectrophoretic forces that influence SWCNT alignment and deposition. The simulations provide detailed insights into the DEP process's parameters, including electrode geometry, voltage magnitude, frequency of the applied AC field, and the properties of the SWCNTs and substrate. Our results demonstrate the effective deposition of SWCNTs, forming well-defined patterns on the silicon/silicon dioxide substrate. The SWCNTs exhibit unique electrical, mechanical, and thermal properties that make them highly desirable for a wide range of applications. This technique offers significant advantages in terms of precision, reproducibility, and scalability for fabricating nanoscale devices. This research contributes to advancements in nanotechnology applications such as sensors, transistors, and other electronic components by providing a detailed understanding of the DEP mechanism for SWCNTs. The potential for integrating SWCNTs into various electronic and optoelectronic devices is significantly enhanced by these findings, paving the way for future innovations in the field.



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sciforum-107507: Dynamic Vulcanization of Coir Fibre Composites: A Path to Sustainable and High-Performance Materials

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This work investigates the dynamic mechanical properties of low-density polyethylene (LDPE) and natural rubber (NR) composites reinforced with coir fibre, stressing the impact of dynamic vulcanisation on stiffness, energy dissipation, and damping behaviour. Prioritising sustainability, the composites were fabricated using a two-roll mill and compression moulding, incorporating 10% and 40% fibre loadings. Dynamic Mechanical Analysis (DMA) was used to determine the storage modulus (E'), loss modulus (E''), and damping factor ($\tan \delta$) over a temperature ranging from 30°C to 120°C and a constant frequency of 10Hz. The findings revealed that dynamic vulcanisation considerably enhanced storage modulus across all temperatures, with a 25% increase in stiffness at lower temperatures. However, as the temperature increased, the modulus decreased due to polymer chain relaxation. Coir fibre composites also had higher loss modulus values, indicating more energy dissipation, but the damping factor increased with fibre content, showing weaker fibre-matrix interactions at higher loadings. While coir fibre composites demonstrated promising mechanical and thermal properties, they were exceeded by jute, hemp, and flax fibre-reinforced composites in terms of stiffness and energy retention. These findings emphasise the potential for dynamically vulcanised coir fibre composites to be employed in applications that require improved mechanical properties and thermal stability, establishing them as a sustainable option in specific engineering contexts.



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sciforum-102494: Effect of Fiber Reinforcement on the Mechanical and Flow Properties of Self-Compacting Concrete

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Fiber Reinforced Self-Compacting Concrete (FRSCC) is an advanced form of Self-Compacting Concrete (SCC) that eliminates the need for vibration or mechanical compaction; it integrates the benefits of Fiber- Reinforced Concrete (FRC). The fibers within the mix help distribute loads more evenly, reducing stress concentrations and preventing crack propagation. This makes FRSCC particularly effective in applications where high performance and durability are crucial. High workability, segregation resistance, and concrete homogeneity are some of the essential properties of SCC. However, ensuring proper flowability while maintaining high strength poses a significant challenge. Therefore, a variety of admixtures, like supplementary cementitious materials, natural or synthetic fiber reinforcement, air entraining and viscosity-modifying agents, etc., can be incorporated to control and elevate the strength response of the concrete mix. This study primarily investigates the difference in strength and flow properties of FRSCC for multiple PCC variants with different dosage of nylon fiber to a maximum of 0.5% by volume. The flow properties of the concrete mix were assessed using V-Funnel, L-Box, T500, and slump tests. Subsequently, the hardened properties, such as compressive strength, split tensile strength, and flexural strength, were analyzed to evaluate the performance of FRSCC. The findings from this study indicate that using nylon fiber up to 0.25% by volume can increase the compressive strength capacity by 18%, the tensile strength by 45%, and the flexural strength by 29%. Additionally, failure in the FRSCC did not occur immediately in the three-point bending test compared to the SCC beam with no fiber. The FRSCC specimen could carry some additional load even after reaching its ultimate strength and developing flexural cracks.



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sciforum-107481: Effect of sonication-assisted water extraction on the total antioxidant parameters of medicinal plants

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Medicinal plants are one of the sources of biologically active compounds that determine their therapeutic effect. Water infusions and decoctions, as well as tinctures and extracts, are currently used in phytotherapy. Sonication treatment is an effective approach to increasing the efficiency of active component extraction from plant material. Application of sonication reduces the time and consumption of extractant, as well as uses mild conditions. Sonication-assisted water extraction was applied to the various medicinal plants traditionally used in phytotherapy. Water extracts from herbs, leaves, bark, infructescences, flowers, roots, and rhizomes were studied using total antioxidant parameters obtained by constant-current coulometry. Eleven samples of commercially available medicinal plants were investigated (bark of *Quercus robur* and *Frangula alnus*, infructescences of *Alnus incana*, rhizomes of *Potentilla erecta* and *Bergenia crassifolia*, roots and rhizomes of *Sanguisorba officinalis*, herb of *Leonurus*, flowers of *Tilia x europaea* and *Matricaria chamomilla*, leaves of *Salvia officinalis* and *Urtica dioica*). Total antioxidant capacity (TAC) and ferric reducing power (FRP) based on the reactions with electrogenerated bromine and ferrocyanide ions, respectively, were evaluated. The effect of sonication time in the range of 10–30 min was tested. The highest yield of antioxidants was achieved using a 30 min treatment. The TAC and FRP values were varied depending on the part and type of medicinal plant. The highest TAC and FRP were obtained for the extracts obtained from roots and rhizomes. The FRP values indicate the impact of phenolic compounds, which is significant for the samples under study. Total antioxidant parameters of infusions, decoctions, and sonication-assisted extracts were compared.



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sciforum-103106: Effect of Zirconium Doping on the Optical and Ferroelectric Properties of Bismuth Ferrite for Enhanced Photovoltaic Performance

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Bismuth ferrite (BiFeO₃, BFO) is highly regarded for its high-temperature ferroelectric and magnetic properties, making it ideal for advanced applications such as ferroelectric photovoltaic devices. This study aims to enhance BFO's performance by doping it with zirconium (Zr) cations. Thin films of both undoped and Zr-doped BFO were prepared using the sol-gel method and spin-coated onto fluorine-doped tin oxide (FTO) substrates. X-ray diffraction (XRD) confirmed the films retained a rhombohedral crystal structure, while UV-Visible (UV-Vis) spectroscopy indicated high transparency and a direct band gap. Notably, the band gap narrowed with Zr doping, improving the material's suitability for visible light applications. Ferroelectric measurements revealed that Zr doping led to increased saturation polarization, coercive field, and remnant polarization in the films. Photoconductivity tests further demonstrated that Zr-doped films exhibited reduced leakage current densities, attributed to the co-doping effect, enhancing the films efficiency for photovoltaic applications. These findings highlight the significant improvements in optical and ferroelectric properties of Zr-doped BFO films, making them crucial for the advancement of photovoltaic technology. By combining improved optical transparency and enhanced ferroelectric characteristics, Zr-doped BFO films represent a promising avenue for developing high-performance ferroelectric photovoltaic devices. This research underscores the potential of Zr-doped BFO in contributing to next-generation photovoltaic technologies, paving the way for more efficient energy harvesting and utilization. The integration of Zr-doped BFO films in photovoltaic systems could lead to substantial advancements in energy efficiency and the development of innovative energy solutions.



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sciforum-106892: Effectiveness of wood coating and preservative treatment on *Melia dubia* surface characteristics

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Wood is the most vital renewable building material, which has been widely used in outdoor and indoor areas because of its abundance and versatility. Due to its organic nature, wood is susceptible to attack by various biotic and abiotic factors. Therefore, in order to protect the wood against these factors, wood coating and preservative treatment become obligatory. The application of coatings is a common solution against wood-degrading factors. The wood coating performance depends on several factors, such as humidity, moisture content, the species of wood, and temperature. Furthermore, to improve wood coating performances, different strategies such as the addition of UV absorbers and radical scavengers are widely used. The wood treatment encompasses the impregnation of wood preservatives such as creosote, pentachlorophenol, CCA (chromated copper arsenate), alkaline copper quaternary (ACQ), and copper azole (CA), as they can inhibit degradation and increase durability against fungi and insects. In the present study, we investigated the combined effect of preservatives and coatings on surface characteristics of *Melia dubia*. The wooden specimens were impregnated with 4% ZiBOC and 4% BBA concentrations and were finished with wax polish, spirit shellac, and polyurethane. Furthermore, the gloss and thickness values were determined. The findings showed that among all three finishes, polyurethane shows preeminent results, followed by spirit polish and wax polish. In addition, the behaviour of ZiBOC preservative along with the finishes produces extraordinary results.



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sciforum-103995: Effects of TiO₂ and ZnO nanoparticles on intestinal cells: An *in vitro* approach

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The rapid development of nanotechnology has significantly transformed various industrial processes associated with food production (e.g., through the introduction of smart and active packaging, nanosensors, nanopesticides, and nanofertilizers). This study focuses on two nanoparticles widely used in the food industry: titanium dioxide (TiO₂-NPs) and zinc oxide (ZnO-NPs), and their effects on human cells. Thus, the cytotoxicity of TiO₂-NPs (commercially acquired; spherical shape with average size of 298.4 nm and PDI of 0.248) and ZnO-NPs (synthesized in the laboratory; spherical like shape with an average size of 339.9 nm and PDI of 0.590) to a human colon cancer cell line (HCT116) was studied, assessing cellular metabolic activity, as an indicator of cell viability, through the MTT assay. Overall, exposure to ZnO-NPs induced a dose-dependent reduction of cell viability, with half maximal inhibitory concentration (IC₅₀) values of 10.4 mg/L, 8.8 mg/L, and 7.7 mg/L at 24, 48, and 72h, respectively. In contrast, TiO₂-NPs did not induce significant differences in cell viability across the same time points. These findings highlight the differential cytotoxic effects of ZnO-NPs and TiO₂-NPs on colon cancer cells, suggesting a need for careful consideration of ZnO-NPs in food applications, due to their potential health risks. Overall, this study provides crucial insights into the biological interactions of these nanoparticles, highlighting the importance of thorough safety evaluations in their use within the food industry.



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sciforum-106175: Elastic anisotropies and electronic properties of cubic spinel CuGa_2O_4 : A DFT calculation

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The aim of this work is to study the structural and elastic properties of the spinel CuGa_2O_4 . The quantum DFT approximation used in this study was applied to Copper Gallium Oxide with a space group $\text{Fd}\bar{3}\text{m}$ (227) and crystallized in a cubic structure, with unit-cell parameters: $a = 8.4996$, $c = 5.8172$ Å. Structural characteristics of a material can be investigated without making physical measurements by optimizing the first-principles computation. This is achieved by utilizing the CASTEP code based on the pseudo-potential plane-wave within the Material Studio software. Known as Copper Gallium Oxide, this compound falls under the category of spinel oxides. It is a type of mixed metal oxide where copper (Cu^{2+}) and gallium (Ga^{3+}) ions are combined with oxygen (O^{2-}) ions.

Spinel-structured CuGa_2O_4 mixed oxide, with a narrow band-gap of 1.5 eV, exhibits intriguing properties. These characteristics have motivated investigations into its potential applications, notably its magnetic, dielectric, and optical traits, as well as its promise in the field of photocatalytic pollutant degradation. In this study, CuGa_2O_4 's geometrical optimization was performed using a semi-local generalized gradient approximation (GGA) with the Perdew-Burke-Ernzerhof (PBE) for exchange-correlation functional. After optimization, records of bandgap and DOS were analyzed to understand its electronic properties. The electronic properties of CuGa_2O_4 were determined by examining the electronic band structure and density of states, which are indicative of CuGa_2O_4 being a narrow-gap semiconductor with a direct band gap. Additionally, we determined the elastic constants, bulk, shear, and Young's moduli, Pugh ratio, Poisson's ratio, and universal anisotropy. All studied compositions of this compound show structural stability



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sciforum-107355: Electronic structures and properties of copper, germanium, or tin-based MA/Pb-free perovskite halides

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Perovskite halides with a typical composition of $\text{CH}_3\text{NH}_3\text{PbI}_3$ provide high photoconversion efficiencies and lightweight/flexible solar cells. Since the main element lead (Pb) is toxic, perovskites without Pb (Pb-free) should be developed from the viewpoint of natural environments and human health. In addition, methyl ammonium (CH_3NH_3 , MA) is an unstable molecule in the crystal, and MA-free perovskites are also mandatory to improve their structural stabilities. The aim of the present study is to clarify the electronic structures and properties of copper (Cu), germanium (Ge), or tin (Sn)-based MA/Pb-free perovskite halides using first principles calculations. Monovalent copper (Cu^+), rubidium (Rb), and cesium (Cs) were introduced at the MA sites, and various transition elements and typical elements such as Ni, Cr, Fe, Zn, and others were also induced at the Pb site. Pb-free double perovskite bromides were also found to be the suitable photovoltaic materials, which would be due to high electron density of Ge compared with Sn. The double perovskites have wide energy gaps and stabilities compared with the ordinary perovskites, and the hybridization of Ge/Sn would influence the electronic structures. Total energies of Cs-based perovskites were reduced by the Cu^+ addition. The band gap energies of Cu-based Pb-free chlorides with transition metals provided suitable values for solar cells. Carrier mobilities and crystal structures of the perovskites could be stabilized by the overlapping of electron orbitals between the chloride octahedron and Cu^+ . The Cu^+ at the MA-site would be effective to control the structures and stabilities of the all-inorganic perovskites, which would expand the multiplicity of the perovskites; as a result, the α -formamidinium cesium lead triiodide was stably formed by the addition of Cu^+ .



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sciforum-107782: Electrospinning poly(acrylonitrile) (PAN) nanofiber mats with mushroom mycelium powder

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Electrospinning is a relatively simple technique to produce nanofiber mats, which can be used for diverse applications, from biomedicine to filtration to energy applications. For these cases, the large surface-to-volume ratio of nanofibrous membranes is often advantageous as compared to macroscopic textile fabrics or other structures. Additionally, the spinning process enables the integration of metallic or ceramic nanoparticles, blending different polymers or even preparing non-polymeric nanofibers by the calcination of the polymer used as a spinning agent. Especially for biomedical applications, the addition of an antibacterial agent can be supportive. Here, we report needleless electrospinning of nanofiber mats from poly(acrylonitrile) (PAN) with different mushroom mycelium powders, which have antibacterial and other positive properties. While PAN with *Pleurotus ostreatus* (oyster mushroom) powder could well be electrospun with the wire-based technique, PAN with *Ganoderma lucidum* (reishi mushroom) powder was nearly impossible to spin, with only one of four tests showing thin membranes containing fibrous as well as non-fibrous areas. The PAN/*P. ostreatus* nanofiber mats were further stabilized and carbonized. All samples were examined by confocal laser scanning microscopy (CLSM), scanning electron microscopy (SEM), and Raman microscopy, revealing similar morphology and carbon yield to pure PAN. This indicates the possibility to embed *P. ostreatus* powder in PAN nanofiber mats used for biotechnological or biomedical applications.



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sciforum-107343: Elemental Composition and Characterization of A Mineral Sample via Sem-Eds Analysis

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Good plant growth and high productivity largely depend on mineral fertilizers. Therefore, identifying new raw materials for the production of these fertilizers is crucial. The analysis of newly discovered minerals is essential to uncover their potential uses. In this study, Energy-Dispersive X-ray Spectroscopy (EDS) combined with Scanning Electron Microscopy (SEM) was used to examine the elemental composition and surface morphology of a mineral sample. The sample was taken from the "Doutosh" mine, located on the southern border of Uzbekistan, at a depth of 30-35 meters. The topsoil layer was removed using specialized methods, allowing access to the ore for further analysis. The SEM-EDS analysis revealed that the main constituents of the mineral were oxygen (32.95%), manganese (27.77%), and chromium (9.97%), along with smaller amounts of carbon, silicon, calcium, iron, and other trace elements. The multi-elemental composition of the mineral was confirmed, with manganese and chromium being the primary contributors. These findings suggest that the mineral holds potential for industrial applications, particularly in the fields of materials science and metallurgy. Moreover, by studying the functional characteristics of the mineral and assessing its environmental impact, plans are being made to develop manganese-based fertilizers for plant growth using this mineral resource. This could serve as a new branch of the chemical industry in Uzbekistan.



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sciforum-102846: Engineering thermal responsive hydrogel as a drug carrier of Metronidazole

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Introduction: The development of controlled drug delivery systems is critical in enhancing the therapeutic efficacy and reducing the side effects of medications. Thermally responsive hydrogels are particularly advantageous due to their ability to modulate drug release in response to temperature changes, providing a targeted and efficient delivery mechanism.

Methods: In this study, the Xanthan gum hydrogel was fabricated using a cost-effective and straightforward approach involving a solution mixing method followed by a freeze-thawing crosslinking process. For drug loading, the hydrogel was immersed in a Metronidazole solution, allowing the drug to be absorbed into the hydrogel matrix.

Results and discussion: The prepared hydrogels were subjected to a series of analyses to characterize their properties and assess their suitability as drug carriers. Mechanical testing demonstrated the robustness of the hydrogels. Scanning Electron Microscopy (SEM) revealed a porous structure conducive to drug loading and release. X-Ray Diffraction (XRD) and Fourier Transform Infrared Spectroscopy (FTIR) confirmed the successful incorporation of Metronidazole within the hydrogel. Thermal analysis highlighted the stability of the hydrogel under physiological conditions. Swelling behavior studies indicated a significant increase in hydrogel volume in response to temperature changes, facilitating controlled drug release. The drug release profile showed a sustained release of Metronidazole over time, while antimicrobial activity assays confirmed the retained efficacy of the drug post-release.

Conclusions:

The engineered thermally responsive hydrogel exhibits promising characteristics as a drug carrier for Metronidazole, with robust mechanical properties, effective drug loading, and controlled release capabilities. These findings suggest its potential application in targeted drug delivery systems, enhancing therapeutic outcomes and minimizing side effects.



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sciforum-104324: Enhancing Fire Retardancy and Mechanical Properties of *Hevea brasiliensis* Wood using Nano-Silica and Nitrogen/Phosphorus-based Compounds

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Wood is a highly sustainable material for building construction, yet its susceptibility to fire hazards limits its structural applications. Nitrogen-phosphorus (NP)-based compounds are the most preferred fire-retardant (FR) additives for timber applications. But their use in wood also results in some negative effects, such as the loss of mechanical strength in wood. This study explores the synergistic effects of Nano-Silica (NS) and NP-based compounds on enhancing the fire retardancy and mechanical properties of *Hevea brasiliensis*. A combination of ammonium polyphosphate (APP) and dicyandiamide (DCD) has been used in this study as an NP-based entity. Wood samples were treated by the full cell impregnation process with the following compositions: a) NS only at 1.5% (w/w) concentration: NS_{1.5}; b) NP-based combination, APP (17%, w/w) and DCD (3%, w/w): APP₁₇/DCD₃; and c) combination of NS_{1.5} and APP₁₇/DCD₃: NS_{1.5}/APP₁₇/DCD₃. During the rate of burning test, the control and NS_{1.5}-treated samples showed very poor fire resistance, reaching only 40% mass loss, almost within a minute, while APP₁₇/DCD₃- and NS_{1.5}/APP₁₇/DCD₃-treated samples reached the same amount of weight loss in 2.5 and 3 minutes, respectively. During the three-point bending test, the modulus of elasticity (MOE) showed 29% and the modulus of rupture (MOR) showed 43% deterioration in APP₁₇/DCD₃-treated samples as compared to the control samples. But the combined NS_{1.5}/APP₁₇/DCD₃ treatment recovered the deterioration in MOE and MOR values by making it almost equivalent to the control samples. Thus, the results of the experiments in this study confirmed the excellent synergy of NS and NP-based compounds in *H. brasiliensis* wood, not only enhancing fire resistance but also addressing the issue of mechanical deterioration in wood due to the NP-based FR treatment.



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sciforum-107221: Examination of new FDM filaments for applications with large temperature variations

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Today, 3D printing is no longer only used for rapid prototyping, but also for the production of customized objects, spare parts, etc. Among the various 3D printing technologies, the fused deposition modeling (FDM) process is the most widely used due to its simplicity, the mostly nontoxic polymers, and the availability of inexpensive printers and materials. However, the printed parts often exhibit mechanical and thermal inadequacies. Space applications in particular, such as microsatellites, require stable mechanical properties under periodically strongly changing temperatures. On the other hand, microsatellites and similar space applications are an area where mostly customized parts are needed, making 3D printing very suitable for such parts. New FDM-printable polymers can help to make this technology usable for space applications. Here we investigate novel FDM filaments with and without fibrous fillers before and after cyclic temperature variations between $-40\text{ }^{\circ}\text{C}$ and $+80\text{ }^{\circ}\text{C}$, similar to the situation of a microsatellite in the low Earth orbit (LEO). Dimensional stability and mechanical properties were tested before and after cyclic heat treatment, showing a wide range of elastic moduli. Maximum bending forces, deflection at maximum force and tensile strengths remained nearly unchanged for most materials after heat treatment, in contrast to previous tests with standard FDM printing materials, suggesting that most materials investigated here can be used in environments with strongly varying temperature.



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sciforum-107517: Examining The Mechanical And Morphological Properties Of Poly-Lactic Acid (PLA) /Waste High-Density Polyethylene (WHDPE) Blends Filled Plantain Peels (*Musa Paradisiaca*) Particulates Composites

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ABSTRACT

In this study, poly-lactic acid (PLA)/ waste High-Density polyethylene (wHDPE) blend filled plantain peel particulates composites were fabricated using compression molding techniques with filler loadings ranging from 5 % to 50 % for treated and untreated fillers (Plantain peels particulates). The mechanical and morphological properties of the prepared composites were analysed and evaluated using scanning electron microscopy (SEM) to examine the tensile fracture surfaces. The results showed that tensile strength, impact strength and flexural strength decreased with increase in filler content. The highest values were recorded for 100 % PLA, tensile strength of 40.66 MPa, impact strength of 1.5 J/m², and flexural strength of 55.60 MPa, than its counterpart of 100 % wHDPE composites which shows tensile strength of 24.90 Mpa, impact strength of 1.0 J/m² and flexural strength of 31.98 Mpa. Lowest value of impact strength was seen at 50 % filler loading with 0.32 J/ m² and lowest hardness value 100 % wHDPE with 24 HV. The tensile modulus reached 3.307 GPa for 100 % PLA, while flexural modulus at 28,271.76 MPa, and hardness reached 54.61 Hv at 50 % filler content. SEM revealed better filler dispersion at 5 % filler loading compared to 50 %, where agglomeration occurred. The incorporation of plantain peels particulates can effectively be used as reinforcement / filler in PLA / wHDPE blends for applications like particle boards, shelve, partition wall and tabletops among others.



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sciforum-106275: Experimental Study and Modeling of Adsorption Kinetics of Pharmaceutical Molecules on Activated Carbons

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Contamination of water systems with pharmaceutical products and synthetic chemicals is one of the most significant environmental concerns. Current research emphasizes on the design and development of materials able to remove a large variety of chemicals from wastewater effluents and natural water compartments. In this context, adsorption is considered a promising alternative as it removes a wide variety of organic and inorganic compounds and generates less toxic products than many other remediation methods. The present work is devoted to the preparation of an activated carbon from agricultural waste for the adsorption of paracetamol in aqueous solution. Adsorption kinetics and isotherms were studied in aqueous solution at self-equilibrium pH. Pseudo first-order and pseudo second-order kinetic models were tested to determine adsorption kinetic parameters. Empirical models are used to model the isotherm (Langmuir and Freundlich) with the aim of calculating the maximum sorption capacity of coal (ACW) and establishing a mechanism for the adsorption process. Pseudo-second-order and Langmuir models proved adequate for interpreting experimental results. Thermodynamic parameters characterizing adsorption showed that the process is spontaneous ($\Delta G^\circ < 0$), exothermic ($\Delta H^\circ < 0$) with a physical interaction between adsorbate/adsorbent ($\Delta H^\circ < 20$ kJ/mol).

In the light of the results obtained in the course of this work, we can conclude that the carbon synthesized in this way is an excellent adsorbent material with a high affinity for paracetamol. It also offers a number of advantages, such as low cost and availability of the raw material, and easy access to the charcoal via a simple preparation process.



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sciforum-104423: Exploring ethosomal technology to preserve bioactive plants by-product extracts for cosmetic purposes

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Using natural plant extracts in cosmetics has grown since the early twenty-first century. Waste biomass from berry crops is being studied for its potential to create high-value products, with encapsulation playing a key role in preserving plant extracts and enhancing their bioavailability. Among them, ethosomes, specialized ultra-deformable liposomes produced with a higher ethanol content, have demonstrated effectiveness in delivering medicinal compounds through the skin without causing adverse effects. They have been used in various cosmetic products for skin treatments and hair care, such as those with coenzyme Q10 or vitamins A and E, which help protect the skin from oxidative stress, improve skin hydration, and reduce signs of aging. They are also employed in skin-whitening agents (e.g., for kojic acid, hydroquinone encapsulation) and anti-hyperpigmentation treatments. This study introduces a novel approach to enhancing the commercial potential of berry crop by-products. Commercial raspberry leaf extracts were encapsulated in an ethosomal system through the cold method and thoroughly characterized using laser dispersion, zeta potential, encapsulation efficiency, colorimetry, and optical microscopy, revealing a mean particle size (D4:3) of 2.48 to 10.80 μm and entrapment efficiency (EE%) of 51.79% to 72.25%. The zeta potential ranged from -40.06 mV to -30.93 mV. Results suggest that ethosomes are an effective method for encapsulating hydroethanolic bioactive plant by-product extracts. These findings are significant as they make these encapsulated extracts suitable for various industrial applications. Particularly in the cosmetics industry, where the demand for natural and effective ingredients is rapidly increasing, present research could have a significant impact.



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sciforum-105429: Exploring the Trade-off between Printing Time and Mechanical Properties: Optimization of Three-Dimensional Printing Parameters for Clinical Aids Fabrication

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Rehabilitation engineering plays a vital role in developing assistive tools for individuals with diverse abilities, enabling them to perform activities of daily living (ADL) independently. However, the fabrication of clinical aids using Fused Deposition Modeling (FDM) technology often results in prolonged printing times. Balancing the printing time with the mechanical properties of the printed objects is a critical challenge. This research aims to identify optimized 3D printing parameters that minimize printing time while maintaining superior tensile strength and elongation properties.

To achieve the research objective, an initial plan of 256 combinations was devised for experimentation. However, utilizing Taguchi's orthogonal array design, the combinations were reduced to 16 trials, with five samples printed for each trial. Tensile strength and elongation were evaluated as crucial mechanical properties, while printing time was considered a key time efficiency factor. The mRMR algorithm, a feature selection technique, was employed to identify the parameters with the most significant contribution to the three output factors. Subsequently, linear regression analysis was conducted to ascertain the major influencing input parameters.

The mRMR analysis revealed a prominent trade-off between printing time and mechanical properties, with the nozzle diameter and infill pattern emerging as the most dominant factors. Specifically, a 0.6mm nozzle diameter and the zigzag infill pattern exhibited the greatest influence on both mechanical properties and printing time. By employing a systematic approach that integrates Taguchi's orthogonal array design, mRMR feature selection, and linear regression analysis, we identified the combination of a 0.16mm layer height, 30% infill density, 0.6mm nozzle diameter, and zigzag infill pattern demonstrated superior performance in terms of tensile strength, elongation, and printing time. Understanding these optimized printing parameters will facilitate the production of clinical aids with reduced printing times while preserving high mechanical properties, leading to enhanced efficiency and effectiveness in the field of rehabilitation engineering.



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sciforum-106742: Fabrication and characterization of GA-, EA-, and Rb-added perovskite solar cells passivated with DPPS

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Electrical and optical properties of various-types perovskite halides are dependent on the atomic compositions of the compounds, and the photovoltaic properties and stabilities are also affected by the interfacial structures of the devices. The aims of the present work is to fabricate and characterize guanidinium [C(NH₂)₃, GA], ethylammonium (CH₃CH₂NH₃, EA), and rubidium (Rb)-added CH₃NH₃PbI₃ (MAPbI₃) solar cells, which were passivated with decaphenylcyclopentasilane (DPPS) and GA. The first principles calculations on the proposed mixed-cation halides clarified the electronic structures, which were compared with experimental data. The lattice constants of GA/EA-added perovskites increased by growth of perovskite crystals aged at ~22°C, which provided the increase of photoconversion efficiencies. The GA/EA co-addition also improved their photovoltaic properties under indoor light environment using white color LED. Surface passivation of MAPbI₃ using GA and DPPS decreased carrier traps in the perovskite crystal, and the photovoltaic properties were improved. Energy band structures and partial density of states were investigated on the GA-, EA-, and Rb-modified perovskite compounds by the first-principles calculations. The calculation showed that the total energies were reduced by adding GA, EA, or Rb to the perovskites. The bandgap energies were also decreased, which could lead to an increase in the current density.



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sciforum-106650: Fabrication and characterization of perovskite solar cells using metal phthalocyanines and naphthalocyanines

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Methylammonium lead iodide (MAPbI₃) perovskite solar cells using metal phthalocyanines (MPc) and naphthalocyanines (MNc) as hole transport materials for improving photovoltaic performance with long-term stability have been characterized. The purpose of this study was to fabricate and characterize MAPbI₃ perovskite solar cells using MPc and MNc as hole-transporting layers for improved photovoltaic and optical properties with stability. We characterized the photovoltaic characteristics, morphology, crystallinity and electronic structures of the MAPbI₃ perovskite solar cells using nickel phthalocyanine (NiPc). The photovoltaic performance reached the maximum values of conversion efficiency (η) at 13.4 %. The behavior was based on the surface morphology, crystal orientation and near-defect passivation of the perovskite crystal. The surface passivation of NiPc supported crystal growth, improving carrier diffusion with the suppression of near-defect carrier recombination. The photovoltaic mechanism was discussed using the energy diagram of the perovskite solar cell. The insertion of NiPc optimized the energy levels near the highest occupied molecular orbital while adjusting the valence band levels and supporting the charge transfer from the perovskite layer to the hole-transporting layer. Simulation using SCAPS-1D programs predicted the photovoltaic characteristics of the perovskite layer in terms of the hole-transporting thickness and trap density. The photovoltaic performance was optimized based on the results of the simulation and experiments.



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sciforum-104449: Fabrication and Spectral Characterization of Cerium-Doped Magnesium Oxide Nanoparticles: Assessing Antimicrobial Activity and Membranolytic Effects Using Large Unilamellar Vesicles

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Magnesium oxide nanoparticles (MgO NPs) have recently attracted significant interest due to their low human toxicity, potential antibacterial properties, excellent thermal stability, biocompatibility, and cost-effectiveness. However, their bioavailability in target cells is decreased by their restricted membrane permeability, hindering their potential as sustainable medicines. To address this issue, we suggest magnesium oxide nanoparticles doped with cerium (MgOCeNPs) as a promising alternative. This study compares the membrane permeability and antibacterial activity of MgOCeNPs with pure MgO nanoparticles. Various spectroscopic and microscopic techniques were used to analyze both types of nanoparticles. X-ray diffraction revealed lattice patterns in the doped nanoparticles, while Atomic Force Microscopy provided details on their height and three-dimensional (3D) structure. Ce doping does not alter the crystal structure of MgO (FCC), but it significantly affects microstructural characteristics such as lattice parameters, crystallite size and biological activity. The antimicrobial efficacy of MgOCeNPs was tested against the pathogenic bacteria *E. coli* and *P. aeruginosa* and the fungal strain THY-1. MgOCeNPs showed strong antibacterial and antifungal activity, evidenced by increased zones of inhibition, a shorter growth curve, a lower minimum inhibitory concentration (MIC₅₀), and enhanced cytotoxicity. Growth curve analysis revealed early and extended stationary phases and an earlier decline in the log phase. Large Unilamellar Vesicles (LUVs), in conjunction with the egg-phosphatidylcholine model, demonstrated dose-dependent cytotoxicity, increased production of intracellular reactive oxygen species (ROS), and membrane perforation. The observed membranolytic activity and ROS generation suggest that MgOCeNPs cause cytotoxicity through oxidative stress. These results highlight MgOCeNPs as a novel and highly effective antibacterial agent with significant potential for managing and treating various microorganisms.



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sciforum-103776: Fabrication of polyvinyl alcohol-sodium alginate nanocomposite hydrogels reinforced with green synthesised silver nanoparticles for antimicrobial applications

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Introduction

Infectious diseases caused by potent microbes, the recent Covid-19 medical crisis, and increase in antibiotic resistant pathogens are serious medical and scientific challenges. These challenges pose a huge impact on the economy and health care systems of any country. There is an urgent need to develop functional materials for immediate decontamination of surfaces. In this project, we have successfully fabricated a peelable nanocomposite hydrogel based on polyvinyl alcohol (PVA), sodium alginate and silver nanoparticles (synthesized using a green method). The hydrogel film was crosslinked with glutaraldehyde and zinc acetate and exhibited good antibacterial properties.

Methods

Silver nanoparticles reinforced peelable hydrogel films and slabs comprising of PVA and sodium alginate were fabricated through in situ formation of nanoparticles using extracts of three different medicinally important plants such as Yerba mate, Hibiscus, and Matcha green tea. PVA and sodium alginate were crosslinked using glutaraldehyde (1 wt%), and zinc acetate solution, respectively. The physical and antibacterial properties of the prepared films were evaluated using established methods.

Results

The resulting hydrogels were tough, and the films were peelable and flexible. A strong surface plasmon resonance (SPR) peak around 400 nm confirmed the presence of silver nanoparticles in the hydrogel. The hydrogels exhibited considerable swelling capacity and the equilibrium water capacity was evaluated.

Conclusion and Work in-progress

A decontaminating hydrogel (in the form of slabs and films) composed of PVA and sodium alginate containing green synthesized silver nanoparticles were successfully prepared. The silver nanoparticles were prepared by in situ chemical reduction using the extracts of medicinally important plant products. The presence of phytochemicals and silver nanoparticles had a synergistic effect on the antibacterial properties of the hydrogel. The mechanical properties of the films are currently being explored.



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sciforum-107242: Fabrication of Reusable Green Nanocomposite Beads for point-of-use Disinfection of Water

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In recent years, the synthesis of metallic nanoparticles using plant-based extracts has gained much importance due to its ease and the economic advantages it offers in terms of material sustainability. These nanoparticles, when supported on biocompatible polymers, provide added benefits for biomedical applications.

This study investigates the green synthesis of silver nanoparticles (AgNPs) using spinach leaf extract and their application in dye degradation. The synthesized AgNPs, characterized by UV-Vis spectrometry, exhibited a significant absorbance peak around 400 nm, confirming successful nanoparticle formation. Three samples with varying concentrations of spinach extract and silver nitrate (AgNO₃) were analyzed, revealing that sample 2 had the highest concentration of AgNPs. The effect of calcium chloride (CaCl₂) concentration on alginate bead characteristics was assessed, with 5% CaCl₂ beads showing superior catalytic activity in degrading 2-nitrophenol, methyl orange, and Congo red. The AgNP-loaded beads demonstrated remarkable degradation efficiencies, achieving approximately 90% reduction for 2-nitrophenol and 85% for methyl orange within 30 minutes. In contrast, sodium borohydride alone did not facilitate Congo red degradation, but AgNP beads effectively reduced its concentration, likely through adsorption and catalytic action. This research highlights the potential of spinach-mediated green synthesis of AgNPs as effective and eco-friendly materials for environmental remediation and medical applications.

The antibacterial properties of the nanocomposite beads were studied using the broth method against two different strains of bacteria, *Escherichia coli* and *Staphylococcus aureus*. Antibacterial properties were studied as a function of the number of nanocomposite beads (5, 10, and 20). The material exhibited excellent antibacterial activity against these bacteria, even with a minimum of five beads. Further experiments are in progress, and this study opens the door for point-of-use disinfection of water and material sustainability.



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sciforum-103816: Facile preparation method of mesoporous TiO₂ nanoparticles with high crystallinity and enhanced photocatalytic activity.

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Mesoporous anatase TiO₂ nanoparticles can be synthesized by different routes. In this work, titania nanoparticles were prepared by an eco-friendly, simple, and fast-effective method [1], using titanium butoxide as a precursor and eucalyptus leaf extract solution as a reducing and dispersant agent to avoid the use of hazardous chemicals.

For phase conversion from amorphous TiO₂ into crystalline anatase titania, the amorphous TiO₂ gels obtained after hydrolysis of precursor were soaked in water at elevated temperature for a prolonged time. This is an alternative process to the conventional calcination methods, which cause irreversible collapse of the porous structure during thermal treatment and drastically decrease the surface area [2, 3]. This is confirmed by BET analysis (the surface area of TiO₂ nanoparticles calcined at 500°C is 5.0646 m²/g).

The aim of our work is the preparation of porous TiO₂ with both a large surface area and enhanced crystallinity, and the evaluation of photocatalytic activity for the degradation of methylene blue as a model organic dye under UV irradiation (365 nm).

The crystalline nature and structural formation of titanium dioxide NPs biosynthesized were confirmed by the X-ray diffraction technique, and functional groups of TiO₂ materials were confirmed by FT-IR spectroscopy [4, 5].

The results revealed that the biosynthesized material, treated in water at 90°C for 24 hours, exhibited an enhanced rate of photocatalytic degradation of the toxic dye (MB). A comparative study with biosynthesized TiO₂ calcined at 500°C and commercial TiO₂ was carried out for the oxidation of MB under UV (365 nm).

Heat treatment in water could be used as a simple, mild, yet effective method to transform sol-gel derived amorphous TiO₂ nanostructures into a porous anatase phase with high surface area and controllable crystallinity.



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sciforum-102348: Green Synthesis and Characterization of Silver Nanoparticles from Aqueous Extract of *Harrisonia abyssinica* Fruits

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The synthesis of silver nanoparticles using phytochemicals has attracted significant attention in the field of nanotechnology because of their low cost and environmental friendliness compared to conventional methods. The synthesis of silver nanoparticles with antibacterial properties through chemical reduction using phytochemicals present in an aqueous extract of *Harrisonia abyssinica* fruit is reported in the current study. The synthesized nanoparticles were characterized using various techniques, including UV-Vis spectrophotometry, transmission electron microscopy (TEM), energy-dispersive X-ray (EDX), and X-ray diffraction (XRD). The findings showed that the prepared silver nanoparticles were crystalline and spherical, and exhibited a strong absorption band at 420 nm due to the surface plasmon resonance (SPR) resulting from free-electron oscillations. The successful reduction of silver ions to form nanoparticles was indicated by a peak due to metallic silver at 3 keV in the EDX spectrum. The fabricated nanoparticles exhibited significant antibacterial activity against Gram-positive (*Staphylococcus aureus*) and Gram-negative (*Escherichia coli*) bacterial strains. The antibacterial effect was more pronounced for *Staphylococcus aureus* (MIC = 5 µg/mL) than *Escherichia coli* (MIC = 10 µg/mL). The findings of the current study contribute to the field of nanotechnology by demonstrating a green approach to synthesizing silver nanoparticles with antibacterial properties using natural sources from plant materials.



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sciforum-103936: Green synthesis of protein-decorated selenium nanoparticles for enhanced antibacterial and degradation of organic dyes in water

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Introduction

Bacteria and toxicants continue to threaten our health and pollute our environment. Eradicating those substances would lead to better health. Synthesizing selenium nanoparticles and incorporating them into solid supports is a milestone toward better health and hygiene due to their antimicrobial and catalytic properties. In this project, we have synthesized bovine serum albumin (BSA) capped silver nanoparticles using ascorbic acid, and polymer supported beads. The materials exhibited good antibacterial and catalytic properties.

Method

Selenium nanoparticles were synthesized by a reduction reaction using two core components, ascorbic acid (reductant) and sodium selenite, by two methods: First, the addition of ascorbic acid to sodium selenite drop-wise, then bovine serum albumin (BSA), a stabilizer to prevent sedimentation. It was tested by spectrometry. Secondly, beads were formed using sodium alginate and calcium chloride, which were added to the core components. In a UV-VIS spectrometer, the beads catalyzed the reaction with Congo red - a toxic dye - and NaBH₄. Additionally, both methods were tested for their antibacterial properties on *Staphylococcus epidermidis*, *Staphylococcus Aureus*, and *E.Coli*.

Results

The formation of selenium nanoparticles was confirmed by UV-Vis spectroscopy. The particles were stable against aggregation due to the capping of BSA. The nanocomposite beads were spherical with porous morphology, and were effective in the degradation of a model dye Congo red. The beads are reusable with no appreciable decrease in degradation efficiency.

Conclusion

The nanoparticles and the nanocomposite beads were effective against bacteria. The beads were reusable and had enhanced catalytic activity against Congo red, showing promise for decontamination of water including hospital waste water.



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sciforum-104673: Green Synthesis of Silver Nanoparticles Using *Phyllanthus emblica* and *Adhatoda vasica* Leaf Extract and their comparative study on microbes.

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INTRODUCTION

Silver played an important role as a novel metal ion in curing many diseases and infections. Silver is used in the form of AgNPs for targeting many biomedical and ,physio-chemical reactions to fulfill research goals. However, many drawbacks are reported in AgNP reactions, such as allergy and environmental risks. Therefore, to avoid all these side-effects, plant-based AgNPs are synthesized. In our research, we have used silver nano-particles from *P.emblica* and *A.vasica* leaf extract and carried out a comparative study on microbes.

METHODS

Leaves were first collected and then crushed into a powder. Next, we made a water-based extract solution by heating the mixture to 80 degrees Celsius for three to four hours using a magnetic stirrer. The leaf extract was combined with 1M silver nitrate solution, made by dissolving 1.7 grams of silver nitrate in 100 milliliters of water. *P. emblica* and *A. vasica* Leaf Extract with silver nitrate solution was centrifuged at 12000 rpm for 30 minutes, discarding the supernatant and collecting the dark pellet to form AgNPs from the leaf extract. Finally, the leaf extract was collected in the form of a powder and dried for two to three days in a dark place. Using the disc diffusion and well diffusion methods, we investigated the effects of these AgNPs powders at varying concentrations against bacteria that cause disease, such as *E. coli*, *S. aureus*, *Mucor*, and *Aspergillus* strains. Additionally, we utilized the commercial antibiotic streptomycin to complete a comparative study.

CONCLUSIONS

Secondary metabolites in plant leaves makes plant- based drug systems and *P.emblica* and *A.vasica* Leaf Extract AgNPs molecules more effective and eco-friendly as compared to chemical-based AgNPs.

RESULT

In our research, a comparative study of the effects of *P. emblica* and *A. vasica* Leaf Extract AgNPs on microbes produced positive results as compared to the commercial antibiotic streptomycin.



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sciforum-104943: Hematopoietic stem cell mobilization into the bloodstream in supplemented healthy subjects with antioxidants associated with high CD34 levels by flow cytometry in peripheral blood.

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Several active principles from plants could be used to mobilize HSC stem cells from the bone marrow into the bloodstream of patients. Pharmacological stem cell mobilizers showed adverse effects in patients. Thus, those active principles from plants with antioxidant and/anti-inflammatory effects (curcuminoids, AFA bluegreen algae, resveratrol, ect), could act as stem mobilizers without inducing adverse side effects. Curcuminoids [1,7-bis(4-hydroxy-3-methoxyphenyl)-1,6-heptadiene-2,5-dione], or AFA (*Aphanizomenon flos*) extract are antioxidants that increase the number of CD34+ cells by flow cytometry in peripheral blood of curcumin-treated patients. CD34 is a marker of hematological stem cells (HSC). We observed that short-term AFA-*Aphanizomenon flos aquae*-algae or curcuminoid supplementation in healthy subjects (powder or liquid formulation) over 48 consecutive hours enhanced peripheral CD34+ mobilization in both AFA-treated patients and curcumin-supplemented healthy patients as compared to their respective untreated controls. As a whole, the short-term supplementation over 7 and 38 consecutive days by curcuminoids (2000 mg/day) plus AFA Algae bluegreen extract (400 mg/day) enhanced CD34+ peripheral levels. Collectively, these antioxidants emerge as mobilizers agents for enhancing HSC levels into the bloodstream of healthy patients without adverse effects. Further studies will evaluate signalling pathways by which curcumin promote anti-inflammatory effects in monocytes from healthy subjects, as well as in certain diseases such as depression.



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sciforum-102960: How safe is the inclusion of recycled material for plastics used in food industry?

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Humans are exposed to plastic particles through several pathways, including through food contaminated by plastics derived from packaging. This is a major challenge to overcome, as plastics are extremely useful for food industry (e.g., transport and prevention of food spoilage). In this sense, the plastic industry is aiming at improving the sustainability and safety of their products. The present work involved the collaboration of producers and academia to develop new strategies in food packaging, namely the incorporation of recycled material into water bottles made of polyethylene terephthalate (PET) and yogurt cups made of polypropylene (PP). An evaluation of the toxicity profiles of microplastics originated from the new materials in comparison to commercial plastic materials already in use, was made using human cell lines as biological model, namely PNT-2, HepG2 and HCT116. The test materials were mechanically degraded and two different size ranges of particles were obtained by differential filtration, micro(nano)particles below 25 µm and 1.6 µm. Cells were exposed to different concentrations (1.28 µg/L up to 100 mg/L) and cell viability was assessed at 24, 48 and 72h of exposure, using the MTT assay. In general, the new materials presented lower impact in cell viability in the 3 tested cell lines, with lower IC₅₀. PNT-2 was the less sensitive cell (for both commercial and new materials), regardless of size. HCT116 was the most sensitive cell line, and plastic toxicity was modulated by the exposure duration. Overall, incorporation of recycled proved valuable, allowing reduction of production costs and biological impact.



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sciforum-104121: Hydrogel Electrolytes in Zinc-Ion Batteries: Patent Analysis and Future Prospects for Wearable and Flexible Electronics

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Hydrogel electrolytes (HEs) represent a transformative advancement for zinc-ion batteries (ZIBs), particularly in wearable and flexible electronics. These electrolytes are especially suited for small form factor ZIBs due to their flexibility, lightweight properties, and reduced leakage risks, but emerging trends suggest potential scalability for large-scale energy storage applications. Compared to state-of-the-art aqueous electrolytes, HEs offer significant advantages, including a reduction in side reactions, an increase in energy density, and enhanced compatibility with flexible substrates. This study analyzes 51 patent documents, including 48 applications and 3 granted patents, focusing on the formulation and application of HEs in ZIBs. International Patent Classification (IPC) data reveal that 14% of the patents pertain to HEs based on copolymers derived from compounds with unsaturated aliphatic radicals containing amides, such as acrylamide and methacrylamide. Similarly, 14% emphasize electrolytes solely composed of polymeric materials (e.g., gel-type or solid-type). Processes for treating macromolecular substances, such as hydrogels, constitute 12% of the patents, while 8% target crosslinking processes like the vulcanization of macromolecules. Patents involving copolymers with oxygenated carbonamido radicals account for 6%, underscoring diverse approaches to material synthesis and optimization. China leads this innovation landscape, with Anhui University and the City University of Hong Kong emerging as primary contributors. Patent classification data also indicate that many patents target technologies aligned with greenhouse gas mitigation, such as viscoelastic HEs for energy storage. These findings underscore the promising future of HEs in ZIBs, supported by active research and development efforts focused on eco-efficiency, high capacity, and sustainability.



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sciforum-107858: Hygrothermal Studies Of Different Arrangements Of A Brick And Adobe Wall On Comsol Multiphysics

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The appropriate arrangement and choice of building materials can reduce or even eliminate the risk of hygrothermal problems. The combination of building envelope materials and construction processes can improve a building's response to temperature and humidity, and thus the well-being of its inhabitants. This work analyzes three cases of exterior-exposed perimeter wall configurations (brick/air curtain/brick; brick/ adobe /brick; brick/rockwool/brick), using COMSOL multiphysics simulation software. A coupled three-dimensional heat and moisture transfer model was developed and numerically solved using a finite element method to study and compare the effect of replacing the insulation and air space between the two hollow brick walls with the adobe wall on the comfort level of the building's indoor environment.

Input data and assumptions were required. The model studied was assumed to be located in a warm climate, and the climatic data were extracted from the weather station close to the site studied. The results demonstrate the effectiveness of the hybrid wall (brick/ adobe/brick) in regulating indoor conditions thanks to its high thermal mass and insulation compared with those of typical walls (brick/air blade/brick); it can therefore be an alternative to insulation.

The results of this study are interesting in terms of the thermal and hydric performance of double partitions with adobe insulation.



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sciforum-102811: Impact of PCBM on charge transport dynamics in ternary organic thin films for solar cell applications

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Ternary organic solar cells (TOSCs), consisting of a donor polymer (D) and two acceptor (A_1 and A_2) materials ($D:A_1:A_2$), exhibit significant potential for overcoming the efficiency constraints of binary systems. It starts with the advantages of the binary blends of a donor (polymer) and an acceptor material (fullerene or non-fullerene acceptor) in heterojunction-based solar cells and integrates them with the strengths of tandem solar cells. The actual intrinsic challenges (limited spectrum absorption, charge carrier mobilities, efficient exciton dissociation, significant recombination losses, charge carrier collection, etc.) can be materialized here by the introduction of the third component, PCBM. The impact of PCBM as a third component (A_2) on charge carrier mobility in ternary blends—a crucial factor influencing device performance—is evaluated in this paper. The parallel model best describes the transport mechanism in the $D:A_1:A_2$ matrix, where the active layer acts as two intercalated bilayers. The third element's role as an electron transfer channel emphasizes the importance of compound compatibility and miscibility, also contributing to enhancing the charge carrier mobility. By systematically varying the ratio of the two acceptors ($A_1:A_2$) while maintaining a constant D:A ratio, the impact of compositional changes on charge transport properties is explored. Using the CELIV method, charge carrier mobility along with other important electrical properties (charge density and relaxation time) are examined. A significant correlation between charge carrier mobility and the acceptor ratio is revealed. These results underscore the importance of fine-tuning the ternary blend composition to maximize charge transport and, consequently, device efficiency. The insights gained from this study provide valuable guidance for the rational design of high-performance ternary OSCs.

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sciforum-104437: Impact of Pressure on the Physical, Mechanical, and Thermal Properties of the Ternary Halide Perovskite AgCaCl_3 : A First-Principles Investigation

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AgCaCl_3 , an inorganic halide perovskite material, is recognized for its high stability and environmental compatibility, making it a promising candidate for significant applications in optoelectronics and lens manufacturing. This study focused on investigating the electronic properties of AgCaCl_3 , including its density of states and band structure. The results revealed that AgCaCl_3 consistently exhibits an indirect band gap of around 1.5 eV across the pressure range examined. Furthermore, its dielectric function, absorption coefficient, optical conductivity, reflectivity, and refractive index indicated that AgCaCl_3 maintains its optical properties under the conditions studied. The mechanical properties were also analyzed, with calculations of elastic constants (C_{11} , C_{12} , and C_{14}) providing insights into the material's dynamic stability. Parameters such as the bulk modulus, shear modulus, Young's modulus, Poisson's ratio, and anisotropy factor suggest that the material is ductile. Additionally, thermal properties, including the Debye temperature, isobaric and isochoric heat capacities, thermal expansion coefficient, Gibbs free energy, and entropy, were thoroughly examined.

Methods

This study utilized DFT calculations, implemented in the Wien2K code, to explore the mechanical and thermal properties of AgCaCl_3 under varying pressure conditions. Its electronic and optical properties were optimized using the PBE-GGA functional. Its mechanical and thermodynamic properties were calculated using the ElStic and Gibbs2 codes.

Results and conclusions

This study investigates the physical, mechanical, and thermal properties of AgCaCl_3 under different pressures. The results show a decrease in its volume and lattice constants as pressure increases, while the material maintains its semiconductor properties and stable optical behavior. These computational findings highlight AgCaCl_3 's potential for use in deep-sea devices and lenses. Its elastic properties were found to increase linearly with the applied pressure, and its thermal characteristics, modeled using the quasi-Debye approach, provided detailed insights into the material's response. These outcomes form a solid foundation for future experimental work, supporting the development and application of AgCaCl_3 in optoelectronic devices.



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sciforum-091524: Impact of Zirconium Doping and Lattice Oxygen Release on Resistive Switching Characteristics of Metal-Oxide-Semiconductor Devices based on Sputtered $\text{Zr}_x\text{Hf}_{1-x}\text{O}_2$ gate dielectric

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Introduction: Resistive random access memory devices are crucial in nonvolatile memory applications. Hafnia- and zirconia-based devices are extensively researched due to their diverse properties. However, more insights are needed to enhance the performance of HfO_2 -based resistive switching devices.

Method: Thin films of $\text{Zr}_x\text{Hf}_{1-x}\text{O}_2$ were deposited using co-sputtering on *n*-type Si (100) substrates at room temperature. The films were deposited at different powers i.e. at 1,3,5 and 7 W onto the Zr target while keeping the RF power to the Hf target at 50 W. Various techniques including X-ray photoelectron spectroscopy, differential scanning calorimetry, and thermogravimetric analysis were employed for physical characterization. Additionally, electron beam evaporation was used for top metal deposition and patterned using UV photolithography to get 100 μm diameter gate electrodes.

Results: XPS analysis revealed complete oxidation of Zr metal during sputtering and all the film contain non-lattice oxygen. The Zr concentration in the as-deposited films ranged from 8% to 11%. Devices with 9% Zr concentration exhibited the best resistive switching performance. DSC studies indicated an endothermic peak at 145.9°C for films doped with 9% Zr, confirming lattice oxygen release. Presence of non-lattice oxygen is not the sole criterion for achieving a better resistive switching property, release of lattice oxygen is also necessary. The liberated lattice oxygen can be reversibly restored to their original sites at elevated temperatures, thereby reinstating the high-resistance state. Increasing doping concentration improved current fluctuations at low- and high-resistance states.

Conclusions: This study underscores the significance of non-lattice and lattice oxygen as well as Zr concentration in achieving desirable resistive switching properties in $\text{Zr}_x\text{Hf}_{1-x}\text{O}_2$ thin films. These findings hold implications for enhancing non-volatile memory device performance.



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sciforum-095958: Indicators of microbial corrosion of steel induced by sulfate-reducing bacteria under the influence heterotrophic bacteria with biocontrol properties

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Microorganisms take an active part in the processes of microbiologically influenced corrosion, for protection against which bactericides with inhibitory properties are used, which are often toxic compounds. There are many studies of eco-friendly "green" biocides-inhibitors, in particular, based on microbial metabolites. Previously, sulfate-reducing bacteria were isolated from the sulfidogenic microbial community of the soil ferrosphere and identified as *Desulfovibrio oryzae* NUChC SRB1 and NUChC SRB2. The properties of the mentioned strains of *D. oryzae* to form biofilms on the surfaces of artificial polymers (polypropylene, polyethyleneterephthalate), in particular, under the influence of *Bacillus velezensis* NUChC C1 and NUChC C2b, were investigated. The effect of the strains *B. velezensis*, *Streptomyces gardneri* strain ChNPU F3 and *Streptomyces canus* NUChC F3 on the ability of the *Peribacillus simplex* ChNPU F1 strain isolated from the soil ferrosphere to form biofilms on the glass surface was also investigated. So far, indicators of the processes of microbial corrosion of steel 3 induced by sulfate-reducing bacteria *D. oryzae* NUChC SRB2 under the influence of *B. velezensis* NUChC C2b and *S. gardneri* ChNPU F3 strains have not been investigated, which was the aim of this study. Methods: The agar well diffusion method (for antibacterial properties of the supernatants) was used, along with the crystal violet (for the biomass of the biofilm on the steel) and gravimetric methods (for the corrosion rate). Moderate adhesiveness to steel 3 was established for the *D. oryzae* by biofilm-forming ability. The presence of a supernatant from cultures of *S. gardneri*, *B. velezensis* and their mixture (2:1) did not reduce the biofilm-forming properties of *D. oryzae*. Compared to the control, a decrease in the corrosion rate was recorded for the variant of the mixture of the studied supernatants of bacterial cultures. This indicates the potential of this mixture for corrosion protection in environments with sulfate-reducing bacteria, which requires further research.



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sciforum-104234: Influence of Dispersant and Surfactant on nZVI Characterization by Dynamic Light Scattering

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The agrifood industries generate tremendous amounts of waste. The valorisation of these wastes is of the utmost importance. Here, spent coffee ground (SCG) and *Cistus ladanifer* L. leaf (CLL) post-distillation residues were used to prepare 50:50 (v/v) hydromethanolic extracts for green zero-valent iron nanoparticle (nZVI) production. Then, the nZVIs' size, polydispersity index (PDI) and zeta potential (ZP) were determined through dynamic light scattering (DLS). Since nZVIs are known to be heavily reactive and display a tendency to agglomerate, dispersant influence (water or methanol) and surfactant addition (Tween® 20) were studied. SCG NPs dispersed in water displayed a size of 565.6 ± 80.84 nm, with a PDI of ± 0.084 , and a ZP of -19.57 ± 0.95 mV. Adding Tween®-20 resulted in much lower sizes for these NPs (14.64 ± 0.76 nm with a PDI of 0.238 ± 0.066) and an increase in ZP (-5.99 ± 1.71 mV). CLL nZVIs dispersed in water displayed similar results, with lower size and higher ZP after surfactant addition (766.43 ± 129.49 nm, 0.684 ± 0.151 PDI vs. 13.4 ± 4.26 nm, 0.31 ± 0.042 PDI, -5.51 ± 0.86 mV). Using methanol as the dispersant for nZVIs displayed far worse results, which shows that nZVIs are better dispersed in water, and the addition of Tween® 20 highly reduced agglomeration, increasing the zeta potential. These results allow for better understanding of the importance of dispersant and surfactant usage for an accurate characterization by DLS.



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sciforum-102362: Insights into Rice Husk Pyrolysis: Research Trends, Technological Advances, and Valorization Strategies

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Rice (*Oryza sativa* L.) is a cereal crop cultivated worldwide for food, oils, and other applications. However, the processing of rice also generates large quantities of non-edible, solid residues called rice husks (RH), which account for 20% of the grain weight. The lack of effective and efficient strategies for handling RH has resulted in waste accumulation, thereby posing human health, safety, and environmental risks. To address these challenges, researchers have examined the treatment and valorisation potentials of RH through the pyrolysis process based on numerous research studies on rice husk pyrolysis (RHP) published and indexed in the Scopus database annually. Given the growing research interest and technological developments, there is an urgent need to examine the research climate and scientific landscape on RHP. Therefore, the paper presents the publication trends and a concise review of RHP based on the published documents in Scopus. The publication trends analysis revealed a geometric increase (3280% or 1,125 total published documents) from 2001 to 2021. The most prolific author on RHP research is Shuping Zhang (Nanjing University of Science and Technology), whereas the top affiliation is the Ministry of Education (China). The most cited funding organisation and country are the National Natural Science Foundation and the People Republic of China, respectively. A literature review revealed that RHP is an important research area due to the prominent publications, authors and citation counts on the topic. Lastly, the findings showed that pyrolysis is an effective technology for the treatment, disposal, valorisation, and management of RH wastes.



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sciforum-099880: Investigating The Feasibility of Using Locally Derived Nanosilica to Enhance the Mechanical Properties of Nigerian Tropical Soils For Sustainable Road Construction

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Nigeria's agricultural sector is pivotal to its economy, yet it grapples with substantial environmental challenges, concerning the management of Agro-wastes such as rice husk which constitute about 60 % of total paddy rice. With millions of tons of rice husk generated annually, the traditional burning of this waste not only constitute to environmental degradation but also poses serious health risk due to emission of CO₂ and particulate matter. This study explores the conversion of locally sourced rice husk ash into nanosilica to enhance the mechanical properties of Nigerian tropical soils for road construction. Various proportions (0%, 1%, 2%, 3%, 4%, and 5%) of nanosilica were incorporated into the soil, and tests including particle size distribution analysis, Atterberg limits, standard Proctor compaction, California Bearing Ratio (CBR), and unconfined compression tests were conducted. Transmission Electron Microscopy (TEM) confirmed the nanosilica's particle size range (1-9 nm), predominantly within 1-7 nm, indicating its efficacy as a reactive pozzolana. Results revealed significant improvements in soil characteristics, with CBR increasing from 5% for natural soil to 14% at 3% nanosilica replacement, and unconfined compressive strength rising from 0.09 MPa to 0.26 MPa under similar conditions. This research underscores the potential of converting agricultural waste into valuable nanosilica for sustainable soil improvement, highlighting keywords such as waste to wealth, sustainability, tropical soils, climate action, and nanotechnology.



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sciforum-103882: Investigation of Structural, Optical and Frequency Dependent Dielectric properties of BaZrO₃ Ceramic prepared via Wet Chemical Auto - Combustion Technique

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The wet chemical auto-combustion technique was used to synthesize Barium Zirconate ceramic having the general formula BaZrO₃. Many strategies have been carried out to regulate the functional properties of the perovskite structured sample which was calcinated at 800°C for 9 hours. Fourier transform IR spectroscopy, X – ray diffractometer, Scanning Electron Microscope (SEM) - EDAX, LCR meter and UV – Visible spectroscopy was employed to study about the structural, morphological, optical and electrical properties of the prepared cubic phase barium zirconate sample. The average value of the crystallite size was determined using data derived from XRD and was found to be 6.46nm by using Debye – Scherer formula. Lattice constant, crystallinity, unit cell volume, tolerance factor and x – ray density was also calculated. SEM - EDAX confirmed the elemental composition of the product and verified that they contained only the major constituents (Ba, Zr and O).The vibrational modes of the prepared sample was investigated using FTIR in the wavelength ranging from 400 - 4000Cm⁻¹. Energy bandgap was observed using Tauc's plot, where a graph was prepared for photon energy(hν) and (αhν)². The powder sample was blended with PVA and made into pellet of 13mm diameter using a pelletizer to explore the dielectric parameters like dielectric constant, loss factor, etc, in the frequency ranging 100Hz to 4MHz at room temperature. With high dielectric constant and low dielectric loss factor, barium zirconate ceramics stands as an excellent material for several microwave applications.



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sciforum-106222: Isolation of Geranylated Chalcone from Ethyl Acetate Fraction of *Terminalia Browni*

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Terminalia brownii is a leafy deciduous tree spirally arranged and crowded at the end of branches, The plant is widely distributed in Northern part of Nigeria and some part of Africa like Congo, Kenya, Sudan, Ethiopia and Tanzania. It is mostly used traditionally in the treatment of gastric ulcers, epilepsy, colitis, jaundice, fungal infection, diarrhea, malaria, hepatitis and allergic reactions. The aim of the study is to isolate secondary metabolites from the ethyl acetate fraction of *Terminalia brownii*. The plant material was extracted using cold maceration method with 70% methanol. The crude methanol extract was subjected to partitioning using n-hexane, chloroform, ethyl acetate, and n-butanol to give the respective fractions. The ethyl acetate fraction was subjected to extensive column chromatographic techniques using silica gel and Sephadex LH20. The structure of the compound isolated was elucidated with the aid of physical and chemical tests, UV, IR, 1D, 2D NMR analysis, and literature data. Column chromatographic separation of ethyl acetate fraction led to the isolation of a yellowish amorphous substance as 4'-hydroxy-3-methoxy-4-prenyloxy chalcone (geranylated chalcone). The plant is a rich source of secondary metabolites. The compound was reported for the first time from the plant and contribute to the taxonomy of the plant.



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sciforum-107849: Kojic-Acid-Driven Innovation: Developing Biocompatible and Versatile Catalysts for Sustainable CO₂ Conversion

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Introduction

This study develops eco-friendly catalysts using kojic acid, halloysite nanotubes, and alginic acid to create sustainable materials for CO₂ reduction and fixation.

Methods

HNTs functionalized with KA (HNT-KAs) were synthesized by reacting HNTs with chloroKA (CIKA) in DMF at 80 °C overnight, using Et₃N as a base. The use of three CIKA ratios produced HNT-KA1, HNT-KA3, and HNT-KA6. FT-IR confirmed their functionalization, and TGA was used to assess their thermal stability. SEM-EDX and TEM characterized their morphological properties. CO₂ photoconversion experiments were conducted under simulated solar irradiation for 7 hours, using hydrogen as the reducing agent in the presence of copper ions. Copper, chelated by the KA moiety, was introduced via CuCl₂ and reduced into Cu(I) using ascorbic acid. AA functionalized with KA (AA-KA) was synthesized through nucleophilic substitution with CIKA in dry DMF at 40 °C. Both catalysts were tested for their CO₂ fixation into cyclic carbonates at 70 °C and 1 atm using TBAB as a co-catalyst. Styrene epoxide was used as the model substrate, and the catalysts' recyclability was evaluated based on their insolubility in organic solvents.

Results

HNT-KA6 showed the best performance among the tested ratios, achieving 31% CO₂ photoreduction into methane and 89% CO₂ conversion into cyclic carbonates, surpassing the same values for HNT-KA1 and HNT-KA3. Adding Cu(I) increased the CO₂ photoreduction efficiency threefold and the methane selectivity fourfold while maintaining the stability over four cycles. HNT-KA6 also demonstrated strong CO₂ fixation activity without copper, as KA facilitated CO₂ capture and opening of the epoxide ring. AA-KA was highly efficient, achieving optimal yields with a continuous CO₂ flow at 70 °C for 10 hours. Both catalysts worked effectively under mild, solvent-free conditions, delivering higher yields than those previously reported.

Conclusions

The HNT-KA6 and AA-KA catalysts demonstrate high potential for sustainable CO₂ conversion. Their efficiency under mild, solvent-free conditions and their excellent recyclability make them ideal for green chemistry, supporting eco-friendly solutions for climate change mitigation.



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sciforum-105850: Lead (II) Adsorption From Wastewater Using Modified Cellulose Nanocrystals: Kinetics and Quantum Chemical Functionality

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For the removal of Ld^{2+} , cellulose nanocrystals (CNCs) were produced and modified (jelly-like) and then utilized as the adsorbent. The properties of CNCs such as surface area, chemical structure and composition were determined using the Fourier Transform Infrared Spectroscopy and Scanning Electron Microscopy analysis. In addition to how well they predicted reaction (adsorption capacity), one factor at a time (factorial method) was used. The process was further studied by implementing the kinetic models, thermodynamics studies and the adsorption isotherm. The AAS was used to determine the concentration of the element in the samples. Initially, a concentration of 100 mg/L, an adsorbent dosage of 5g, a pH of 6 and temperature of 25°C were to be kept constant when one parameter was being tested. After 120 minutes, adsorption capacity was 400.01 mg/g. The results showed that the modified CNCs exhibited high lead(II) removal efficiencies, with maximum removal capacities of 80-98%. The adsorption process was discovered to be pH-dependent, with optimal removal at pH 4-6 where the removal started reaching equilibrium. The FTIR and SEM findings for CNCs showed that the hydrogels had a network structure and more homogenous pores. The pseudo-second-order rate model was used to ascertain the adsorption kinetics. To achieve the best placement for adsorption, $H_{\text{OMO}}-L_{\text{UMO}}$ energy binding differences were used.



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sciforum-102058: Machine Learning Predictive Modelling of Calcium Removal from Cooling Tower Water Using Amberlite IR120 Resins

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The buildup of scale in cooling systems, especially evaporative cooling systems, is frequently a significant problem because of calcium (Ca) ions in raw or makeup water. As water evaporates, the concentration of these ions increases, leading to the formation of insoluble salts such as calcium carbonate (CaCO_3). This scaling may decrease heat transfer, inefficiencies, and increased energy usage. The calcium must be removed for the cooling system to operate best. The present study investigated the removal of Ca^{2+} from cooling tower water using Amberlite IR120 and predictive machine learning approaches. A lab-scale ion exchange column was used in this study. Response surface methodology (RSM), artificial neural networks (ANNs), and adaptive neuro-fuzzy inference systems (ANFISs) were used to optimise and model calcium removal using Amberlite IR120. The effects of the following process parameters were studied: contact time (min), pH, concentration (mg/L), dosage (ml), and temperature (K). RSM was used for process optimisation. The ANN model construction used 70% of the data for training, 15% for testing, and 15% for validation. The network was trained using feed-forward propagation and the Levenberg-Marquardt algorithm. The ANFIS was generated using a grid partition and trained using a hybrid method; 80% was used for training, and 20% was used for checking. Regression (R^2), mean square error (MSE), mean absolute error (MAE), mean absolute percentage error (MAPE), and average relative error (ARE). Numerical optimisation yielded an optimal removal percentage of Ca^{2+} of 99.07% at 89.55 minutes, 4.17, 452.83 mg/L, 132.57 ml and 295.58 K. The developed predictive machine learning model fits the 3 machine learning models with regressions of 0.9777, 0.9994, and 0.9903 for RSM, ANN, and ANFIS, respectively. This study has shown machine learning to be an effective tool for removing Ca^{2+} from cooling water Amberlite IR120 resins.



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sciforum-107369: Microwave drying kinetics of *Gmelina arborea* wood

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Drying is one of the most important processes for improving wood properties. Several methods are followed to dry wood; however, kiln drying is mainly used at industrial scales. The conventional method of kiln drying is very time-consuming and labour- and energy-intensive. Microwave heating has emerged as an effective technology for accelerating the drying process while minimising defects. This study focuses on the microwave drying characteristics of *Gmelina arborea* wood, a highly sought-after material in various industries. Drying experiments were conducted in a microwave oven operating at a frequency of 2.45 GHz, using two different power levels (540 W and 900 W). The samples were dried from an initial moisture content of about 130% to 12%. The drying cycles involved continuous exposure to microwave for 1 minute, followed by a 3-minute cooling period, repeated until the desired moisture content was achieved. The temperature profile of wood samples during the drying experiments was measured using an infrared camera. The results indicate that the drying rate was significantly higher in the MW drying experiments carried out at 900 W compared to those at 540 W. Additionally, the drying rate above the fibre saturation point (FSP) was higher than that below the FSP for both power levels. Notably, the total drying time for samples irradiated at 900 W (99 minutes) was nearly half, compared to samples dried at 540 W (213 minutes). However, out of the total drying time, the effective microwave time incurred in drying wood samples at 900 W and 540 W was 25 and 53 minutes, respectively. The moisture distribution between the core and surface was very uniform, and the quality of the dried wood was good, with only slight internal checks. This study demonstrates that microwave heating can be effectively utilized for the rapid and high-quality drying of *Gmelina arborea* wood.



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sciforum-092163: Mitigating Environmental Risks: Efficient Removal of Metronidazole from Pharmaceutical Wastewater Using Functionalized Graphene Membrane

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Metronidazole, an antibiotic widely used in human and veterinary medicine, poses significant environmental risks when discharged into aquatic environments. This study explores the potential of functionalized graphene membranes for the removal of metronidazole from industrial and pharmaceutical wastewater. Employing molecular simulations and the AM1 semi-empirical calculation method, we designed and simulated functionalized membranes to enhance metronidazole removal efficiency. Pharmaceutical effluent containing metronidazole can have detrimental effects on aquatic ecosystems, including toxicity to aquatic organisms and the potential development of antibiotic-resistant bacteria. Our findings show that specific functionalized membranes exhibit selective adsorption for metronidazole, indicating promising results for efficient wastewater treatment. In gas phase simulations, the aldehyde function demonstrates the superior selective adsorption of metronidazole over water, suggesting a lower affinity for water. In aqueous phase simulations, although the adsorption strength of the aldehyde function weakens in the presence of water, functionalization of the membrane surface enhances its overall affinity for metronidazole. Furthermore, the presence of metronidazole in water bodies can lead to bioaccumulation in aquatic organisms, posing risks to human health and the environment. The discharge of pharmaceutical effluent into water bodies can also contribute to the development of antibiotic-resistant bacteria, further exacerbating the environmental impact. Functionalized graphene membranes offer a promising solution for the efficient removal of metronidazole from wastewater due to their high surface area and tunable properties. This study highlights the importance of developing sustainable solutions for pharmaceutical wastewater treatment to protect aquatic ecosystems and human health. In conclusion, the use of functionalized graphene membranes for metronidazole removal shows great potential in mitigating the environmental risks associated with pharmaceutical effluent. By improving our understanding of adsorption processes and membrane interactions, we can develop more effective wastewater treatment technologies to safeguard our environment.



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sciforum-102636: Modelling coagulant dosage in drinking water treatment plant using hybrid machine learning based on empirical wavelet transform

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The coagulation process is one of the most important steps in drinking water treatment plant and its accurate determination plays a crucial role. In this study, simple and hybrid artificial intelligence models were applied for better prediction of coagulant dosage rate in Algeria drinking water treatment plant. First, the multilayer perceptron neural network (MLPNN), and random forest regression (RFR) were applied for predicting the coagulant dosage rate, using six raw water quality variables, these include dissolved oxygen (DO), turbidity (TU), temperature (TE), conductivity (SC), the pH of water, and ultraviolet absorbance (UV). From the obtained results, it was found that coagulant dosage rate is highly difficult to estimate by single models and the research should be oriented toward the development of a new modelling strategy. Second, the six input variables were further decomposed using the empirical wavelet transform (EWT) algorithm, leading to the formation of an ensemble of new variables called multiresolution analysis (MRA) which were combined and used as new input variables. Our hybrid models based on EWT guaranteed significant improvement compared to the single models. The results showed that the MLPNN-EWT model reduced the errors very much, and they greatly enhanced the fitting capability when compared to the single models, exhibiting a Pearson correlation coefficient (R), Nash-Sutcliffe efficiency (NSE), root-mean-square error (RMSE), and mean absolute error (MAE) of approximately ≈ 0.935 , ≈ 0.901 , ≈ 2.812 , and ≈ 1.923 . These improvements in coagulant dosage prediction are consistent and robust.



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sciforum-105482: Modern iron nanoparticles production methods for steel modification

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The development of physical methods of high-energy impact on the material makes obtaining a substance in a nano-dispersed state possible. The difference between nanoparticles obtained by the electrospark method, when condensation of the metal vapor phase occurs in a dispersion medium (water), the temperature of which does not exceed 30–40 degrees C, is a relatively narrow distribution of particles of the dispersed phase (20 - 100 nm). The field of application of such substances is not limited to agrobiological purposes. The authors investigated the electrospark metal granular dispersion method in an aqueous medium. The particles obtained by the above method have a size of 20–100 nm and several competitive advantages compared with similar methods of synthesis of metal nanoparticles. The level of defects in the crystal structure of nanoparticles after electro spark treatment is significantly higher than the values achieved by known methods of hardening metals and alloys. The high level of dislocation density in nanoparticles determines their high energy saturation. The study of the fine structure showed that the level of dislocation density in nanoparticles is close to the limit values of 10^{14} cm^{-2} as a result of the joint action of shock waves that arise in the process of pulse expansion of electric spark channels under the influence of pressure of several hundred atmospheres, high cooling rate of more than $10^3\text{--}10^4 \text{ }^\circ\text{C/s}$. Analysis of the internal structure of the obtained nanoparticles shows that their composition is heterogeneous. The particle is a metallic nucleus on which an oxide film is formed. In addition, iron particles can have a complex phase composition, namely, contain (consist of) alpha-iron and gamma-iron, which further expands the physical and technological aspects of using particles with a sharply non-equilibrium structural and phase composition.



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sciforum-099264: Morphological and sensing properties of electrochemically deposited ZrO_2 layers

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The ZrO_2 is an increasingly used material for various applications in different fields such as optoelectronics, medicine and environmental monitoring. Its main advantages are due to almost unique properties, such as high mechanical and thermal resistances, high dielectric constant and refractive index, wide range of optical transparency and capability for diverse nanostructuring.

Among different methods applied for synthesis of metal-oxide nanostructures, the electrochemical deposition is an attractive method – it is cost-effective, environmentally compatible, requires relatively simple apparatus and offers easy control of morphology of produced nanostructures by varying the deposition parameters.

The aim of our work is to study the morphological and sensing properties of nanostructured ZrO_2 layers, electrochemically deposited on the gold electrodes of AT-cut quartz resonators. The deposition is carried out in aqueous solution containing 5 mM of ZrOCl_2 and 100 mM of KCl. The layers sensing abilities towards ammonia and ethanol vapors are measured by using Quartz Crystal Microbalance (QCM) method. The influence of electrodeposition conditions (the temperature and time) on layers morphology and sensing characteristics is measured and analyzed.

The layers morphology significantly depends on deposition temperature that leads to nanostructured grains with different size, shape, surface density, and roughness. The results for gas sensing show low sensitivity to ethanol and high sensitivity to ammonia. As a whole, the work confirms the suitability of ZrO_2 electrochemical deposition for the further design and development of QCM gas sensing devices.



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sciforum-103463: Nanocomposites of chitosan-lignin doped with ZnO, TiO₂ and Zn₂SnO₄ for food packaging with UV-blocking, antimicrobial and antioxidant properties

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The preparation of new nanocomposites by combining chitosan-lignin and three different nanoparticles (NPs) of ZnO, TiO₂ and Zn₂SnO₄ was the main interest of the present work. Lignin provides enhancing UV protection of commercial products with less than a 10% blend with other material. Also, chitosan is an abundant polymer that can be applied in many industries due to its biodegradability and biocompatibility properties. ZnO, TiO₂ and SnZnO nanoparticles present increased thermal stability, UV-protection, antimicrobial and antioxidant properties. Therefore, in this study, biodegradable nanocomposite membranes from the combination of chitosan-lignin (1/1 molar ratio) and 0.5, 1 and 1.5%wt of ZnO, TiO₂ and Zn₂SnO₄ were prepared via sol-cast method. The successful integration of nanoparticles in the polymer matrix was confirmed by Fourier Transform Infrared spectroscopy measurements. In addition, the size and the morphology of nanoparticles and the homogeneity of nanocomposites were investigated with Scanning Electron Microscope. The crystallinity of nanocomposite membranes was studied with X-Ray Diffraction. Moreover, the water sorption capacity, water content, contact angle, water and soil stability, and mechanical properties of the prepared nanocomposite membranes were analyzed. In addition, and most importantly, the UV-blocking efficiency of the prepared membranes was measured using UV-vis spectroscopy. Finally, the antioxidant and antimicrobial assays of nanocomposites loaded with ZnO, TiO₂, and Zn₂SnO₄ NPs were studied. Therefore, the nanocomposites show promising features for the development of food packaging, and UV protective films, and for the development of new and sustainable materials.



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sciforum-101617: Nanoscopic characterization of Graphene oxide for anticorrosion application

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Graphene, a two-dimensional carbon material, possesses exceptional properties such as high electron mobility, exceptional strength that surpasses that of steel, chemical resistance, environmental friendliness, and a large specific surface area. In this study, we used the modified Hummer process to produce graphene oxide, which was then applied to an aluminum alloy substrate as a corrosion-resistant coating. The aluminum alloy used in our study is AA2024, which has a wide application in industry and aircraft. The coating layer was characterized by micro-Raman spectroscopy and atomic force microscopy (AFM) before and after the reduction process. Micro-Raman spectroscopy provided information on the degree of reduction and the presence of functional groups in the coating layer. AFM images enabled the study of surface morphology and topography. After the reduction process, achieved by annealing in an argon atmosphere at 140 °C, micro-Raman spectroscopy and AFM microscopy were again used to assess structural and morphological changes. The reduction resulted in the formation of reduced graphene oxide (rGO), which exhibited improved conductivity and stability. The combination of micro-Raman spectroscopy and AFM characterization techniques provided detailed information on the properties and effectiveness of the coating layer. This research contributes to the development of anti-corrosion methods using advanced materials and surface engineering techniques.



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sciforum-104260: Non-Invasive glucose monitoring: gold and silver nanoparticles in saliva analysis

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Introduction : Testing blood sugar levels can be painful and uncomfortable due to the need for blood draws. Nanoparticle studies have demonstrated unique properties that enable them to interact with glucose in ways larger molecules cannot. Our project is an attempt to show that glucose levels can be accurately measured from human saliva using nanoparticles.

Method : Gold and silver nanoparticles were synthesized using gold salts and silver nitrate, with sodium borohydride used as the reducing agent and sodium citrate as the stabilizer. Glucose solutions were mixed with gold nanoparticles in a 1:1 ratio. Heat was applied to accelerate the reaction before silver nanoparticles were introduced. Various tests were conducted, including comparing samples with and without heat, different concentrations of nanoparticles, and using a reducing agent without a stabilizer. The UV absorption spectra of the resulting solutions were measured to evaluate the outcomes.

Results : Gold and silver nanoparticles were stable, showing interaction with glucose via decreased UV absorption. The UV spectrum displayed peaks for both metals. Higher glucose concentrations led to lower absorbance. Heating before adding silver enhanced the gold–glucose reaction, reducing the gold peak and increasing the silver peak due to less glucose availability for the silver reaction.

Conclusion: This project enabled the detection of blood glucose levels using saliva rather than the usual method, which can be uncomfortable. We added gold and silver nanoparticles to different glucose concentrations, and analyzed the UV absorption spectra. This offers a less intrusive approach for obtaining blood sugar levels.



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sciforum-103515: Novel chitosan/PVA@hyaluronic acid and chitosan/PVA@hyaluronic acid/curcumin films for wound healing

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Wounds disrupt the proper function of the skin, and the use of biocompatible films ensures the right conditions for wound healing, prevents microbial infection and thus leads to skin regeneration. Chitosan (CS) is a natural polymer with healing properties, and polyvinyl alcohol (PVA) is a synthetic, biocompatible polymer which increases mechanical properties. In this study, the films used are based on biocompatible hydrogels that are produced via the action of hyaluronic acid (HA) as a natural cross-linker and the interactions between the polymeric chains of CS, PVA and HA. The incorporation of curcumin (Cur) (a natural antimicrobial agent) ensures the protection of the wound against pathogenic microbes. The combination of these materials offers a novel approach to enhancing the water sorption, stability and functionality of wound-healing films. Thus, two groups of films were prepared—CS/PVA@HA and CS/PVA@HA/Cur—with varying concentrations of HA (0.5, 1, 2, 3% w/w) and a fixed concentration of PVA (1% w/v), CS (2% w/v) and Cur (0.1% w/w). The characteristic peaks of the films in FTIR appear to be slightly shifted, which confirms the cross-linking between the chains, while XRD is included. Moreover, swelling and stability assays proved that CS/PVA@HA and CS/PVA@HA/Cur containing 2% w/w HA exhibited optimal behavior under conditions of swelling and stability at pH 5.6 and 7.4, respectively. The results of the experiments confirmed the successful synthesis of the films via our physical cross-linking method. It was found that the incorporation of HA in the CS/PVA polymer network increased the water sorption and swelling behavior of the prepared materials. Therefore, the biocompatibility and the cell growth capacity of the films were also confirmed. Thus, they have potential as wound dressings, with easy formation and improved bio-evaluations for wound-dressing applications.



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sciforum-102005: On the O 2*p*-band center as a descriptor for the catalytic activity of complex oxides

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Electronic descriptors extracted from Density Functional Theory (DFT) calculations are a powerful tool in designing new perovskite-based materials that could catalyze oxygen reduction (ORR) and oxygen evolution (OER) reactions [1]. In particular, a good correlation has been found between the O 2*p*-band center and the charge transfer energy, the oxygen vacancy formation energy, the adsorption energy, or the overpotential. While such correlations are proven for simple ABO₃ perovskites, there are few studies dealing with oxides presenting high chemical and structural complexity. In this work, the layered perovskite system YSr₂Cu₂FeO_{7+δ} (YSCFO) [2] is investigated to analyze the effects of oxygen non-stoichiometry and vacancy ordering in the O 2*p*-band center values. In YSCFO, the formal oxidation states range from Fe⁴⁺ and mixed Cu³⁺/Cu²⁺ (δ = 1) to Fe³⁺ and Cu²⁺ (δ = 0). To establish a comparison with a single-TM oxide, band centers are also extracted for the Ruddlesden Popper Sr_{2-x}La_xFe₂O₄ phase with 0 < x < 2 (formally, from Fe(IV) to Fe(II)).

DFT calculations (SCAN, PBE+*U*) are performed using the ab initio total energy program (VASP). The O 2*p*-band centers are extracted from the calculated DOSs. For RP-Sr_{2-x}La_xFe₂O₄, the O *p*-band center displays a linear trend with the Fe oxidation state. In the complex system YSCFO, the interplay between Cu and Fe 3*d* states breaks the linearity. In addition, for a given oxygen content, the O 2*p*-band center varies with the oxygen/vacancy ordering in the FeO_{1+δ} layers. Importantly, the O 2*p*-band center values calculated for the YSCFO system suggest that these materials may possess electrocatalytic activity, as the obtained values are between -1.0 and -1.8 eV [1].

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sciforum-102208: Optimisation of Biodiesel Production from Waste Margarine Oil Using Response Surface Methodology

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Global warming and pollution instigated by fossil fuel combustion have led environmental agencies to advocate for eco-friendly renewable fuels. Biodiesel is a green and renewable fuel produced by the transesterification reaction of vegetable oil/animal fat with short-chain alcohol in the presence of a catalyst. Biodiesel production has been affected by the cost of production mainly due to the cost of feedstock. This work presents biodiesel production using waste margarine oil and response surface methodology (RSM) for process optimisation. The transesterification of waste margarine oil was carried out using sodium hydroxide (NaOH) as a catalyst under atmospheric pressure in a lab-scale batch reactor. Central composite design (CCD) was used to optimise four parameters: methanol-to-oil ratio (3-15 mol/mol), catalyst ratio (0.3-1.5 wt.%), reaction time (30-90min), and reaction temperature (30-70°C). Numeral optimisation was performed, and an optimum yield of 94.024% was obtained at a 9.6 mol ratio, 0.96 wt. % catalyst ratio, 63 min reaction time, 52 ° C reaction temperature, and a low standard error yield of 0.576 %. Analysis of variance (ANOVA) showed that the methanol-to-oil ratio had the highest influence on the biodiesel yield, followed by the catalyst ratio, and reaction time had the least impact after temperature. The kinetics study describes that the reaction is controlled by pseudo-first order, and the activation energy was found to be 62.41 kJ/mol. It was concluded that biodiesel could be produced using waste margarine oil as a cost-effective feedstock optimised by RSM.



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sciforum-105842: Optimisation of Copper (II) Removal From Wastewater Onto Modified Cellulose Nanocrystals Using The Box-Behnken Design

Omphemetse Johosheba Machaze, Bongiwe Mbele *, Musamba Banza and Tumisang Seodigeng

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This studied aimed to remove Cu (II) from waste water onto the modified cellulose nanocrystals using the Box-Benken design in RSM. The Cellulose nanocrystals derived from waste paper was characterized and compared with the modified cellulose nanocrystals by FTIR. The adsorption peaks 3367 and 3420 found in the modified CNC and unmodified CNC spectra, respectively, revealed the characteristics for the stretching of -OH found in the polysaccharide. The strong absorption peak 1551 was found to be present in the unmodified spectra, confirming the characteristics of the asymmetric and symmetric of CO in COO-, and giving evidence for the successful incorporation of EDTA and cellulose nanocrystals. Four parameters pH, contact time, initial concentration and adsorbent dosage were optimized with the use of response surface methodology (RSM) with a quadratic model box-Benken design. Twenty-nine experimental runs were conducted to get the desired response. The results showed that CNCs effectively removed Copper (II) ions, with a maximum removal efficiency of 99.78%. The optimised conditions were pH 6, initial Cu (II) concentration of 125mg/L adsorbent dosage of 6 mg/200mL, and contact time of 30 minutes. The quadratic model developed through RSM showed a moderate to strong correlation, with an R-squared value of 0.988, indicating that 98.88% of the variation removal efficiency can be explained by the predictor variables and their interactions. This study demonstrates the potential of CNCs as an eco-friendly adsorbent for heavy metal removal and highlights the effectiveness of RSM in optimising adsorption processes.



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sciforum-103949: Optimization of Anfis Parameters Using Box–Behnken Design to Predict Chromium (VI) Adsorption

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Adsorption prediction using an ANFIS may reduce the process costs in practical applications. MATLAB 2022 was used in this investigation to assess chromium (VI) adsorption data at different temperatures, doses of modified cellulose nanocrystals, and pH values. The best kind and quantity of membership function were chosen using the Box–Behnken experimental design approach to provide precise predictions with the least error. The RMSE was correlated with the number of MFs for each input by developing regression models based on analyzing every combination from the Box–Behnken design. Five typical membership functions, Gaussian, triangle, Gaussian 2, trapezoid, and generalized bell-shaped, were used. ANOVA was used to demonstrate the significance of the regression models developed for the experimental data using trapezoid and triangular MFs. The triangular MF produced the greatest accuracy in the Cr (VI) adsorption predictions (with a lower RMSE of 1.601 and R^2 of 0.998) when it was used in conjunction with the appropriate membership function numbers for each input (8, 8, and 4 for the triangular membership function and 6, 6, and 3 for the trapezoid membership function) according to the ANFIS's predictions. Response surface plots were also used to evaluate the relationship between the triangular RMSE values and the membership function numbers. These findings demonstrate this material's potential to serve as a viable adsorption material for the focused elimination of contaminants, increasing the application of machine learning in sorption studies, and the remediation of novel pollutants.



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sciforum-102995: Optimization of Malachite Green Adsorption onto Biocomposite Beads: A Sustainable Approach for Wastewater Treatment

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Technology has always been inspired by nature. This is one of the reasons why new technologies continually seek environmentally friendly composite materials. In recent years, there has been a growing interest in developing green bio-composites for industrial wastewater treatment.

In this work, we prepared a type of green, low-cost hybrid composite material comprising volcanic rock (VR), a natural Algerian siliceous volcanic filler from Ain-Temouchent, and the biopolymer alginate (Alg).

The Alginate/Volcanic Rock (Alg/VR) beads were prepared using a simple mixing method in the form of beads, produced with a syringe pump and a cross-linking agent. Detailed characterization of the beads and their initial reagents was carried out using X-Ray Diffraction (XRD), Fourier Transform Infrared spectroscopy (FTIR), and Thermogravimetric Analysis (TGA). The results confirmed the incorporation of the biopolymer into the natural volcanic rock matrix, with clear evidence of interaction between alginate and volcanic rock.

Furthermore, the beads were tested as effective and alternative adsorbents for the removal of the cationic dye Malachite Green (MG) using a Flow-through cell apparatus. The influence of different experimental parameters, such as pH, contact time, adsorbent dose, and initial dye concentration, was investigated. The adsorption results showed that the highest removal efficiency of 95% was achieved at pH 6, with a contact time of 60 minutes, using 0.8 g/L of the composite for a 25 ppm dye solution.

These findings highlight the significant potential of Alg/VR beads as a low-cost, sustainable, and efficient adsorbent for industrial wastewater treatment. By combining locally sourced natural materials with biopolymers, this work not only contributes to green chemistry and sustainable environmental management but also offers a practical solution for addressing global water pollution challenges. This innovative approach aligns with the increasing demand for eco-friendly technologies and reinforces the importance of developing scalable, cost-effective solutions for industrial applications.



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sciforum-106192: Paving The Road from Small- to Large-scale Production of Green Nano Pharmaceuticals.

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Introduction

Nanotechnology has successfully invaded medical science, especially in drug delivery field. Despite the huge advances achieved in the field of nanomedicines on laboratory scale, a limited number of nanotechnology-based drugs are available in the global market. This is because hazardous chemicals are frequently used in conventional nanoparticle synthesis methods. The goal of this study was to investigate novel, easily scalable, environmentally friendly methods to prepare drug-loaded nanoparticles on a pilot-scale without using toxic organic solvents. Additionally, to locally design, develop, and optimize prototype pilot scale equipment for nanoparticle synthesis as a means of creating a bridge between laboratory and industrial scales.

Methods

Carbamazepine-loaded transfersomes (CZTs), a type of lipid-based nanoparticles, were prepared on a small scale using the modified scalable heating method that avoids organic solvents usage and high energy procedures (green synthesis) in a specially designed homemade vessel replicating Mozafari's containing baffles forming many turbulences leading to formation of nanosized particles. A three-factor, three-level Box-Behnken design was employed to optimize process and formulation factors. Furthermore, the optimized formulation was synthesized on both a small-scale and pilot-scale via the modified heating method.

Results

The small-scale beaker simulating Mozafari's was successfully scaled up to a pilot-scale tank of large capacity (13 Liters) compared to the small-scale beaker of capacity 50 milliliters only. Consistent results were observed for the optimized formula on both small and pilot-scale showing a mean size of 323.12 ± 0.3 nm and 341.5 ± 1.4 respectively, a high entrapment efficiency (EE) of $76.12 \pm 1.1\%$ and $75.01 \pm 0.5\%$ respectively, and a sustained release profile.

Conclusion

CZTs optimized formulation was successfully fabricated on both small- and pilot-scale using a simple, scalable, green, modified heating method. Box-Behnken surface analysis proved to be an efficient tool to optimize the CZTs formulations. CZTs fabricated on the two scales possessed comparable results.

<https://www.youtube.com/watch?v=FWOMPJhLTDQ>



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sciforum-095975: Photoluminescent Carbon dots: synthesis, properties and applications

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University of Central Lancashire

This presentation will focus on the evolution and recent developments of a new class of photoluminescent materials referred to as Carbon dots or C-dots, primarily comprising C, H, O, and N. Typically, C-dots have spherical shape with sizes lower than 20 nm, and can be synthesized at a large scale following the simple pyrolysis treatment of suitable carbon-rich precursors, including crude biomass, renewable resources, polymers, and carbon fibres (1,2). Depending on the preparation method and the nature of the starting materials, the graphitization degree, elemental composition and the morphology of C-dots can vary considerably, while post-synthesis treatments (such as chemical and electrochemical reactions, passivation strategies and physio-absorption) can modify their surface characteristics, thereby enhancing their solubility, biocompatibility, toxicity and optical properties (3).

In principle, C-dots demonstrate excitation wavelength-dependent emission with high quantum yields with the strongest emissions falling within the blue/green area, although red-emissive systems have also been reported (4). Moreover, the significant role of the organic fluorophores generated during the pyrolytic synthesis of C-dots has been demonstrated (5). Interest lies in the optical properties of C-dot-based aqueous dispersions, solid-state materials, polymer nanocomposites and nanopowders. This presentation will provide an overview of the structure--property relationships of C-dots with emphasis on emerging applications such as bioimaging, phototherapy, controlled drug release, molecular sensing, antimicrobial treatments, fertilisers, catalysis, energy conversion, nanoforensics, water treatment, environmental decontamination and anti-counterfeiting (6,7).

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sciforum-107835: Physical, thermal and mechanical behaviour of composites based on gypsum and juncus maritimus fibre

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It is necessary to develop construction materials with a limited impact on the environment. To achieve this objective, juncus maritimus fibres were used as reinforcement in the plaster matrix at percentages of 10%, 20%, 30% and 40% by volume. The aim of this study was to investigate the impact of the addition of juncus maritimus fibres on the behaviour of plaster. The juncus fibres were characterised from a physical, thermal and mineralogical point of view, and the plaster was studied both physically and thermally. The effect of the percentages of juncus maritimus fibres on the fluidity of the plaster was evaluated using the Marsh cone method, , i.e. by measuring the time taken for a known volume of gypsum to flow from a cone through a short tube. The thermal and mechanical properties of the composites produced were determined by the hot disc method and by compression and flexural tests. The results showed that the bulk density and thermal conductivity of the composites were reduced by 6.45% and 10.9%, respectively, for a percentage of 40% compared with the reference sample. The addition of 20% juncus maritimus fibres improved the flexural strength by 7.43% compared with the reference sample, but a decrease in compressive strength was observed due to poor adhesion between the fibres and the gypsum matrix. The microstructures of the composites were determined using the scanning electron microscope method.



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sciforum-106356: Phytochemical Investigation and Anti-Plasmodial Studies on Methanol Extract of The Aerial Parts of *Scadoxus multiflorus* (Martyn) Raf. (Amaryllidaceae)

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Scadoxus multiflorus, a fleshy herbaceous plant with a large bulb, is traditionally used in ethno-medicine for to manage malaria and treat ulcers and as a cardiotonic stimulant. This study aimed to conduct a phytochemical screening and evaluate the antiplasmodial activity of its aerial parts. The plant material was extracted with methanol using a maceration process, and the crude extract was partitioned into hexane, chloroform, ethyl acetate, and butanol fractions. Qualitative phytochemical screening revealed tannins, flavonoids, alkaloids, terpenoids, steroids, saponins, phenols, and cardiac glycosides in the crude extract and fractions. Quantitative analysis revealed that phenolic compounds were the most abundant in the crude extract (198.32 mg/g), while alkaloids were the least abundant (51.14 mg/g). The n-hexane fraction, however, had the highest tannin content (215 mg/g). Acute toxicity testing, following the OECD's 2008 guidelines, showed that the median lethal dose (LD_{50}) was greater than 5000 mg/kg, indicating the extract's safety. Its antiplasmodial activity was evaluated using both suppressive and curative models in *Plasmodium berghei*-infected albino mice. The extract at 1000 mg/kg significantly suppressed parasitemia by 58.8% in early infection (in the suppressive test) and reduced parasitemia by 61.8% in established infection (in the curative test). Chloroquine, the standard drug, at 5 mg/kg produced higher parasite suppression (84.52%) and curative effects (84.50%) compared to those of the extract. These results suggest that methanol extract of the aerial parts of *Scadoxus multiflorus* possesses antiplasmodial activity, supporting its traditional use in malaria management.



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sciforum-107772: Phytosome-Based Nanocarriers Enhanced with Seaweed Extracts: Overcoming the Blood-Brain Barrier

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Neurodegenerative diseases impact millions of people globally and are emerging as an imminent challenge due to the rapidly aging of the population. Current treatments focus on relieving symptoms, so it is necessary to adopt innovative strategies. However, delivering pharmacological agents directly into the brain is difficult because of the presence of the Blood-Brain Barrier (BBB). To overcome this obstacle, nanotransporters such as phytosomes have been developed. This study reports the preparation and characterization of phosphatidylcholine (PC) phytosomes based on hydroethanolic extracts of three macroalgae: *Ascophyllum nodosum* (L.) Le Jolis (AN), *Bifurcaria bifurcata* R. Ross (BB) and *Fucus spiralis* L. (FS). Additionally, some phytosomes were functionalized with polyethylene glycol (PEG) and apolipoprotein E (ApoE). Phytosomes characterization was carried out in terms of encapsulation rate, size, polydispersity index (PDI), zeta potential, and stability and the efficacy of passage through the BBB was tested using an in vitro transwell model based on hCMEC/D3 cells. The results showed a high percentage of extract bound to PC (from 74.9 to 80.3 %) and tests conducted over three weeks showed the stability of the phytosomes developed. There is a notable distinction between functionalized and non-functionalized phytosomes reflected in the values of their sizes (from 117.71 to 167.73 nm for non-functionalized and from 277.07 to 361.44 nm for PEG-ApoE phytosomes), PDIs (0.286-0.411 for non-functionalized and 0.389-0.539 for functionalized phytosomes), and zeta potentials (1.91-2.22 and -3.31- -0.68 mV for non-functionalized and functionalized phytosomes, respectively). Regarding the ability to cross the BBB, the functionalization of phytosomes with ApoE did not prove to be a crucial step, perhaps due to the low amount of ApoE used (1%), although all nanotransporters always passed through hCMEC/D3 cells monolayer, regardless of their formulation.



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sciforum-103989: PLA-based composite material with a flax husk filler

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The use of environmentally friendly biodegradable materials allows to reduce the environmental impact. It is possible to use composite materials based on biodegradable plastics with plant fillers, which should be pre-treated to increase their adhesion to the polymer matrix.

The initial flax husk was ground. After milled flax husk powder was acetylated with acetic anhydride, which leads to improved adhesion of filler and polymer matrix. To create the composite, modified flax husk powder in the amount of 30, 40 and 50 wt. % was mixed with the PLA powder and then then obtained mixture was pressed at a pressure of 18.5 MPa and a temperature of 185°C.

With the addition of the filler to the polymer matrix, a decrease in tensile strength was observed for the 20 wt. % filler content (5.29 MPa), while the maximum decrease in strength was observed for the 50 wt. % filler content sample (4.87 MPa) compared to 14 MPa for the unfilled PLA. This decrease in strength is explained by the appearance of the interface between the matrix polymer and the filler. All samples are biodegradable, with the maximum degree of biodegradation observed after 90 days of testing at a temperature of 29°C and humidity of 75% for the sample containing 50 wt. %. The testing simulated a natural environment based on the assessment of the impact of resident biocenoses according to the ISO 846:2019 methodology. It should be noted that increasing the filler loading from 30 wt. % to 50 wt. % does not lead to a significant decrease in strength, while increasing biodegradability and reducing production costs.

The composite material obtained in this study can be used in products that do not require significant strength properties, while reducing the environmental impact.

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sciforum-089128: Polymeric Membranes in Water Treatment: Insights into Contaminant Removal Mechanisms and Advanced Processes

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The accelerated urbanization and industrialization have significantly heightened water contamination risks, posing severe threats to public health and ecological balance. Polymeric membranes stand at the forefront of addressing this challenge, revolutionizing water and wastewater treatment. These membranes adeptly remove a broad spectrum of contaminants, including organic compounds and heavy metals, thereby playing a crucial role in mitigating environmental pollution. This research delves into the sophisticated mechanisms of polymeric membranes in filtering out pollutants, with a spotlight on the enhancements brought about by nanotechnology. This includes a detailed examination of their inherent antibacterial properties, showcasing their innovative design and potential for extensive application. The study further investigates advanced techniques like electrochemical processes and membrane distillation, particularly focusing on desalination. These methods are central to the advancement of water purification, emphasizing efficiency and environmental sustainability. However, challenges such as membrane fouling pose significant hurdles, necessitating ongoing research into surface modifications and antifouling strategies. This paper offers a comparative analysis of various membrane technologies, highlighting their manufacturing complexities and efficiency benchmarks. In summation, the paper underscores the importance of continuous innovation in membrane technology, aiming to develop sustainable and effective water treatment solutions. By bridging the gap between basic science and technological advancements, this review aims to guide practitioners and researchers towards a future where clean water is universally accessible, ensuring the preservation of our ecosystems.



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sciforum-107823: Polyvinyl chloride-based polymeric nanocomposites for X-ray shielding

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Different materials are used as barriers to protect patients and medical staff in hospital radiological areas. A suitable shielding material needs to have a high atomic number (high Z) to protect against X-ray or gamma radiation, such as lead (Pb), barium (Ba), and bismuth (Bi). However, traditional shielding materials have cost, weight, and toxicity limitations. Therefore, there is a need for alternative materials for radiation shielding, one of which could be polymeric matrix nanocomposites. These materials have important properties such as elasticity, biocompatibility, low cost, and lightness, making them good candidates for attenuating different types of radiation. This study focuses on synthesizing different oxides and their use in developing polyvinyl chloride (PVC)-based polymeric nanocomposites. The structural and morphological properties of oxides and nanocomposites were studied by X-ray diffraction (XRD) and scanning electron microscopy (SEM). The X-ray shielding property for the radiodiagnostic energy range of 50 to 129 kV was measured by mass attenuation coefficient (μ_m), half-value layer (HVL), and tenth-value layers (TVL). The flexible nanocomposites were cross-linked with ionizing radiation treatments to enhance toughness and further analyzed for their cytotoxic properties. This analysis involved exposing the nanocomposites to 1132sk fibroblast cells and measuring their viability, providing insight into the safety of these materials for medical applications.



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sciforum-103471: Properties of Colored Phosphate Coatings for Corrosion Protection of Steel

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Phosphate coatings obtained from solutions based on the drug containing $\text{Mn}(\text{H}_2\text{PO}_4)_2 \cdot 2\text{H}_2\text{O}$ (proportion of phosphoric acid, in terms of P_2O_5 46-52 % ; mass fraction of manganese not less than 14 %), used to protect steel products from corrosion. Phosphating solutions are widely used to produce protective films at low temperatures. To obtain colored coatings, it is proposed to introduce the dyes procyon olive green and methylene blue in the amount of 8 g/L into phosphating solutions. Colored phosphate films unevenly cover the surface of steel samples. The protective and physical and mechanical properties (thickness, heat resistance, wear resistance, breakdown voltage value) of colored phosphate coatings obtained on steel by the cold method are studied. The protective properties of phosphate coatings strongly depend on their thickness and the nature of the crystal structure, since the thickness and structure determine the porosity of the coatings, and, consequently, the freedom of access of the aggressive medium to the metal surface. It was found that phosphate coatings can withstand short-term heating up to 100 °C, after which their protective ability is greatly reduced. Colored phosphate films produced on steel by the cold method have low values of the coefficient of friction, but this disadvantage can be eliminated by impregnation with lubricants. The breakdown voltage of colored phosphate coatings is about 200 V. Its electrical insulation properties can be improved by impregnation with oil and bakelite lacquers.



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sciforum-103800: Protein blowing agents based on hydrolysates of keratin-containing raw materials obtained by hydrolysis using sodium hydroxide and sodium sulfide

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The production of a cheap industrial protein foaming agent with optimal foaming properties is an important research area. Protein foams based on keratin hydrolysates, obtained by alkaline hydrolysis, have complex properties, The European Union has a number of important international agreements on this subject. The dependence of protein foaming properties on alkali hydrolysis conditions of keratin-containing raw materials allows to optimize the hydrolysis process with the result hydrolysate core component protein foamer. During the work, foaming agents were prepared on the basis of hydrolysates obtained using sodium hydroxide and sodium sulphide at different concentrations in hydrolysing solutions. The evaluation of the foam forming properties obtained in the experiment was carried out on such indicators of foam formation as foam multiplication, volume weight of foam, Foam stability during the regulated time and average rate of reduction of foam resistance.

The analysis of the results of the experiment showed that the quality of the protein foaming agent directly depends on the qualitative and quantitative composition of the hydrolyzing solution when producing a keratin-containing hydrolysate. From the blowing agents obtained in the experiment only some of them corresponded to the established ones and were characterized by high foam resistance in the range of 1.5 hours, which made it possible to select optimal compositions of hydrolyzing solutions for obtaining a blowing agent based on keratin-containing raw materials.



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sciforum-095296: Quest for piezoresistive strain sensors based on polymer nanocomposites for human motion monitoring

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sciforum-103874: Rationalizing the Physical Mechanisms behind the Amplified Spontaneous Emission Signatures in CsPbBr₃ Nanocrystal Films

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Thanks to their optical and electronic properties, lead halide perovskites have become prominent materials in optoelectronics. CsPbBr₃ nanocrystals (NCs) stand out as excellent candidates for implementing lasers due to their excellent photoluminescence quantum yields and their facile and low-cost production. Elucidating their stimulated emission mechanisms is fundamental in addressing their possible limitations and to achieve more efficient perovskite lasers, specially continuous wave or electrically excited ones. Two questions remain open: why the Amplified Spontaneous Emission (ASE) band is shifted from the fluorescence one, and why the former seems to coexist with the latter. These characteristics have led to a debate about which is the mechanism behind the ASE band shift. Some reports claim that the fluorescence comes from single excitons, while the ASE has a biexcitonic origin. Others defend that both fluorescence and ASE are generated by localized single excitons, and the shift owes to reabsorption.

In this communication, we address these questions through experimental ASE measurements, combined with numerical simulations, and the use of a novel analytical expression to retrieve the optical gain from these experiments [1]. We show that the ASE behaviour in CsPbBr₃ NCs thin films stems from four processes: reabsorption due to a large overlap between the absorption and fluorescence spectra, a strong contribution of excited state absorption at the fluorescence window, the excitation of differently polarized waveguide modes, and the coexistence of short- and long-lived localized single excitons. The results in this work establish guidelines with which to analyse the optical gain in perovskite samples, which can help in rationalizing the ASE signatures of both CsPbBr₃ NCs and perovskites in general, and which provide insightful information on research avenues to increase the efficiency of perovskite light-emitting devices.

Reference:

[1] S. Milanese, M. L. De Giorgi, M. Anni, M. Bodnarchuk, and L. Cerdán, Adv. Opt. Mater., 2401078 (2024)



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sciforum-107752: Recent advancements in bismuth complexes: Computational studies and biological applications

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Bismuth and its compounds are generally recognized for their biological safety and non-toxicity, making them highly valuable for large-scale synthesis of various bismuth-based complexes for their use in diverse biological applications. Bismuth complexes have shown promising antiviral, antifungal, antibacterial, antileishmanial, and anticancer properties. Notably, bismuth drugs are among the few antimicrobial agents that have not developed drug resistance and have a synergistic effect with antibiotics. Studies have explored that the biological activity of bismuth-containing compounds is closely related to the type of ligand and the geometry of the complex, emphasizing the importance of these factors in drug development. The biological activities of the resulting bismuth complexes are often influenced by the properties and positions of the substituted groups on ligand, indicating that even slight modifications can have profound effects on their efficacy. Computational studies provide a detailed insight for understanding the structure, stability, and reactivity of compounds, which can be difficult to achieve only through experimental methods. By utilizing computational methods like DFT and molecular docking, we can predict how ligands will interact with different drug targets. This approach makes it easier to design and develop more effective compounds for various applications. In this study, we present several factors that can influence the optimization of geometry, vibrational frequencies, HOMO and LUMO energies, quantum chemical parameters, as well as biological activities for the ligand and its bismuth complexes.



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sciforum-104306: Recent Development and Future Aspects of Metal–Organic Frameworks (MOFs) as Adsorbents

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Metal–Organic Frameworks (MOFs) have garnered significant interest in the field of advanced adsorbent materials due to their exceptional surface areas, customizable pore sizes, and diverse chemical functionalities. Recent advancements in MOF research have focused on enhancing their adsorption capabilities, selectivity, and robustness, making them highly effective for applications in gas storage, environmental remediation, and related areas. This paper explores the latest progress in the synthesis, alteration, and application of MOFs as adsorbents, including advancements in high-pressure gas storage, the selective separation of gases, and the removal of heavy metals and organic pollutants from water. Improvements in MOF production, incorporating environmentally friendly techniques and scalable manufacturing processes, have increased their feasibility and reduced their environmental impact. Advancements in functionalization strategies, such as post-synthetic modifications and the incorporation of functional groups, have enhanced the selectivity and adsorption capacity of MOFs for specific adsorbates such as CO₂, CH₄, and various contaminants. This study also examines the integration of green chemistry principles, the scalability of MOF production, and the use of advanced analytical techniques like real-time analysis and computational simulations. Furthermore, this paper highlights future prospects in the field, including targeted adsorption applications in healthcare and energy storage, as well as strategies to improve the sustainability and recyclability of MOF-based adsorbents. The development of water-resistant and acid/base-tolerant MOFs, along with the creation of hybrid composite materials, presents promising avenues for expanding the use of MOFs in various industrial and environmental settings. The combination of advanced characterization techniques and computational modeling will further drive the design of next-generation MOFs with tailored properties for a wide range of industrial and environmental uses.



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sciforum-105838: Removal of Chromium (VI) From Hydrometallurgical Effluents Using Moringa Waste: Isotherm, Kinetics and Thermodynamic Studies

Sharon Makgoga *, Musamba Banza and Tumisang Seodigeng

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Heavy metal ions are harmful to aquatic life, people, and the environment, and they have been a significant source of concern for researchers for a long time. They are a public health concern since they do not biodegrade as organic contaminants do in industrial effluents. This study uses moringa waste as a bio-sorbent to remove Cr (VI) from hydrometallurgical effluents. Cr (VI) is more harmful because of its high mobility in the environment and capacity to cause cancer in organisms. Moringa waste was pyrolyzed and modified with phosphoric acid to develop a bio-sorbent. FTIR and SEM were used to determine the surface functional groups and examine the bio-sorbent's morphology and microstructure. FTIR examination revealed the moringa waste structure's stability and aromaticity, confirmed by peaks around 1600 cm^{-1} . Because aromatic rings contribute to a large surface area and porosity and are stable, they are important for adsorption applications. At 75 minutes of contact time with 6 pH and a 1.5g adsorbent dosage at $55\text{ }^{\circ}\text{C}$, the removal percentage was found to be 68%. Adsorption data indicated a good fit to the Langmuir isotherm model, indicating that chromium VI was covered in a monolayer on the surface of the moringa waste. It could be that the adsorption rate is affected by the amount available of sites on the bio-sorbent, as the pseudo-second-order model indicated the kinetics that followed. The thermodynamic study showed that the process is endothermic and spontaneous, hence making the application of moringa waste in wastewater treatment viable.



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sciforum-104379: Repercussions On The Shear Force Of An Internal Beam–Column Connection From Two Symmetrical Uniformly Distributed Loads At Different Positions On The Beam

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A basic element in frame construction is the beam–column joint. Despite numerous studies, there is still no uniform procedure for designing shear force in different countries. We are still witnessing serious problems and even the destruction of buildings under seismic effects caused by failures in the frame beam–column connection. Over the past six decades, a huge number of experimental studies have been carried out on frame assemblies, where various parameters and their compatibility under cyclic impacts have been tracked. What continues to remain incompletely understood is the magnitude and distribution of the forces passing through the joint. The creation of a new mathematical model of the beam and column that transmit their forces in the frame joint contributes significantly to clarifying the flow of forces. For this purpose, the full dimensions of the beam, as well as its material properties, are taken into account. All research was performed for a stage before the opening of a crack and after its appearance and growth on the face of the column separating it from the beam. In the present paper, the loading of two transverse, uniformly distributed loads, remaining symmetrical on the beam, is considered. The position of the loads for which there is an extremum of the forces contributing to the shear force is investigated. Numerical results are demonstrated for the influence on the magnitudes of the support reactions from different concrete strengths of the beam. The obtained results are compared with those specified in Eurocode for shear force design. It was established that at the appearance of the crack, the shear force determined with the proposed new model exceeds the magnitude of the force calculated by Eurocode.



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sciforum-105857: Response Surface Approach For Recovery And Optimization Of Copper (II) From Polluted Soil

Tshepiso Khumalo *, Musamba Banza and Tumisang Seodigeng

Vaal University of Technology, South Africa

Copper (II) extraction from polluted soil is crucial for environmental remediation. This study employed the Response Surface Method (RSM) to optimize the recovery of Copper (II) from contaminated soil. The effects of pH, stirring rate and ratio of solid to liquid and concentration of sulphuric acid on Copper (II) recovery from the contaminated soil were investigated. A quadratic model was developed to predict the recovery efficiency, and the optimal conditions were identified. Results showed that the maximum Copper (II) recovery of 98% was achieved, and it was found that the ideal values for the solid-to-liquid ratio, pH, sulphuric acid concentration, and stirring speed were 6.5 g/100 mL, 300 rpm, and 0.25 mol/L, respectively. The elemental analysis by XRF showed that the contaminated soil is composed mainly of 10.5% Al₂O₃, 54.2 SiO₂, 1.93 P₂O₅, 2.90 CaO, 2.14 TiO₂, 23.5 Fe₂O₃, 0.26 ZrO₂ and 3.11% CuO. Moreover, FTIR revealed the presence of Si-O-(Si) and Si-O-(Al) vibrations. The CCD model accurately predicted the recovery efficiency, with an R² value of 0.98. This study demonstrates the effectiveness of Central composite design in optimizing Copper (II) recovery from contaminated soil, providing a valuable approach for soil remediation and sustainable management. According to the results of these experiments, the leaching rate rose as the pH, stirring speed, acid concentration, and solid-to-liquid ratio decreased.



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sciforum-102135: SEM-Tilting for the Imaging of Two-Dimensional Nanomaterials

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Two-dimensional (2D) nanostructures can be both single-atomic layers (e.g., graphene, graphite oxide, reduced graphite oxide) and lamellas made of a few atomic layers (e.g., Molybdenum disulphide, Tungsten disulphide, gold nanoplatelets). The small thickness of 2D nanostructures, frequently of only a few angstroms, is needed in order to allow for the arising of anomalous physical properties in the solid phase as a consequence of quantum-confinement effects, prevalence of surface on bulk atoms, high surface free-energy content, etc. Owing to the strict correlation existing between structure and properties in nanomaterials, their morphological characterization represents the first essential information that is required. Electron microscopy techniques (SEM and TEM) are commonly used as approaches for investigating the structure of this very tiny matter form. However, the observation of 2D nanostructures by SEM needs suitable expedients to achieve highly informative images. Indeed, the extremely thin thickness of a single-layer nanostructure makes really challenging the microscopical characterization. Here, a special approach, based on specimen tilting from the 90° sample positioning, has been used to allow for the imaging of single 2D layers of graphene and MoS₂ and WS₂. Usually, the standard operation of sample tilting from the 0° positioning is unable to provide images with enough contrast. Sample morphology is clearly visualized by using this tilting approach and a number of morphological features (e.g., presence of ripples in the layer, edge structure and defects, holes, etc.) appears in the electronic micrograph. In order to evidence the efficacy of the proposed method, a comparison with the classical top view SEM observation is also provided for these selected 2D nanostructures.



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sciforum-106774: Silver Nanoparticles as a Breakthrough Therapy for Irritable Bowel Syndrome

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The urgent need to address new health issues and enhance the effectiveness of treatment for a wide range of illnesses motivates the search for novel therapeutic agents as a current task in medicinal chemistry. Irritable bowel syndrome (IBS) is a multifactorial disorder characterized by altered intestinal motility, visceral hypersensitivity, dysfunction of the gut-brain axis. The nanoparticle system is one of the best ways to provide medication in a controlled manner. This study aims to develop drug-loaded silver nanoparticles (AgNPs) with mebeverine to improve the treatment of IBS.

A green, glucose-assisted method for the rapid synthesis and stabilization of AgNPs as a drug-delivery system is presented. The synthesized AgNPs were characterized by their UV-Vis spectra, TEM, zeta potential, and drug release. To assess their pharmacological potential, a series of ex vivo and in vitro experiments were conducted.

The mebeverine-based AgNPs were designed to relax smooth muscle tissue, providing a novel treatment option for IBS patients. Biological experiments showed that drug-loaded AgNPs have better spasmolytic activity compared to mebeverine.

In *in vitro* and *ex vivo* experimental models of inflammation, the nanoparticles significantly inhibited the production of pro-inflammatory cytokines and other mediators of inflammation. This activity suggests that synthesized AgNPs could be effective in treating chronic inflammatory conditions such as IBS, rheumatoid arthritis, and other autoimmune disorders.

Based on the results, synthesized AgNPs might be a promising medication delivery system and a useful treatment option for IBS. Our research into the synthesis and biological evaluation of drug-loaded AgNPs reveals their potential as novel therapeutic agents, capable of modulating multiple inflammation pathways. The promising results achieved so far underscore the importance of continued exploration and development in this area.

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sciforum-107103: Simulation of the Optoelectronic Section of an Interferometric Fiber-Optic Gyroscope

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This paper presents a comprehensive stochastic model of the optoelectronic and photonic components of an interferometric fiber-optic gyroscope (IFOG), which plays a critical role in inertial navigation systems, especially for aerospace applications. The model accounts for various noise sources and disturbances, including power drift, the Kerr effect, and electronic noise generated by the photodetector and transimpedance amplifier. These elements are crucial for accurately simulating the real-world behavior of the IFOG system. Experimental validation was carried out using a prototype integrated from commercially available components, with a 500-meter fiber coil as the sensing element.

The experimental results showed strong agreement with the numerically simulated waveforms, demonstrating the model's ability to predict the IFOG's behavior under different operating conditions. The noise sources were modeled using Gaussian and Poisson distributions, capturing the stochastic nature of the disturbances. The Kerr effect, in particular, was identified as a significant influence but was mitigated by employing a broadband light source.

This validated model offers a valuable tool for the development of more advanced IFOG systems, including those that integrate readout electronics. It enables better interpretation of experimental data and paves the way for future improvements in precision, making it suitable for applications requiring highly accurate angular velocity measurements.



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sciforum-104251: Solvothermal Synthesis of Nanomagnetite-Coated Biochar for Efficient Arsenic Adsorption

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Arsenic contamination in water poses a significant health risk, making effective removal methods essential. Low-cost biosorbents and easy magnetic separation are desirable for this purpose. While various magnetic adsorbents have been developed using the coprecipitation method, challenges remain due to arsenic's toxicity and WHO limitations. This study introduces nanomagnetite-coated biochar derived from pecan nutshells as an efficient arsenic adsorbent, utilizing a solvothermal method. This controlled synthesis enables the precise growth of magnetite crystals on biochar, resulting in uniform particle size and morphology. The process occurs in Teflon-lined stainless-steel autoclaves at 200°C, with reaction times ranging from 6 to 12 hours. Iron chloride acts as the iron ion precursor, and ethylene glycol serves as the solvothermal medium. Pecan nutshell biochar particles, sized 0.10-0.18 mm and 0.18-0.38 mm, are produced via pyrolysis at 700°C for 1 h under nitrogen. Following solvothermal treatment, the resulting particles are magnetically separated from the solution. Characterization via XRD, SEM, TEM, and FTIR confirms the formation of homogeneously magnetite-coated biochar particles. This method yields homogeneous nucleation and the growth of nanometric magnetite crystals on the surface of biochar particles, leading to a narrow size distribution and consistent morphology without other crystalline phases, enabling high arsenic adsorption rates (97.30–98.76%) from water. Notably, biochar with varied particle sizes synthesized at a short reaction time (200°C, 6 h) demonstrates the highest arsenic removal efficiency (98.76%) and adsorption capacity (7.974 mg/g), comparable to magnetite nanoparticles. The development of nanomagnetite-coated biochar derived from pecan nutshells showcases significant innovative potential in addressing arsenic contamination. This is due to several factors: the sustainable use of biochar from pecan nutshells, nanomagnetite coating for efficient arsenic removal, the controlled synthesis process, high adsorption capacity, low-cost biosorbents, ease of magnetic separation, and versatility for removing other contaminants.



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sciforum-103965: Structural analysis of zinc oxide nanostructures and study of the influence of the hydrothermal method on nanowire preparation

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The researchers paid increasingly more attention to the creation of materials which would be cheap, have good sensitivity and be, environmentally benign. Zinc oxide (ZnO) has multiple applications due to its unique physical, chemical, and optoelectronic properties. This makes it ideal for usage on solar cells, light-emitting diodes, and gas sensors. There is increasing interest in ZnO nanostructures especially the one-dimensional forms since they can easily and rapidly respond to external influences of temperature and humidity. High-quality ZnO nanowires are of great scientific interest, however, there is no universal method to produce them in a simple and economical way with all important parameters accurately specified.

The objective of this study to produce more oriented and purer one-dimensional ZnO nanostructures using a simple and fast method, in this case the synthesis of ZnO Nanowires. Synthesis of ZnO nanowires was accomplished in a two-step process. The initial step involved applying a seed layer onto the surface of the substrate that was aimed to anchor ZnO molecules. The molecular structures were observed using Atomic Force Microscopy (AFM). Nanowires' second step included growing the structures with the use of a hydrothermal method, where the size of the synthesized ZnO nanowires was 100-150 nm.

The findings show that this approach leads to the successful fabrication of ZnO nanowires with great uniformity, large surface area and well-defined geometric shapes. The nanowires are also shown to possess good structural as well as chemical integrity, establishing their application in the domains of optoelectronic devices and gas sensors. In addition, the hydrothermal method is simple and reliable, and ZnO nanowires appear to be of good quality; therefore, this method is low-cost and easily up-scaled with great potential for industrial applications.



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sciforum-102112: Structural Insights into Molybdenum Schiff Base Complexes: Impedance Spectroscopy and Coordination Behavior

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Molybdenum, a transition metal, is well regarded for its diverse applications due to its ability to adopt multiple oxidation states and form various complexes. Molybdenum Schiff base complexes, which are created by coordinating molybdenum with Schiff base ligands, resulting from the condensation of primary amines and carbonyl compounds, demonstrate unique and valuable properties [1]. These complexes are extensively documented for their significant roles across various fields. Biologically, molybdenum is crucial as a component of several key enzymes [2]. Industrially, these complexes are essential in processes like petroleum refining and chemical manufacturing. They are especially notable for their catalytic activity in oxidation, hydrogenation, and olefin metathesis reactions, contributing to various chemical synthesis processes [1]. In material science, they are instrumental in developing advanced materials with distinctive electronic and structural properties, which are beneficial for enhancing energy conversion and environmental remediation [3,4].

In the current study, a Schiff base ligand was synthesized via the condensation of salicylaldehyde and oxalylhydrazide and then coordinated to the $[\text{MoO}_2]^{2+}$ core. This synthesis, performed in methanol, resulted in the formation of the complex $[\text{Mo}_2\text{O}_4(\text{L})(\text{MeOH})_2] \cdot 2 \text{H}_2\text{O}$. The complex was exposed to vapors of water, methanol, ethanol, and propanol, leading to the desolvatation and decoordination of solvent molecules and the coordination of vapor molecules. Characterization was conducted using IR-ATR spectroscopy and thermogravimetric analysis (TG), with molecular and crystal structures determined through X-ray diffraction. Impedance spectroscopy (IS) confirmed structural changes. Additionally, these complexes were tested as catalysts for the oxidation of benzyl alcohol, demonstrating their potential in catalytic applications.

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sciforum-103864: structural, morphological, optical and dielectric examination of magnesium chromite (MgCr₂O₄) spinel oxide

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The citrate–nitrate method was employed to synthesize the magnesium chromite (MgCr₂O₄) spinel, followed by calcination at 700°C for 3 hours. The synthesized compound was analyzed using techniques including powder XRD, SEM-EDAX, FTIR, UV-DRS and LCR Meter. The structural analysis was carried out using X-ray diffraction, which revealed the formation of the cubic crystal symmetry of the sample with the corresponding Fd-3 m space group. The average particle size of the sample was calculated around 13.26 nm. Further, the diffraction pattern was refined by Fullprof Software which validated the single phase cubic structure formation. Using tetrahedral and octahedral positions, the lattice vibrations of the associated chemical bonds were identified using Fourier transform infrared (FTIR) spectroscopy. SEM (Scanning electron microscopy) micrographs showed the spherical nature of the particles and the constituent particles were between 10 and 40 nm in size. The optical bandgap value was evaluated using the Tauc's plot. Pellets of the powdered sample were prepared for determining the dielectric aspects including dielectric constant (ϵ'), tangent loss ($\tan\delta$) and ac conductivity (σ_{ac}) in the frequency range of 100 Hz–4 MHz, at room temperature. The charge transport mechanism was explored from the complex impedance spectroscopy study. The obtained results indicate that magnesium chromite may be a potential candidate in the fabrication of sensors, micro-electronic devices, and other electronic equipment.



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sciforum-103876: Structural, optical, and dielectric properties of lead-free double perovskite $\text{La}_2\text{FeMnO}_6$ for possible application in storage devices.

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Double perovskite oxides A_2BBO_6 have attracted significant attention because of its eccentric multiferroic properties. Among such materials, double perovskites containing rare earth metals are widely studied due to their interesting physical, optical and chemical properties. Presently, the lead-free double perovskite $\text{La}_2\text{FeMnO}_6$ was synthesized using citrate combustion method. The orthorhombic phase formation of $\text{La}_2\text{FeMnO}_6$ with $Pbnm$ space group was confirmed using powder X-ray diffraction (XRD) technique. The grain size was calculated to be 47.5 nm computed using Debye-Scherrer formula. The characteristics of double perovskites was investigated using Fourier Transform Infrared Spectroscopy (FT-IR) technique. The band gap energy properties were studied using Ultra-violet Visible Diffusive Reflectance Spectroscopy (UV-DRS). The calculated band gap of $\text{La}_2\text{FeMnO}_6$ was about 1.53 eV. The calculated experimental band gap value of $\text{La}_2\text{FeMnO}_6$ suggests that it could be a better candidate for light harvesting applications and other energy storage devices. The dielectric properties of $\text{La}_2\text{FeMnO}_6$ was studied using Dielectric Analyser in the range of 100 Hz – 1 MHz at room temperature. From the observed results, impedance, dielectric and modulus studies support the existence of a non-Debye type relaxation peak. The material's polarization mechanism was explained using Koop's theory and the Maxwell-Wagner interfacial polarization model highlighting the presence of relaxation behaviour in $\text{La}_2\text{FeMnO}_6$. These findings render that $\text{La}_2\text{FeMnO}_6$ a fascinating material for scientific research as well as for practical uses.



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sciforum-103855: Study of factors affecting the process of complexation of nimesulide - γ -cyclodextrin

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Complexation helps to increase the solubility as well as improve other qualities of drug substances. To study this process and subsequent preparation of compounds, we chose γ -cyclodextrin and nimesulide, a widely used drug for the treatment of acute and chronic pain.

To obtain the inclusion complexes we used a combination of methods: co-evaporation, coprecipitation. Varying some parameters of complexation (pH of the reaction mixture (pH = 3, pH = 7), presence and volume of additional solvent (acetone)), several samples of putative complexes were obtained as a result of the experiment. Qualitative analysis was carried out by FTIR spectroscopy on a Fourier spectrometer ('FMS 1201', Russia). The obtained IR spectra suggest that some functional groups of nimesulide (S=O, R-NO₂) interacting with functional groups of γ -CD lead to a shift of the corresponding absorption bands. The formation of the complex was further confirmed by differential scanning calorimetry. The change in the enthalpy of phase transition with respect to the pure substance indirectly testify to the formation of the complex compound. The quantitative composition of inclusion complexes was studied by calibration plot method on a Shimadzu UV-1800 UV spectrometer. Quantitative analysis showed that the most complete incorporation of nimesulide into the cavity of γ -CD is achieved with the addition of an additional solvent - acetone and the observance of an acidic environment in the reaction mixture. Change of other parameters (temperature, time of mixing the reaction mixture) did not have a noticeable effect on the process. Toxycological activity of the obtained compounds was not studied. Based on the confirmed safety of nimesulide and γ -CD, we assume that the complexes are also non-toxic.

Thus, knowing the factors that have a predominant influence on the process of complexation, it is possible to obtain inclusion complexes of cyclodextrins with various drugs, creating new modified forms.



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sciforum-107669: Study Of Ldh Growth On Magnesium Biodegradable Alloy: The Effect Of Microstructural Changes Due To Ecap Processing

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Introduction

Magnesium alloys are under intensive investigation because of their possible use in the biomedical field thanks to their good biocompatibility and mechanical properties which are similar to human bones and biodegradation. For instance, they have been used to produce a biodegradable bone fixator that does not require a second surgery. The main issue is the high corrosion rate in respect to tissue remodelling. The principal strategies to overcome this problem are: tailoring the alloy composition, inducing microstructural changes, employing surface treatments and coatings.

Several authors observed that the Layered Double Hydroxides (LDH) coatings improve the biocorrosion behaviour of the Mg-alloys and also permit drug delivery.

The aim of present work is to investigate how the microstructural changes induced by Equal Channel Angular Pressing (ECAP) affect the LDH films growth on the AZ31 surface.

Methods

The commercial AZ31 alloy was processed by 0, 1, 2 and 4 ECAP passes.

LDH structures were grown on AZ31 samples using the co-precipitation technique. The nutrient solution was: $\text{Zn}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ (5 mM) and urea (15 mM) in 150 mL of distilled water. After preliminary cleaning the samples were immersed in the nutrient solutions, and kept there for 12 h at 90 °C. Finally, they were cooled in the nutrient solution, extracted from the reactor, rinsed in distilled water and ethanol and air-dried.

The microstructural characterisation of the samples was performed by LM, XRD, SEM, EBSD technique.

Results

The LDH film was successfully grown on the surface of all the samples. The LDH crystals mostly present a dendritical shape. It was observed that the LDH film was more uniform after 1 ECAP pass with an average crystal size of 200 nm.

Conclusions

The microstructural evolution induced by ECAP favours a more homogeneous LDH growth due to the best trade-off between texture and presence of nucleation sites (twins, dislocations, GB etc.).



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sciforum-103236: Study of the dependence of the Amplified Spontaneous Emission (ASE) and sensing properties on the capping ligand in CsPbBr₃ nanocrystal thin films

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Over the last decade, fully inorganic lead halide perovskite nanocrystals (NCs) have received a lot of attention as active materials for photonic and optoelectronic devices. Despite their high sensitivity to ambient conditions typically inducing irreversible degradation mechanisms, some experiments have evidenced reversible environmental effects, clearing the way for their application as active materials for resistive and optical sensors. In particular, the sensitivity of CsPbBr₃ NC thin films to ambient air was demonstrated, noticeable as reversible modulation of the PL and ASE intensities, which is a sign of physical perovskite–air interactions, ruling out degradation effects. The air's humidity determines the solvation of the surface and the hydrophilic ligand's head group, resulting in the formation of surface trap states that modulate the emitted PL intensity; in a vacuum, water molecules can be desorbed, restoring pristine conditions. Moreover, the stimulated emission demonstrated a higher sensitivity (up to 6.5 times higher) to ambient air compared to that of the spontaneous emission, opening the way for the realization of ASE-based optical gas sensors with perovskites.

Since the PL and stability properties of the NCs strongly depend on their surface chemistry and, in particular, on the surfactant molecules used to passivate the surface defects, we performed a systematic investigation of the effects of the NC capping ligands on the ASE and sensing properties of CsPbBr₃ thin films. In particular, our experiments were performed on four different samples, representatives of three generations of capping ligands: oleic acid and oleylamine (OAc/OAm) as the first, didodecyldimethylammonium-bromide (DDAB) as the second, and 3-(N,N-dimethyloctadecylammonio)propanesulfonate (ASC18) and lecithin as the third. The lowest ASE threshold was reported for the lecithin-capped NC sample, together with the strongest sensitivity to air. On the other hand, the OA-capped sample, which showed one of the highest ASE thresholds and the lowest sensitivity to air, was demonstrated to be highly stable under strong laser irradiation.



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sciforum-107768: Study Of The Solubility Of The Calcium Chlorate–Monochloroacetic Acid–Triethanolamine–Water System

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The development of sustainable and environmentally friendly defoliants has become a critical area of research due to the increasing demand for eco-conscious agricultural practices. Traditional chemical defoliants used in cotton harvesting have raised concerns over their environmental toxicity and adverse health effects. In this context, the calcium chlorate–monochloroacetic acid–triethanolamine–water system has emerged as a promising alternative, offering a less toxic and biodegradable solution. However, the solubility and crystallization behavior of this system, particularly under varying temperature conditions, remain poorly understood, limiting its large-scale application in the field. This study investigates the solubility diagrams and crystallization phases of the calcium chlorate–monochloroacetic acid–triethanolamine–water system across temperatures ranging from -52°C to 47°C. The goal is to optimize the defoliant formulation by identifying key phase boundaries and new crystalline phases. The study identified several crystalline phases, including $\text{Ca}(\text{ClO}_3)_2 \cdot 6\text{H}_2\text{O}$, $\text{Ca}(\text{ClO}_3)_2 \cdot 4\text{H}_2\text{O}$, and $\text{Ca}(\text{ClO}_3)_2 \cdot 2\text{H}_2\text{O}$, as well as a novel compound, $\text{ClCH}_2\text{COOH} \cdot \text{Ca}(\text{ClO}_3)_2 \cdot (\text{C}_2\text{H}_4\text{OH})_3\text{N}$, which was confirmed through infrared spectroscopy (IR) and scanning electron microscopy (SEM) analysis. These findings provide valuable insights into the phase behavior of this system, potentially leading to the production of more efficient and sustainable defoliants for the cotton industry. Future research should focus on scaling up these results for field applications and exploring additional environmentally friendly compounds to further enhance agricultural sustainability.



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sciforum-107506: Syntheses And Application Of Triphenylamine Dyes As Efficient Sensitizers In Dye-Sensitized Solar Cells

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Five new organic sensitizers of type Donor- π -Acceptor (D- π -A) were designed and synthesized to investigate the effect of anchoring mode and conjugation length towards TiO₂ film which leads to influence the efficiency of the fabricated dye sensitized solar cells. These dyes were synthesized based on the triphenylamine as electron donor, a series aromatic amine as π -conjugated spacers and anchoring/acceptor groups. The optical absorption of sensitizers shows red shift as well as high molar extinction co-efficient with extension of the π -conjugation. The DSSC based on AD series show power conversion efficiency (PCE = η) ranging from 1.53 – 6.89 % under simulated AM 1.5 G. DSSCs based on AD4 and AD5 produce maximum IPCE of 74.8% and 71.9%, respectively while those based on AD1 and AD5 in particular produce maximum IPCE below 50%. This variation is due to an increase in conjugation and the number of anchoring groups. The short circuit current (J_{sc}), open circuit voltage (V_{oc}), field factor (FF), and quantum efficiency (η) also increased with increase in IPCE values. High J_{sc} values signified high electron collecting efficiencies, which in turn denote faster electron diffusion rates. Additionally, a rise in the value of the V_{oc} might raise the life time of the DSSC. The PCE (η) values of AD dyes especially those of AD4 and AD5 (η = 6.86% and 6.89% respectively) were seen to be higher than those of some triphenylamine based DSSCs (SD series with elongated thiophen units) whose PCE values ranged from 1.91% to 3.92%.



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sciforum-103511: Synthesis and characterization of chitosan/PVA/starch/ZnO/camphor and chitosan/PVA/carboxymethyl cellulose/ZnO/camphor patches for potential hemostatic application

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Hemostasis is the first stage of the wound healing process activated upon injury, that results in the control of bleeding and the formation of a protective barrier. The mechanism of hemostasis includes 1) vasoconstriction, 2) the formation of a platelet plug, and 3) blood coagulation. During the hemostasis process, wound infection can exist, inhibiting epidermal maturation, and may cause bacteremia, sepsis, and multiple-organ dysfunction syndrome. In cases of severe wounds, the use of hemostatic products with antimicrobial properties is necessary to compensate for the compromised first step of wound closure. Chitosan (CS) is a naturally derived polymer that plays a leading role in the development of new hemostatic products. CS is a cationic polysaccharide with bactericidal properties; it is renewable, nontoxic, biodegradable, and hydrophilic with high reactivity, and promotes coagulation, flocculation, and biosorption. The hemostatic properties of chitosan are due to direct electrostatic interactions between negatively charged red blood cells and platelets and the positively charged CS. Researchers and pharmaceutical companies are focusing on the hemostatic properties of CS by formulating it into several hemostatic products. Ongoing research is focusing on advanced hemostatic CS-based materials with enhanced antimicrobial properties, good biocompatibility, rapid hemostatic ability, and low manufacturing cost. Hence, in this work, CS was combined with polyvinyl alcohol (PVA) and carboxymethyl cellulose or starch to prepare well-cross-linked patches with enhanced mechanical properties and blood sorption as well as immediate hemostatic properties. Additionally, ZnO and Camphor were added as natural antimicrobial agents to ensure a healthy environment, avoiding potential infections during hemostasis treatment. The successful synthesis of the fabricated CS-based patches was confirmed by FTIR, their crystallinity was researched by XRD, and water swelling was also investigated. Moreover, an investigation of the hemostatic capacity of the dressings was carried out via hemolysis and blood clotting time experiments.



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sciforum-103999: Synthesis and characterization of nanostructured α -MnO₂ and its composites with SnO₂ and TiO₂ for efficient gas sensing

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INTRODUCTION

Manganese dioxide exhibits polymorphism. Attributing to its unique framework, abundant oxygen species, catalytic nature, large surface area, nanostructured MnO₂ is considered a vital gas sensing material. This study focuses on the synthesis of α -MnO₂, its composites and their structural, optical, morphological analysis via X-ray diffraction, UV-Visible, FT-IR, FE-SEM respectively.

METHOD

α -MnO₂ is synthesized via a co-precipitate route. For this purpose 2M solution of KMnO₄ and 3M solution of Mn(NO₃)₂ are prepared separately in 20ml deionized water under vigorous stirring. KMnO₄ solution is added to Mn(NO₃)₂ followed by the drop wise addition of 4M solution of NaOH. The precipitate obtained is filtered, dried at 120°C overnight and annealed at 400°C for 4 hours to obtain the MnO₂ powder. Composites of α -MnO₂ is obtained via solid state reaction method wherein α -MnO₂ is grinded (1:1 ratio by weight) respectively with SnO₂ and TiO₂ using agate mortar and pestle followed by annealing them at 400°C for 2 hours.

RESULTS

The structural analysis reveals the formation of tetragonal α -MnO₂, SnO₂, TiO₂. The average crystallite size of α -MnO₂, α -MnO₂-TiO₂ and α -MnO₂-SnO₂ is 15.04nm, 24.25nm and 19.33nm respectively. The crystallinity increased from 81% in α -MnO₂ to 92.98% α -MnO₂-TiO₂ and 94.75% in α -MnO₂-SnO₂. The optical band gap of 5.05eV for α -MnO₂ decreased to 3.16eV and 3.4eV for α -MnO₂-TiO₂ and α -MnO₂-SnO₂ respectively. The morphology discloses the formation of nanorods of α -MnO₂, granular structure of SnO₂ and TiO₂. The gas sensing is due to adsorption of gas on the surface of thin film and depends on the crystallite size, morphology, porosity.

CONCLUSION

The gas sensing can be enhanced by the formation of nanocomposites with small crystallite size, increased crystallinity, reduced optical band gap, porous morphology and abundant oxygen species. The thin films fabricated using the nanocomposite can be used to detect analyte gas at room temperature.



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sciforum-103470: Synthesis and characterization of reduced graphene oxide from pomegranate peels, banana peels, cotton waste and corn leaves

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In this work, four different types of agricultural waste, specifically pomegranate peels, banana peels, cotton waste and corn leaves, as well as different combinations of the previous biomasses, were used in order to produce reduced graphene oxide (rGO). Reduced graphene is a one-atom-thick sheet of sp^2 -hybridized carbon atoms arranged in a honeycomb lattice form with a large surface area, high electrical conductivity, strong chemical stability and superior tensile strength. rGO was synthesized directly from agricultural waste via direct carbonization at 300°C in a muffled furnace under atmospheric conditions for 15 minutes in the presence of ferrocene as an oxidizing catalyst. Ferrocene is an orange-coloured organometallic compound which creates extensive structural changes in carbon materials, promoting the oxidation of porous carbon to graphene-like formations. The treated material, after cooling to room temperature, was collected in the form of a dark brown and black powder. These powders were then put through further study and analyses. The materials' morphology and structure were characterized via XRD, FT-IR, SEM and BET analyses. According to the above characterizations, rGO nanomaterials were successfully synthesized from different types of biomasses, each demonstrating the potential use of waste as raw feedstock for the production of useful materials with attractive properties and wide ranges of applications.

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sciforum-107146: Synthesis and structural characterisation of novel urethane-dimethacrylate monomers with two quaternary ammonium groups based on cycloaliphatic diisocyanates

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Introduction: The World Health Organization report from 2022 points to caries being a meaningful problem worldwide. Such a state results from poor oral hygiene, huge sugar consumption and the effect of oral bacterial metabolism. The treatment of caries is based on the removal of the affected tissue and filling the cavity with dental filling. The disadvantage of this solution is the lack of antibacterial activity of dental fillings, which may result in secondary caries. The materials used in dental fillings can be modified with compounds possessing quaternary ammonium groups to achieve microbiocidal properties. This research aims to synthesize novel dimethacrylate monomers possessing two quaternary ammonium groups. The novelty of this study was the use of two cycloaliphatic diisocyanates in the synthesis of these compounds—*isophorone diisocyanate (IPDI)* and *4,4'-methylenebis(cyclohexyl isocyanate) (CHMDI)*.

Methods: A three-step procedure was utilized to obtain the novel monomers:
I. Transesterification of MMA;
II. N-alkylation of semi-product with 1-bromododecane;
III. Addition of a second semi-product to diisocyanate.
The chemical structures of the obtained monomers were confirmed with ^1H and ^{13}C NMR and FTIR spectroscopy.

Results: The synthesis resulted in two novel monomers—QA12+IPDI and QA12+CHMDI—which are viscous, yellowish liquids. ^1H and ^{13}C NMR and FTIR spectroscopy confirmed the structures of the obtained monomers.

Conclusions: The spectroscopy methods confirmed the structures of our novel monomers. Future research will be focused on the characterization of these monomers' properties.



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sciforum-107591: Synthesis Of Herbicides Based On P-Chlorophenol: Study Of Polythermal Solubility Of System NaOH – Cl-C₆H₄OH – H₂O

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This study investigates the synthesis of herbicides based on p-chlorophenol (Cl-C₆H₄OH) and focuses on the polythermal solubility behavior of the NaOH – Cl-C₆H₄OH – H₂O system. Understanding the solubility and phase transitions within this system is essential for optimizing the synthesis of herbicides. Solubility measurements were performed over a temperature range of -54.3°C to 59.0°C. A polythermal solubility diagram was constructed, identifying crystallization fields of ice, NaOH, NaOH•3.5H₂O, NaOH•5H₂O, NaOH•7H₂O, Cl-C₆H₄OH, and Cl-C₆H₄ONa. The compound Cl-C₆H₄ONa was isolated from its predicted crystallization region and identified using chemical and physico-chemical analysis, including infrared (IR) spectroscopy and scanning electron microscopy (SEM). The solubility diagram revealed distinct crystallization fields for various hydrates of NaOH and p-chlorophenol derivatives. Despite the high solubility of the initial components, the system exhibited a slight salting-out effect on the Cl-C₆H₄OH compound. The structure of the isolated Cl-C₆H₄ONa was further characterized using IR and SEM analyses, confirming its composition and morphology. The study provides valuable insights into the polythermal solubility of the NaOH – Cl-C₆H₄OH – H₂O system and the conditions necessary for the efficient synthesis of herbicides. The identification of specific crystallization fields and the detailed analysis of the isolated compound enhance the understanding of the phase behavior, contributing to more effective herbicide production processes.



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sciforum-093405: Synthesis, characterization, and application of Iron copper phosphate nanoparticles

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Phosphate material have a wide range of applications in biological, and catalysis. It also showed fluorescence capacity, where lanthanide orthophosphate demonstrated a fluorescent properties during their internalization into human umbilical vein endothelial cell. In addition, it has been considered as ceramic materials with high magnetic and electrochemical properties [1].

Since the calcium phosphate nanoparticles utilization in biological, therapeutic, and bio-medicinal fields such as treatment of cancers, caries inhibition, researchers decrease; the researches increase the studies using other metals including phosphate materials. For example cobalt phosphate nanoparticles, which were modified by Nickel, and Zirconium and used as electro-catalyst for water treatment, dyes removal and treatment of cancers [2]. Considerable methods were used to synthesize phosphate material, such as precipitation, co-precipitation, impregnation, deposition, and hydrothermal route. This later can be lead to different shape and structure.

In this study, we prepared iron copper phosphate nanoparticles (FeCuP) using hydrothermal route. During preparation, several conditions were used modifying the urea amount. So, different structures were achieved. The material was characterized by SEM, EDX, UV-Vis and XRD. The material was used as catalyst for the synthesis of propargylamines and pyrroles. The nanoparticles catalyst was reused with high activity and stability.

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sciforum-104510: The chemical composition of clay soil analysis and potential health risks: an experimental study in Tshwane District, Gauteng Province.

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Geophagy is the deliberate ingestion of earthly materials such as chalk, kaolin, soil, clay, and sand amongst pregnant women and women of childbearing age in African countries such as South Africa. This study aimed to examine the chemical composition and potential health risks of clay soil consumed by women of childbearing age. An experimental study was conducted to examine the chemical composition of clay soils ingested by pregnant women and women of childbearing age in Tshwane District, Gauteng Province, South Africa. Thirty-nine clay soil samples were collected from study participants attending antenatal care services and family planning at public healthcare facilities of Tshwane District, Gauteng Province, and were subjected to biochemical analysis. The study detected 18 trace elements that were present in clay soil eaten by women of childbearing age of Tshwane in different concentrations. The practice of geophagy amongst women of childbearing age has been reported to be associated with detrimental health outcomes and risks such as iron deficiency anaemia, constipation, shortness of breath, maternal and childhood mortalities and morbidities, neurological and central nervous system disorder, death, appendicitis, cancers, teratogenic risks and ulcers. The practice of geophagy amongst women of childbearing age is toxic and should be discouraged and abolished.



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sciforum-103857: The development of a multifunctional high-swelling alginate silver nanocomposite for water decontamination

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Introduction

Sodium alginate nanocomposites containing metallic nanoparticles have found various biomedical and environmental applications. These materials are easy to prepare and sustainable. In recent years, such materials have been widely used for the adsorption/degradation of toxic substances such as organic dyes, pharmaceuticals, heavy metals, etc. In this project, we have developed reusable sodium alginate–poly sodium acrylate silver nanocomposites with a high swelling capacity for enhanced degradation of toxic organic materials.

Methodology

Polymer beads based on sodium alginate–poly sodium acrylate containing silver nanoparticles were synthesized by means of a combination of ionotropic crosslinking in calcium chloride solution and free-radical polymerization using ammonium persulfate. The beads were characterized using various advanced methods such as UV-Vis absorption spectroscopy, Fourier transform infra-red spectroscopy, and electron microscopy. The swelling capacity was evaluated using the gravimetric method. The antibacterial property was studied using the incubation method against three clinically important pathogens: *Escherichia coli*, *Staphylococcus aureus*, and *Pseudomonas aeruginosa*. The catalytic degradation of Congo red and 2-nitrophenol achieved by the beads was studied in the presence of sodium borohydride.

Preliminary results

The nanocomposite beads were spherical and porous and exhibited a high swelling capacity due to the presence of poly sodium acrylate. A strong plasmon resonance (SPR) peak at around 400 nm confirmed the presence of silver nanoparticles. The nanocomposites were effective against the growth of *E. coli* and *P. aeruginosa*. Almost 100% degradation of Congo red and 2-nitrophenol was achieved in about 30 min.

Conclusion and work in progress

The nanocomposite beads showed both antibacterial and catalytic properties, showing promise for detoxification of hospital wastewater in the future. The reusability of the material and the use of real-life samples are currently in progress.



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sciforum-107754: The impact of cytostatics on the toxicity of BSA-Stabilized gold nanoclusters

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Gold nanoparticles are promising candidates as vehicles for drug delivery systems and could be developed into effective anticancer treatments. Gold nanorods (GNRs) have suitable optical and thermal properties, which allows them to be used in techniques such as photothermal therapy and photoacoustic imaging.

GNRs with an absorbance peak near 650 nm were synthesized via a seed-mediated method and coated with cross-linked BSA as a stabilizer. New cancer treatment approaches involve the use of several cytostatics to target cancer cells. Therefore, in our work a mixture of cytostatics doxorubicin and dacarbazine were loaded onto the GNRs. The effectiveness of drug loading was determined using UV spectroscopy. TEM and dynamic light scattering were used to verify the structural integrity of the BSA-coated GNRs.

Cytocompatibility of bare and BSA-coated gold nanorods with different ratios of doxorubicin and dacarbazine was assessed by MTT assay, a common method to evaluate the biocompatibility of nanomaterials. 3D tumor spheroids were used to assess the drug gradient uptake and the effect of localized photothermia mediated by GNRs coated with cross-linked BSA alone or in combination with doxorubicin. The results of experiments using GNRs and doxorubicin on irradiated cells and on cells that were not irradiated showed significant differences.

The work was carried out with the financial support of the Ministry of Health of the Russian Federation 'Molecular design and creation of drugs based on conjugates of carbon nanostructures, vectors of targeted delivery and cytotoxic agents for inactivation of stem tumour cells and components of the tumour microenvironment', No. EGISU:1022040700957-7-3.2.21;3.1.3.

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sciforum-107640: The optimization of processes of electrochemical synthesis of ortho- and para-hydroxybenzoic acids in the presence of CO₂

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The electrochemical synthesis of ortho- and para-hydroxybenzoic acids (HBAs) using CO₂ presents a sustainable alternative to traditional methods. These acids, essential intermediates in the production of pharmaceuticals such as aspirin and in polymer manufacturing, are typically synthesized through energy-intensive processes. Given increasing concerns over carbon emissions, optimizing electrochemical approaches that incorporate CO₂ as a reactant is vital for improving both economic and environmental sustainability. This study focuses on optimizing the electrochemical synthesis of ortho- and para-HBAs in CO₂-saturated environments, aiming to enhance reaction efficiency, and selectivity, and reduce energy consumption. Cyclic voltammetry and constant potential electrolysis were employed, with various electrode materials tested to improve process efficiency. Results indicate that electrode material significantly influences both product selectivity and reaction efficiency. Platinum electrodes exhibited a 15% higher current efficiency and favored para-hydroxybenzoic acid, while carbon-based electrodes showed a 20% increased selectivity for ortho-hydroxybenzoic acid. Additionally, CO₂ improved the electrochemical environment by stabilizing radical intermediates and reducing overpotential by 30%. These findings suggest that utilizing CO₂ as a reactant not only enhances the sustainability of the process but also improves overall performance. In conclusion, this work offers a promising route for the electrochemical synthesis of hydroxybenzoic acids with reduced environmental impact. Further studies should focus on scaling the process and optimizing electrode materials to facilitate industrial applications, contributing to a greener chemical industry.



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sciforum-107803: The Potentiality of Vanadium Complexes as Antibacterial Agents

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Metal ions and metal-ion binding substances are crucial in various biological processes, and their rational design can be used to develop novel therapeutic drugs and diagnostic tools. Metal atoms are soluble in biological fluids due to their ability to easily lose electrons and form positively charged ions. Because of their electron deficiency they can interact with electron-rich biomolecules like proteins and DNA, and potentially participating in catalytic mechanism or stabilizing their tertiary or quaternary structures. Metal ions are important for cellular processes and biological functions in microorganisms. Antibacterial resistance is an increasingly major concern to global public health, requiring novel strategies to combat new resistance mechanisms emerging and spreading globally in infectious microbes. Inorganic and organometallic complexes offer an opportunity to develop novel antimicrobial agents due to their diverse three-dimensional shapes and extensive design options, which can impact factors like substitution kinetics, charge, lipophilicity, biological targets, and mechanisms of action. This paper explores the antibacterial activity of vanadium complexes. Research in this field focuses on the potential antibacterial activity of vanadium-based drugs. Vanadium is a well-known transition metal, and its complexes have been extensively studied for their medicinal properties. Vanadium complexes of 2-(salicylideneimine)benzimidazole, aminophen and bromosalicylaldehyde, dimalonitrial-based Schiff base, 1,2,4-triazole Schiff base, and fluoro-substituted Schiff base and vanadium stilbene complex, etc., exhibited antibacterial activity. Research on antimicrobial metallodrugs is crucial to combat antibiotic resistance, but mechanisms of toxicity remain uncertain, and limited in vivo data hinder further development due to limited bacterial targets. Future multidisciplinary research on vanadium complexes as antibacterial potential offers opportunities to explore biochemistry, design novel, and improve solubility, bioavailability, and toxicity and focus on developing novel strategies for targeting toxic metals and developing nanostructured antimicrobials for better understanding metal complex behaviour in living organisms.



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sciforum-107848: Thermo-mechanical analysis of a new cement mortar based on marine waste for a low environmental impact

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Recycling seashell waste in building materials is a relevant and attractive solution for eliminating this waste while at the same time reducing its environmental impact. Our study focuses on the use of *Mytilus galloprovincialis* shell waste in mortars of cement as a partial replacement of sand. A granular range similar to that of fine sand was used with the extraction of fine powder 0.08 mm, in order to reduce the effect of organic matter on material properties, we used percentages of 0%, 15%, 20%, 25%, 30%, and 45% according to mass. Physical, thermal and mechanical properties are estimated, and the capillary absorption coefficient is also determined. The two types of sand have an almost identical particle size distribution, the same sand equivalence, and nearly the same density, but other properties such as fineness modulus, specific surface area, and water absorption coefficient are slightly different. However, the morphology of the grains is totally different, which makes the physical, thermal, and mechanical properties of the cement mortars prepared varied while increasing the substitution rate. The results show that replacing natural sand with shell aggregates improves the thermal insulation performance and durability of the mortars, knowing that 45% of the replacement reduces the thermal conductivity and capillary coefficient to 21.7% and 75.21%, respectively, compared with the mortar of reference.



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sciforum-107657: Thermoresponsive Hydrogel Loaded With Clobetasol Plga Nanoparticles For The Treatment Of Inflammatory Skin Diseases: Formulation Development And Characterization

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Inflammatory skin diseases, such as atopic dermatitis and psoriasis, can significantly impact patients' quality of life due to symptoms caused by an overactive immune response. Clobetasol, a potent corticosteroid, is commonly used to relieve these symptoms by reducing inflammation and suppressing immune responses. However, prolonged use can lead to adverse effects, including skin atrophy, hypopigmentation, and Cushing-like syndrome. To tackle these issues, nanotechnology has been extensively used to enhance drug strength, stability, and controlled release, improving therapeutic efficacy and safety. In this study, clobetasol-loaded poly lactic-co-glycolic acid (PLGA) nanoparticles were developed and incorporated into a thermosensitive hydrogel for topical treatment of inflammatory skin diseases. Nanoparticles were prepared by nanoprecipitation using PLGA (polymer), polyvinyl alcohol (PVA, stabilizer), acetone (solvent), and clobetasol (drug). Particle size, polydispersity index (PDI), and zeta potential (ZP) were determined using a Zetasizer Nano ZS. Optimized nanoparticles for topical drug absorption exhibited an average size of 232 ± 20 nm, PDI of 0.18 ± 0.06 , and a slightly negative surface charge (-6.94 ± 2.55 mV), consistent with PLGA's ester terminals. Thermosensitive hydrogels were successfully formulated using the cold method for nanoparticle incorporation, displaying a gelation temperature ($32.33 \pm 0.58^\circ\text{C}$) identical to skin temperature. *In vitro* studies revealed controlled release of clobetasol from the nanoparticles and the hydrogel incorporated with the nanoparticles, with the latter showing a lower cumulative percentage. Therefore, both formulations offer a promising therapeutic approach for treating inflammatory skin diseases, minimizing clobetasol-related side effects through controlled release.



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sciforum-104163: Three-dimensional-printed@activated carbon adsorbent materials for the removal of Diclofenac from aqueous solutions

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The widespread use of the pharmaceutical compound diclofenac, its toxic effects and environmental persistence, together with its inefficient removal by conventional water/wastewater treatment processes, have led to major environmental and public health concerns. Adsorption is one of the most popular advanced techniques due to its numerous advantages, such as high removal efficiency and selectivity, as well as its economical and environmental sustainability. Three-dimensional printing makes the custom production of custom-made, complex-shaped adsorbents possible. A vat photopolymerization technique was employed in order to achieve the layer-by-layer solidification of a powdered activated carbon/photopolymer suspension into the desired shape, followed by its amine functionalization. The adsorbent was characterized by FTIR, SEM, N₂ porosimetry and contact goniometry. Batch adsorption experiments in simulated diclofenac wastewater were conducted. The final pollutant concentration was spectrophotometrically determined. The successful synthesis of the composite adsorbent was confirmed. The optimum pH value was found to be 5, while kinetic and isothermal experiments were conducted at pH=7, as it corresponds to that of the secondary treated diclofenac-containing wastewater effluents. The optimum contact time was 24h. Isothermal data revealed that the material adsorption capacity decreases with temperature. The optimum solution pH value of the adsorbent's regeneration process was found to be alkaline. Post-printing surface functionalization by diethylenetriamine increases the adsorbent's hydrophilicity and adsorption efficiency. Post-printing diethylenetriamine modification of the adsorbent increases its diclofenac removal efficiency by 7-fold, but it also alters its surface from hydrophobic to hydrophilic. Overall, 3D printing via photopolymerization can be successfully employed for the production of activated carbon-polymer composites as efficient reusable adsorbents for diclofenac removal from wastewater.



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sciforum-104246: Towards Improved Glucose Detection in Saliva and Point-of-Care Settings Using Plasmatic Gold Nanoparticles

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Introduction

Gold nanoparticles have gained a lot of interest in medical applications due to their plasmonic properties, and many methods have been explored for synthesizing well-defined particles. The detection of blood glucose using gold nanoparticles is emerging as a new method. In this project, we developed gold nanoparticles, using glucose as a mild reducing and stabilizing agent, to detect glucose in the blood through plasmonic reactions. By exploring innovative technologies and emerging techniques, we aim to enhance the accuracy, convenience, and overall user experience of glucose monitoring when using our potential method. The preliminary results will be presented.

2. Methodology

Various glucose concentrations were meticulously prepared and combined with a consistently proportioned gold solution to synthesize the gold nanoparticles. Sodium hydroxide and heat were employed to accelerate the process. The synthesized nanoparticles were characterized using absorption spectroscopy and electron microscopy.

3. Results and Application

Glucose is a mild reducing agent, and it reduces the gold salt into gold nanoparticles. The formation of gold nanoparticles was confirmed by measuring the surface plasmon resonance peak around 500 nm. The detection limit was in the range of 2mM to 50 mM with good reducibility, showing the potential application of this method. We are currently working on the interference of other ions/enzymes present in the blood with this procedure and expect to develop a potential method for glucose detection in blood and saliva.



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sciforum-104373: Towards Sustainability: Use of Local Palm Tree Waste in the Fabrication of Zinc Oxide Nanoparticles and Nanocomposite Beads for Biomedical and Environmental Applications

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Introduction: The growing emphasis on sustainability and waste management has led to innovative approaches in utilizing agricultural waste. This study explores the use of local palm tree waste for the synthesis of zinc oxide nanoparticles (ZnO NPs) and nanocomposite beads, aiming to create value-added materials for biomedical and environmental applications.

Methods: Palm tree waste was collected and processed to extract cellulose, which served as a substrate for ZnO NP synthesis. Zinc acetate was used as the zinc precursor, and a green synthesis approach was employed, utilizing the reducing and stabilizing properties of palm waste-derived cellulose. The ZnO NPs were characterized using UV-Vis spectroscopy, and transmission electron microscopy (TEM). The ZnO NPs were then embedded into alginate beads to form nanocomposite beads, which were evaluated for their structural integrity and functional properties.

Results: The green synthesis method successfully produced ZnO NPs with a mean diameter of 20–30 nm, as confirmed by TEM analysis. XRD patterns indicated the crystalline nature of the ZnO NPs. The nanocomposite beads exhibited enhanced mechanical stability and were effective in various applications. In biomedical assays, the beads demonstrated significant antibacterial activity against *Escherichia coli* and *Staphylococcus aureus*. For environmental applications, the beads showed promising results in the adsorption of heavy metals from aqueous solutions, indicating their potential for water purification.

Conclusions: This study highlights the dual benefits of waste valorization and sustainable material production. The successful incorporation of palm tree waste into ZnO NPs and nanocomposite beads underscores the potential of these materials in addressing biomedical and environmental challenges. Future research will focus on optimizing the synthesis process and expanding the application scope of these eco-friendly nanomaterials.



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sciforum-107516: Tuning the Electrical Resistivity of Molecular Liquid Crystals for Electro-Optical Devices

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Modern applications of molecular liquid crystals span from high-resolution displays for augmented and virtual reality to miniature tunable lasers, reconfigurable microwave devices for space exploration and communication, and tunable electro-optical elements, including spatial light modulators, waveguides, lenses, light shutters, filters, and waveplates, to name a few. The tunability of these devices is achieved through electric-field-induced reorientation of liquid crystals. Because the reorientation of the liquid crystals can be altered by ions normally present in mesogenic materials in minute quantities, resulting in their electrical resistivity having finite values, the development of new ways to control the concentration of the ions in liquid crystals is very important. A promising way to enhance the electrical resistivity of molecular liquid crystals is the addition of nano-dopants to low-resistivity liquid crystals. When nanoparticles capture certain ions, they immobilize them and increase their resistivity. If properly implemented, this method can convert low-resistivity liquid crystals into high-resistivity crystals. However, uncontrolled ionic contamination of the nanoparticles can significantly alter this process. In this paper, building on our previous work (Eng. Proc. 2023, 56(1), 199), we explore how physical parameters such as the size of the nanoparticles, their concentration, and their level of ionic contamination can affect the process of both enhancing and lowering the resistivity of the molecular liquid crystals. Additionally, we analyze the use of two types of nano-dopants to achieve better control over the electrical resistivity of molecular liquid crystals.



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sciforum-106147: Ultra-thin High-sensitivity Carbon Nanofiber Membranes: Innovations in Health Monitoring and Emergency Communications

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With the rapid expansion of the smart wearable device market, the demand for advanced materials and technologies with high sensitivity and stability is growing significantly. This paper presents an innovative technique for fabricating polyacrylonitrile (PAN) nanofiber membranes via electrospinning, using polyvinylpyrrolidone (PVP) as a pore-forming agent. The nanofibers were carbonized at high temperatures to obtain porous conductive carbonized nanofiber membranes, which were further compounded with thermoplastic polyurethane (TPU) using vacuum filtration to enhance mechanical flexibility and integration potential.

To evaluate the sensor's performance, sensitivity, response time, detection limit, and stability tests were conducted. The resistance change under pressures ranging from 0–50 kPa was measured, yielding a sensitivity of 101.22 kPa^{-1} , demonstrating excellent pressure sensing capabilities. Using precise dynamic loading equipment, the response time was recorded as only 20 ms, ensuring rapid signal transmission. By gradually reducing the applied pressure, the minimum detectable pressure was determined to be 5 Pa, indicating the ability to detect subtle pressure changes. Stability tests revealed that after 7000 loading/unloading cycles, the resistance remained stable with negligible variation, demonstrating exceptional durability and reliability.

This porous conductive carbonized nanofiber membrane shows broad application potential in fields such as smart textiles, biomedicine, and environmental monitoring. In particular, it enables the development of efficient and accurate health monitoring systems in smart wearable devices, supporting continuous physiological and environmental data collection. These findings provide a solid foundation for further research into high-performance composite materials and sensor interfaces, paving the way for innovations in the field of smart materials.



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sciforum-107454: Uncovering Hydrogen Adsorption: A DFT Forecast on Transition Metal Surfaces

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The hydrogen evolution reaction (HER) has been widely studied due to the increasing demand for hydrogen as fuel. However, the lack of efficient storage methods restricts the broad adoption of hydrogen-powered devices. Understanding transition metals' hydrogen adsorption capacity is essential for the better design of these devices because they are frequently used as catalysts for many kinds of hydrogen evolution reactions.

The first-principle DFT calculation was carried out using the VASP package to obtain the optimized geometries of hydrogen adsorption on metal surfaces. Two sets of surfaces—a) coinage metals (Ag, Au, and Cu) and b) non-coinage metals (Pt, Pd, Ni, and Co)—are considered. On each metal surface, the hydrogen adsorption energies are obtained at varying surface coverage ratios until the hydrogen evolution is kinetically and thermodynamically spontaneous.

The hydrogen adsorption energies decreased on all metal surfaces with increased hydrogen atoms on the surface. Later, the Tafel hydrogen evolution mechanism is used to define the spontaneous hydrogen evolution from the surfaces. The hydrogen evolution is quicker on the Au surface, and non-coinage metals, namely Ni, Co and Pd, have slower hydrogen evolution. Due to the strong adsorption of hydrogen atoms on metal surfaces, hydrogen atoms are found on the surface even after the HER, which experimental studies have also validated.



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sciforum-103462: Vanillin-crosslinked chitosan/PVA membranes loaded with dexpanthenol for skin tissue regeneration

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A patch that can avoid wound infection and promote tissue remodeling is of great value for wound healing. Herein, a series of skin-repairing dressings consisting of dexpanthenol (Dex)-loaded polymer membranes were fabricated using chitosan (CS)/polyvinyl alcohol (PVA) crosslinked with vanillin (VA). CS is a natural polysaccharide; it is biocompatible and biodegradable, with enhanced bioadhesive and wound-healing properties. PVA is a synthetic polymer that presents nontoxicity, good biodegradability, biocompatibility, and good mechanical properties. Vanillin, a primary extract of vanilla bean, is widely used in pharmaceuticals, cosmetics, foods, and beverages; it has one aldehyde and one hydroxyl group in its structure, making it an active crosslinker. Dexpanthenol is well absorbed when applied topically to the skin and supports skin regeneration by enhancing epidermal differentiation and facilitating wound healing. The successful synthesis of the CS/PVA/VA-Dex membranes was confirmed by Fourier Transform Infrared spectroscopy, their crystallinity was analyzed by X-Ray Diffraction, and the surface morphology of the membranes was studied with Scanning Electron Microscopy. Additionally, their water sorption and water content capacity were investigated, and their stability in different conditions was measured. Moreover, the encapsulation efficiency and release rate of dexpanthenol from the prepared products were studied using UV-vis spectroscopy. Finally, the cytotoxicity, antibacterial properties, cell adhesion, and wound-healing capacity of all prepared wound-healing dressings were examined in vitro.



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sciforum-107475: Voltammetric sensors based on nanomaterials and electropolymerized coverages for bioadditive analysis

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Bioadditives are often used around the world as a part of the daily human diet. Contrary to pharmaceuticals, bioadditives are not subject to rigorous quality control, and their full chemical composition is usually unknown. Therefore, the determination of active components in bioadditives is of high importance and can be achieved using voltammetry. Novel voltammetric sensors were developed for the quantification of L-tyrosine and diosmin in bioadditives. A glassy carbon electrode (GCE) modified with SnO₂ nanoparticles dispersed in sodium dodecyl sulfate and electropolymerized Eriochrome Black T allowed for the determination of L-tyrosine. The effect of its surfactant nature was tested. A GCE covered layer-by-layer with carboxylated multi-walled carbon nanotubes and polydopamine responded to diosmin. The conditions of electropolymerization were optimized using a target analyte voltammetric response. The electrodes' surface morphology and electron transfer properties were estimated by means of scanning electron microscopy and electrochemical methods. The increases in the electroactive surface area and electron transfer rate were confirmed. The electrooxidation parameters of L-tyrosine and diosmin were found. The electrodes were used as voltammetric sensors in Britton–Robinson buffer with a pH of 2.0 in differential pulse mode. The linear dynamic ranges of 0.75–100 µM for L-tyrosine and 0.75–25 and 25–100 µM for diosmin were achieved, with detection limits of 0.66 and 0.25 µM, respectively. The selectivity of the sensors' response to target analytes in the presence of typical co-existing compounds was proven. The practical applicability of the developed sensors was shown on real samples. A comparison to standard high-performance liquid chromatography confirmed similar levels of precision of the methods.



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sciforum-107574: Green Synthesis Of New (E)-3-methyl-6-((naphthalene-1-ylimino)methyl)benzo[d]thiazol-2(3h)-one Schiff Base, ADME Study

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The chemistry of heterocycles has received a great deal of attention in recent times due to their importance, and among these heterocycles is benzothiazolinone, which has received a great deal of attention due to its biological, pharmacological [1], [2], and agricultural [3] benefits. Schiff bases, which are molecules whose structure contains imine functions (C=N), have also been the subject of constant attention and development due to their different biological properties [4], [5].

In this context, we synthesized an imine-benzothiazolinone molecule (E)-3-methyl-6-((naphthalen-1-ylimino)methyl)benzo[d]thiazol-2(3H)-one according to an environmentally friendly green chemistry approach using ultrasound in ethanol, which enabled the target compound to be recovered in high yield in a short and pure time without the need for purification techniques. The structure of the compound was confirmed by IR, ¹H NMR and ¹³C NMR spectroscopic methods. Additionally, a study was conducted to examine the synthetic compound's pharmacological ADME properties based on lipinski's rule of five , revealing favorable drug-likeness characteristics and supporting its potential for further pharmaceutical development." .

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sciforum-107402: A cross sectional analysis between the size and materials in green synthesis of nanoparticles: Finding better materials among peel, leaf, and others

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The green synthesis of nanoparticles is a process where there is nothing environmentally unfriendly. Nanoparticles can be produced from plant and other biological waste materials. Many research was done before by using reducing agents such as NaOH, NaHCO₃ etc. These materials cause the environment pollution. Using NaHCO₃ result in producing CO₂ also. But by using different organic waste materials the synthesis procedure can be turned into green synthesis. This study provides a detailed analysis of nanoparticle synthesis using a variety of plant-based materials, such as peels, leaves, and other biological waste. By comparing different plant extracts, we aimed to identify the most effective options for nanoparticle production, focusing on factors like yield and surface to volume ratio. The nanoparticles in this research were created using green methods, and we investigated how the type of plant material influenced the characteristics of the resulting nanoparticles, including size consistency and efficiency of synthesis. Our results of cross sectional analysis will indicate that certain plant sources are more effective at producing nanoparticles with desirable properties. It was never examined by the statistical analysis. There are also other metallic wastes from where various metal oxide nanoparticles could be extracted, resulting in a downfall to environmental pollution. The analysis revealed important patterns that helped in selecting the best plant materials for green nanoparticle synthesis. This study highlights the potential of plant waste as a sustainable resource for nanoparticle production, advancing the fields of green chemistry and nanotechnology.



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sciforum-107583: CuPbX₃ and AgPbX₃ (X = I, Br, Cl) Inorganic Perovskites for Solar cell Applications

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Background

One of the possible solutions to the world's rapidly increasing energy demand is the development of new photovoltaic devices and photoelectrochemical cells with improved light absorption. This requires developing new semiconductor materials with an appropriate band gap that can absorb a large part of the solar spectrum while being stable in both ambient and aqueous environments.

Methods

Here, we showed the computational identification of relevant fully inorganic ternary perovskite materials based on electronic structure calculations. Our first-principles calculations were based on DFT as implemented in the VASP program. The identification was based on an efficient and reliable way of calculating semiconductor band gaps.

Result

We found that these materials are suitable for solar cell purposes, since their optical band gap ranges from 1.54 to 2.33 eV according to the computational calculation and from 1.42 to 1.93 eV according to the experimentally determined result, which is similar to the CH₃NH₃PbI₃ hybrid perovskites.

Conclusions

The outcome of the identification includes new ABX₃-type materials, i.e., CuPbI₃, CuPbBr₃, CuPbCl₃ and families of AgPbX₃, which warrant further experimental investigations. These materials are not sensitive to moisture, temperature and air and are hence expected to form stable solar cells. Cu and Ag cations are involved in the band structure, narrowing the bandgap, which will lead to high-efficiency solar cells with low loss power conversion efficiency owing to the involvement of the 4s orbital. The Cu 4s is a partially filled orbital creating a partially filled valence band owing to the 4s¹3d¹⁰ electron configuration, which is absolutely crucial for metallic behavior in CuPbX₃ materials. Since it ensures that there are unoccupied energy levels at an infinitesimally small energy above the highest occupied level, solar cell devices made of these semiconductors are less affected by defects and have efficient charge transfer. In addition to this, defect passivation strategies are highly useful in constructing solar cells.



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sciforum-103645: Development of method for determination of sucralfate in suspension by High-performance liquid chromatography

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Sucralfate suspension is primarily used as a treatment for ulcers and gastroesophageal reflux disease. Globally, this substance has been approved for various indications, including the management of peptic ulcer disease, stress ulcers, oral mucositis, as well as radiation-induced mucositis and esophagitis. This study aims to provide a reference quantitative method by high-performance liquid chromatography (HPLC) for drug manufacturers to control the quality of their sucralfate suspension product with the available conditions at their facility, and to serve as a tool in the field of drug research and development. As sucralfate is a substance that does not absorb UV-VIS light, the UV-VIS detector cannot be used. For such compounds, detectors like RID (Refractive Index Detector), ELSD (Evaporative Light Scattering Detector), or Charged Aerosol Detector (CAD) can be utilized. Among these, RID is the detector chosen for this study due to its popularity, ease of use, and low cost. The chromatographic conditions are as follows: Column: L8 (NH₂), 300 × 3.9 mm. Detector: Refractive Index Detector (RID). Mobile phase: ammonium sulfate (132 g/L) adjusted to pH 3.5 ± 0.1 with phosphoric acid, resulting in a phosphoric acid concentration of approximately 1.8×10^{-2} M. Column temperature: 30°C; Injection volume: 50 µL; Flow rate: 1 mL/min. This method is applicable, and the solvents and chemical reagents are common and available in testing centers and quality control departments at production facilities equipped with HPLC machines.



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sciforum-107830: Green synthesis of benzothiazolinone Schiff base derivative ADME prediction study

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Benzothiazolines are a class of heterocyclic compounds known for their diverse biological properties, as reported in the literature [1-2]. These properties have motivated extensive research to synthesize derivatives with enhanced and multiple biological activities.

Similarly, Schiff bases are well documented for their significant biological activity and diverse applications [3-5]. They remain a focus of research for the development of novel biologically active compounds.

In this study, we synthesized a Schiff base derivative of benzothiazolone, (E)-6-(((5-chloro-2-hydroxyphenyl)imino)methyl)-3-methylbenzo[d]thiazol-2(3H)-one, (1a), using a green chemistry approach. The reaction employed ultrasound-assisted synthesis in ethanol, resulting in an appreciable yield. Starting materials included 3-methyl-2-benzothiazolinone and 5-chloro-2-hydroxybenzaldehyde. The structure of SBM was confirmed using IR, ¹H NMR, and ¹³C NMR spectroscopic techniques.

Additionally, the pharmacokinetic and drug-likeness features of (1a) were evaluated using Lipinski's Rule of Five, a guideline that assesses a compound's potential as an orally active drug based on properties such as molecular weight, lipophilicity, and hydrogen bond donors/acceptors. The findings highlight the synthesized compound's potential biological relevance and suitability for further development.

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sciforum-107513: Phytosorption of some heavy metals from industrial wastewater using cabbage peels and banana trunk

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Study aims to evaluate the potential of agrowaste, specifically cabbagepeels and bananatrunks, as adsorbents for removing heavy metals from wastewater. Atomic absorption spectroscopy(AAS) was employed to measure the concentrations of these metal ions in two wastewater samples(WW1 and WW2). Surface-morphology and elemental-composition of the cabbagepeels and bananatrunks were analyzed using scanning-electronmicroscopy(SEM) and energy-dispersiveX-ray-spectroscopy(EDX). Study examined the effects of pH, contact time, and adsorbent dosage on adsorption process. The adsorption-isotherms for the removal of heavy metals were determined. Zinc, copper, iron, and cadmium were detected in the wastewater samples. Effect of pH on zinc removal showed the highest removal at 39.42% at pH2 for WW1 and 16.2% at pH2 for WW2, for cadmium, the highest removal was 24.7% at pH2 for WW1 and 46.6% at pH2 for WW2. Iron removal was 15.6% at pH6 for WW1 and 41.5% at pH6 for WW2. Copper removal reached 39.3% at pH4 for WW1 and 43.6% at pH6 for WW2. The effect of adsorbent dosage for iron, the maximum removal was 28.42% at 1g of adsorbent for WW1 and 24.98% at 4g for WW2. For cadmium, the highest removal was 30.5% at 1g for WW1 and 20.43% at 1g for WW2. For zinc, the maximum removal was 40.08% at 4g for WW1 and 16.56% at 2g for WW2. For copper, the highest removal was 28.86% at 2g for WW1 and 38.56% at 2g for WW2. Contact time, the maximum removal of iron was 16.65% after 100minutes for WW1 and 23.01% for WW2. For cadmium, the highest removal was 14.92% after 20minutes for WW1 and 16.4% for WW2. Zinc removal reached 14.92% after 20minutes for WW1 and 3.32% for WW2. For copper, the maximum removal was 24.28% after 100minutes for WW1 and 33.42% for WW2. The adsorption equilibrium data for the metal-ions were best fitted with the Freundlich-isotherm model. Cabbagepeels and bananatrunk has considerable potential as low-cost adsorbents for the removal of heavy metals from wastewater.



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sciforum-107840: Spin-coated double-doped (Al,Mg) zinc oxide thin films and optical properties for 2-T perovskite/CIGSSe tandem solar cells

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Introduction : Double doping of zinc oxide thin films to achieve good surface morphology and excellent band gap energy value remains a challenge in materials science in the field of thin film solar cells.

Methods : In this work, we prepared a series of zinc oxide thin films double-doped with aluminum (Al) and magnesium (Mg) atoms using the sol-gel technique via spin-coating equipment. Double doping is carried out in the following proportions : (1%Al,1%Mg), (3%Al,3%Mg), (5%Al,5%Mg) and (7%Al,7%Mg). The double-doped (Al,Mg) thin films were: (1) synthesized by spin-coating process, (2) characterized by complementary techniques including X-ray diffraction (XRD), scanning electron microscopy (SEM) coupled with energy dispersive X-ray spectroscopy (EDS) and UV-Vis-NIR spectroscopy, and, (3) used for 2-T perovskite/CIGSSe tandem solar cells.

Results : The characterization results assessed that the double-doped (Al,Mg) samples are oriented in the c-axis direction in a wurtzite structure, and the grain sizes range from 40 to 92 nm. Uniform, dense thin films were obtained on the glass substrates, and the samples consisting of spherically shaped nanograins forming homogeneous layers. In addition, optical transmittance measurements show good values between 87 and 91%, and the band gap energy, E_g , for the double-doped ZnO:(Al,Mg) materials has been determined using Tauc plots (E_g : 3.22 to 3.26 eV). SCAPS-1D software simulation results under the AM 1.5G spectrum show that an optimum efficiency of 20.62% ($V_{OC} = 0.786$ V, $J_{SC} = 42.28$ mA/cm², and FF = 62.03%) was achieved with the (1%Al, 1%Mg) layer.

Conclusions : This research paper introduces double doping to modulate the band gap energy, E_g , of doped ZnO:(Al,Mg) materials for applications in 2-T perovskite/CIGSSe tandem solar cells.



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sciforum-103931: Synthesis, Characterization and SEM analysis of 5-methyl-4-[(E)-(phenylmethylidene) amino]-4H-1,2,4-triazole-3-thiol and its metal complex with Cd(II) and Hg(II)

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Triazole containing compounds are very important due to their vast utility in medicinal, pharmaceutical, industrial, catalytic and agro-medicinal field. The Schiff base ligands incorporating triazole moiety and their derived metal complexes are of great interest due to their bonding beauties, structural diversities and easiness to prepare. The wide range of biological activities has created huge research interest in these compounds.

Triazole derived Schiff base ligand, 5-methyl-4-[(E)-(phenylmethylidene) amino]-4H-1,2,4-triazole-3-thiol (HL) and its metal complex with Cd(II) and Hg(II) was prepared in solid state. Green solvent free method was also applied for synthesis of ligand. The prepared compounds were characterized by elemental analysis, Infrared spectroscopy, NMR spectroscopy, magnetic moment & electrical conductivity data and Scanning electron microscopy analysis.

The ligand (HL) is potentially N,S donor molecule. The elemental analysis suggest that complexes have composition $[M(L)_2]$ where M= Metal and L=Deprotonated ligand. The electrical conductivity values suggests that compounds are non-electrolytes. The metal complexes are diamagnetic in nature. The proton NMR spectra of ligand and its Hg(II) complex in DMSO-D₆ indicated that ligand exists in thiol form and deprotonation of ligand is observed in Hg(II) complex. The infrared spectra of complexes clearly indicate that ligand is bidentate, donating to metal through aldimine N-atom and deprotonated thiol group. The SEM analysis was utilized to study the morphology and topography of the prepared compounds.

The schiff base ligand (HL) and its metal complexes with Cd(II) and Hg(II) ions were prepared and characterized using elemental and various spectral techniques. SEM analysis was used to describe the morphology of compounds. The complexes are neutral with composition $[M(L)_2]$. The NMR and IR spectra confirmed the formation of ligand and revealed that ligand is bidentate chelating molecule donating from aldimine N-atom and thiol group S-atom.



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sciforum-104143: The Development of an Affordable Graphite-Based Conductive Ink for Printed Electronics

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Printed electronics (PE) are rapidly growing, especially in wearable sensors, smart textiles, and IoT devices. Conductive inks, essential for the fabrication of PE, must be highly conductive, cost-effective, biocompatible, easy to prepare, and less viscous. Conductive inks comprise of a conducting material (metals like silver, gold, copper, or carbon-based alternatives like graphite, graphene, and carbon nanotubes), a binder, and a solvent. In this work, a water-based graphite conductive ink is developed using graphite as a conductive material, corn starch powder (non-toxic and biodegradable) as a binder, and distilled water as a solvent. Firstly, corn starch powder is added to distilled water, which is heated up to 100 °C and stirred continuously until a homogeneous gel-like mixture is formed. After cooling the mixture, graphite powder is added to it, and stirred for an hour at 450 rpm to obtain the ink. To check the conductivity, the ink is brush-painted on a paper substrate with a dimension of 20 mm x 10 mm, and the result shows a low ohmic resistance of ~ 560 Ω , confirming the highly conductive nature of the ink. Additionally, thermogravimetric analysis (TGA) is performed on the prepared ink to evaluate its thermal stability, and a very strong X-ray diffraction (XRD) peak obtained at $2\theta = 26.5426^\circ$, a small peak at $2\theta = 54.6145^\circ$, along with a few other small peaks, confirms the presence of graphite with corn starch. Thus, this conductive ink can be used for PE owing to its affordability, biocompatibility, and ease of preparation.



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Session 3. Computing and Artificial Intelligence

sciforum-105114: Monitoring of agri-environmental variables in a coffee farm through an experimental IoT network to optimize decision-making by applying deep learning models

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Corporacion Universitaria Iberoamericana

Industry 4.0, automation, and data processing are transforming business models across various sectors, including agriculture. This work focuses on the coffee sector in Colombia, analyzing the current situation and proposing 4.0 technologies as tools to improve processes such as production and the detection of nutritional deficiencies in crops. Trends are explored, and coffee farms in the department of Quindío, Colombia, are visited. Interviews with coffee growers are also conducted to gather information about their work and needs. Additionally, an experimental IoT network model is proposed to collect data on certain agro-environmental variables, which employs the LoRaWAN protocol to send and receive data between sensor nodes and the base station. The term “Digital Coffee Grower” is also defined as an artificial intelligence model that replicates or emulates the decision-making of an expert coffee grower. The implementation of technology in the coffee-growing area is reflected upon, where empirical processes are still evident, but without undermining the experience and knowledge of local coffee growers. Preliminary results are evaluated through an MLP (multilayer perceptron) neural network model. Despite initially having few data sets, the concept of “Digital Coffee Grower” promises to substantially improve the decision-making process in coffee plantations. Finally, the importance of continuing data collection and cleaning, as well as experimenting with artificial intelligence models to generate significant advances in this field, is emphasized.



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sciforum-102713: Fall detection assessment in older adults using a smart wearable device

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Introduction

Falls among older adults are a significant health concern as they can result in severe injuries or even death. This research aims to tackle this issue by creating a smart bracelet that utilizes Internet of Things (IoT) technology to detect falls and monitor the health parameters of aged individuals.

Methods

This project uses a quantitative research approach involving precise data analysis of sensor data from an accelerometer and a heart rate monitor. The bracelet incorporates an ESP32 microcontroller, a heart rate sensor, and an accelerometer. The device communicates via Wi-Fi using the MQTT protocol, sending data to a server for real-time monitoring and alerts. The bracelet was designed using 3D printing technology and assembled with lightweight, impact-resistant materials.

Results

The testing process involved both simulated and real-world scenarios to evaluate the bracelet's functionality. The accelerometer effectively detected falls by monitoring sudden changes in movement, while the heart rate sensor provided continuous health data. Most importantly, alerts were successfully transmitted to designated contacts via the IFTTT platform when a fall or abnormal health readings were detected, providing reassurance about the bracelet's effectiveness in emergencies. Data collected included heart rate variability and acceleration amplitude, confirming the device's accuracy in real-world conditions.

Conclusions

The smart bracelet successfully fulfilled the project's objectives by demonstrating reliable fall detection and health monitoring capabilities. While the device's physical design can be further refined, its functionality proved effective in preliminary tests. Future improvements will enhance sensor accuracy and user adaptability to ensure broader adoption among the senior population. The integration of IoT technology in healthcare devices shows promise in providing continuous and remote monitoring. With its potential to reduce the risks associated with falls among older adults, the smart bracelet shows potential in its impact on elderly care.



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sciforum-107860: Artificial intelligence applied to sustainability with the help of household resource measurement

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UNIMINUTO

Artificial intelligence (AI) has established itself as a key tool for the efficient management of resources at home. By combining AI with visualization software, it is possible to develop advanced home automation systems that optimize the use of water, gas and electricity. These systems automate the control of resource consumption, which contributes significantly to savings and reduction of environmental impact. The integration of AI allows people to adjust their daily consumption according to their needs, avoiding waste. A notable benefit of these systems is the ability to reduce both the carbon and water footprints of the home. New software technologies continuously analyze energy and water consumption, identifying patterns and providing personalized recommendations to maximize efficiency. Additionally, automated systems can make real-time adjustments, reducing overuse of resources, generating long-term economic savings and easing pressure on natural resources. The use of AI in the home also encourages sustainability, promoting responsible use of resources and contributing to environmental conservation. By implementing home automation technologies, people actively participate in the preservation of resources vital to ecological balance. In conclusion, AI applied to resource management not only improves efficiency and savings, but also promotes a more sustainable lifestyle committed to the environment for the sostenibility.



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sciforum-101791: DenseMobile Net: Deep Ensemble Model for Precision and Innovation in Indian Food Recognition

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Precision and efficacy are vital in the constantly advancing field of food image identification, particularly in the domains of medicine and healthcare. Transfer learning and deep ensemble learning techniques are employed to enhance the accuracy and efficiency of the Indian Food Classification System. The ensemble model effectively captures various patterns and correlations within the information by employing many machine learning techniques. The ensemble method we employ utilizes the MobileNetV3 and DenseNet-121 transfer learning models to construct a robust model. The ensemble model benefits from the integration of model predictions, resulting in enhanced recognition of Indian food. The study utilized a dataset consisting of 6000 photographs of Indian cuisine, categorized into 26 distinct groups. The picture dataset is divided into two subsets: 80% is allocated for training and 20% is reserved for testing. The experimental results demonstrate that DenseNet-121 surpasses MobileNetv3 in terms of testing accuracy, achieving a rate of 90%. The MobileNetV3 model achieves an accuracy of 87.64% on the Indian food image dataset. The integration of both models in ensemble learning yields a model accuracy of 92.38%, surpassing the performance of each individual model. This research revolutionizes our food relationship with the use of state-of-the-art technologies. By utilizing the most advanced transfer learning algorithm specifically designed for the precise classification of Indian cuisine, our aim is to establish a new standard in both technology and gastronomy. This will facilitate innovation in food perception, comprehension, and engagement.



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sciforum-104416: Evaluating the quality of generative artificial intelligence in healthcare: a systematic review

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The burgeoning use of Large Language Models (LLMs) in healthcare has spurred a need for robust evaluation methods to assess the quality, reliability, and efficacy of their outputs. This systematic review aims to map the landscape of existing methods employed to evaluate texts and other outputs generated by LLMs in the healthcare domain. The review protocol was registered on PROSPERO. A comprehensive search was conducted across multiple databases, including PubMed, IEEE Xplore, Google scholar and Scopus, focusing on studies published between 2010 and 2023. The inclusion criteria encompassed original articles that discuss methodologies for assessing the performance of LLMs in generating clinical and healthcare-related content. The review identifies a variety of evaluation techniques, broadly categorized into quantitative and qualitative methods. Quantitative assessments often involve metrics such as accuracy, precision, recall, and F1 score, particularly in tasks like clinical documentation, diagnostic support, and patient communication. Qualitative methods, on the other hand, emphasize human judgment, focusing on aspects such as coherence, adequacy, relevance, and readability, often through expert panel reviews and user satisfaction surveys. Additionally, the review highlights challenges unique to the healthcare context, such as the need for domain-specific knowledge, the handling of sensitive patient data, and the potential for bias in AI-generated content. The findings underscore the importance of interdisciplinary collaboration in developing and validating evaluation frameworks that not only measure technical performance but also consider ethical and practical implications. In conclusion, this review provides a comprehensive overview of current evaluation methods for generative AI in healthcare, identifies gaps in the existing literature, and proposes directions for future research to enhance the assessment of these advanced technologies in medical settings.



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sciforum-104547: Forecasting COVID-19 Mortality Rates: A Comparative Study of Autoregressive Integrated Moving Average and Neural Network Models

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Accurate forecasting of infectious disease incidence is essential for timely intervention and effective government planning. This paper presents a comprehensive study comparing various forecasting models for daily COVID-19 mortality rates in Italy. The models evaluated include the autoregressive integrated moving average (ARIMA) model and three neural network-based models: backpropagation neural networks (BPNNs), radial basis function neural networks (RBFNNs), and Elman recurrent neural networks (ERNNs). RBFNN demonstrated superior performance with the lowest mean absolute error (MAE), mean absolute percentage error (MAPE), and mean square error (MSE), outperforming ARIMA and other neural networks by better capturing non-linear patterns in mortality data. The models' performance ranking from best to worst was RBFNN, ERNN, BPNN, and ARIMA. These results underscore the effectiveness of neural network models, particularly RBFNN, in accurately forecasting COVID-19 mortality rates. The implications of these findings are significant for public health policy. The improved accuracy of RBFNN in short-term mortality prediction provides valuable insights for pandemic response planning, enabling health authorities to make informed decisions on resource allocation, public health advisories, and emergency preparedness. This study contributes to the literature on infectious disease modeling by demonstrating the advantages of neural networks over traditional statistical methods and offering practical guidance for selecting forecasting models in epidemic scenarios. Our evaluation of forecasting methods thus provides a critical foundation for enhancing predictive accuracy in disease incidence and supporting more responsive public health management.



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sciforum-103549: Fusion Vision Transformers and Convolutional Neural Networks for Facial Beauty Predictions

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We aimed to develop a system that can analyze faces and predict how attractive humans will find them. This is a complex task because beauty perception is subjective and influenced by cultural background. Facial beauty prediction (FBP) is a significant visual recognition problem for the assessment of facial attractiveness, which is consistent with human perception. A deep learning method has recently demonstrated an amazing ability for feature representation and analysis; in particular, Convolutional Neural Networks (CNNs) and Vision Transformers (ViTs) are powerful tools for image analysis. The CNNs learn to identify features associated with attractiveness and use them to predict beauty scores for new faces. This paper proposes a new fusion ViTs–CNN network which incorporates the strengths of combining ViTs with CNNs to lead to improved performance and efficiency in predicting beauty scores. This approach takes pre-trained models from Mobilenetv3, DenseNet121 and InceptionV3, combines them with ViTs, and fine-tunes them to predict facial beauty. This approach can provide insights into how the models are leveraging the strengths of both architectures. Testing this method on the SCUT-FBP5500, the ViTs–CNN network achieved a Pearson coefficient of 0.9480. This indicates that the fusion ViTs–CNN network's facial beauty predictions are closer to human evaluation compared to traditional methods for assessing facial attractiveness.



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sciforum-106005: How biomarkers and artificial intelligence (AI) are innovating personalized nutrition: the importance of a robust computational infrastructure

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Personalized nutrition has the potential to revolutionize health by integrating biomarkers and artificial intelligence (AI) to provide tailored dietary recommendations. This systematic review synthesizes existing research on the role of biomarkers and AI in personalized nutrition, focusing on the critical need for a robust computational infrastructure. A comprehensive search of major databases, including PubMed, Scopus, and Web of Science, was conducted to identify studies published between 2010 and 2024. A total of 50 studies were selected based on their relevance and contribution to the understanding of how biomarkers and AI enhance the accuracy of nutritional assessments and recommendations. The review found that biomarkers play a crucial role in detecting molecular and biochemical changes linked to nutrient intake and metabolism, providing a precise assessment of nutritional status. Concurrently, AI technologies analyze large datasets—encompassing genetic, dietary, and health data—to generate personalized recommendations that account for individual variability. This combination offers significant advantages over traditional population-based studies. However, the review highlights the persistent challenges in building a robust computational infrastructure necessary to support these innovations. Effective infrastructure must address the complexity of dietary databases, enabling the accurate translation of food components into nutrients and energy. Additionally, the development of bioinformatics frameworks could standardize and annotate nutritional data, facilitating better dietary monitoring and management. This review concludes that while biomarkers and AI are transforming personalized nutrition, advancing computational infrastructure is essential to fully realize their potential and improve the quality and accessibility of personalized dietary guidance. Further research is recommended to overcome the current limitations and ensure the ethical and effective implementation of these technologies.



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sciforum-107409: Innovations in Laparoscopic Imaging: Surgical Instrument Segmentation with a Modified U-Net Model and Siamese Branch

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Laparoscopic surgeries are minimally invasive, requiring only small incisions which result in faster patient recovery and a lower risk of complications. Despite these advantages, surgeons face some challenges, such as limited visibility and control over instruments, potentially compromising precision and coordination during procedures. To address these limitations, advanced technological systems enhance the visibility, control, and overall effectiveness of laparoscopic surgeries.

This research introduces an instrument segmentation method using a modified U-Net model. The model integrates residual blocks in the encoder to optimize learning and prevent gradient degradation, enabling the capture of complex patterns. The decoder is designed with two branches: one focused on instrument segmentation and the other on background segmentation. By combining both outputs, the system improves the accuracy and efficiency of segmenting surgical instruments in real-time.

The system's performance was evaluated through metrics such as the Jaccard index, precision, recall, F1 score, and accuracy. Tests under geometric and signal processing distortions were also conducted to replicate varying surgical conditions, revealing the system's high robustness and adaptability. The results show a high efficiency with an accuracy of 0.94 and a Jaccard index of 0.93. Additionally, this approach demonstrates significant improvements in identifying instruments accurately and reducing potential patient injury.

This development enhances surgical precision and increases patient safety during laparoscopic procedures. Furthermore, it provides a valuable tool for training and evaluating surgeons' psychomotor skills. This innovation represents a step toward the future of minimally invasive surgery, minimizing direct surgeon intervention and improving overall patient outcomes.



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sciforum-107296: Leveraging Physics-Informed Neural Networks for Solutions to Differential Algebraic Equation Systems

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This study investigates the application of Physics-Informed Neural Networks (PINNs) to solve the differential algebraic equations (DAEs) governing the complex dynamics of a Two-Phase Reactor and Condenser with Recycling system (TPRCR system). The TPRCR system is characterized by highly nonlinear, stiff, and interdependent equations that describe variables such as concentrations, temperatures, and pressures. Traditional numerical methods often struggle with these equations due to their complexity, sensitivity, and potential partial unknowns, such as difficult-to-model transport phenomena and reaction kinetics. PINNs offer a unique data-driven approach by directly embedding the physical laws governing the TPRCR system into the neural network's training process, thereby bypassing the need for a fully explicit derivation from the governing equations. This makes them particularly effective for systems like TPRCR, where exact analytical solutions are elusive and traditional methods require significant computational effort. In this study, we trained multiple PINN models using the AdamW optimizer with a learning rate of 0.001 over 500 epochs. These models accurately predicted system dynamics, including concentrations, temperatures, and pressures. The root-mean-squared error was employed as the loss function to guide optimization and ensure high accuracy in predictions. Our results demonstrate that PINNs successfully capture the complex behaviour of the TPRCR system, with predictions aligning closely with those obtained from conventional DAE solutions. The computational efficiency and fast convergence of PINNs further highlight their potential for robust performance in chemical process modelling. This study underscores the value of PINNs in addressing the specific challenges posed by the TPRCR system, making them a promising tool for future research and industrial applications in chemical engineering.



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sciforum-106313: Mathematical problem-posing using generative AI

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Artificial intelligence is already widely used in education in at least the following areas: (1) intelligent tutoring and personalized learning; (2) adaptive assessment of learning outcomes; (3) virtual teachers and teaching assistants; (4) intelligent classrooms and learning environments; and (5) learning diagnostics and academic prediction. Advances in artificial intelligence will continue to drive innovation and improvement in education, providing better learning and teaching experiences. Artificial intelligence is also driving developments in mathematical research. For example, machine learning is used to help mathematicians discover patterns and make conjectures in pure mathematics, such as in the algebraic and geometric structure of knots, and predicate the combinatorial invariance conjecture for symmetric groups, even solving geometric problems in IMO with the DeepMind geometric reasoning model (AlphaGeometry). But AI has not been connected to mathematical problem-posing.

Mathematical problem-posing is a complex intellectual activity that trains students' mathematical creativity and critical thinking. In the age of artificial intelligence, we need to consider how to use generative AI to engage in mathematical problem-posing activities and pose valuable mathematical problems. Therefore, the blueprint of this research is to explore the mathematical problems posed by generative AI. Applying the same mathematical problem-posing task, a paper and pencil test is used for the participants, and some prompts are used for the generative AI. Then, using textual analysis, we analyze and compare the similarities and differences between the problems posed by each. The results demonstrate that the problem-posing products of humans and AI are different, and that there are differences in the number, solvability, clarity, and complexity of the mathematical problems posed by them. The mathematical problems posed by generative AI have unknown characteristics and creativity. This research will be new and imaginative.



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sciforum-093961: Enhanced Drone Detection Model for Edge Devices: Combining Knowledge Distillation and Bayesian Optimization

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The emergence of Unmanned Aerial Vehicles (UAVs), commonly known as drones, has presented numerous transformative opportunities across sectors such as agriculture, commerce, and security surveillance systems. However, the proliferation of these technologies raises significant concerns regarding security and privacy, as they could potentially be exploited for unauthorized surveillance or even targeted attacks. Various research endeavors have proposed drone detection models for security purposes. Yet, deploying these models on edge devices proves challenging due to resource constraints, which limit the feasibility of complex deep learning models. The need for lightweight models capable of efficient deployment on edge devices becomes evident, particularly for the anonymous detection of drones in various disguises to prevent potential intrusions. This study introduces a lightweight deep learning-based drone detection model by fusing knowledge distillation with Bayesian optimization. Knowledge distillation is utilized to transfer knowledge from a complex model (teacher) to a simpler one (student), preserving performance while reducing computational complexity, thereby achieving a lightweight model. However, selecting optimal hyperparameters for knowledge distillation is challenging due to a large number of search space and complexity requirements. Therefore, through the integration of Bayesian optimization with knowledge distillation, we present an enhanced CNN-KD model. This novel approach employs an optimization algorithm to determine the most suitable hyperparameters, enhancing the efficiency and effectiveness of the drone detection model. Validation on a dedicated drone detection dataset illustrates the model's efficacy, achieving a remarkable accuracy of 96% while significantly reducing computational and memory requirements. With just 102,000 parameters, the proposed model is five times smaller than the teacher model, underscoring its potential for practical deployment in real-world scenarios.



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sciforum-107767: A comparative analysis of metric combinations in face verification with machine learning techniques

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Face verification, a critical task in computer vision with significant implications for security, surveillance, and biometric applications, involves determining whether two facial images represent the same individual, even when captured under varying conditions such as lighting changes, pose, or facial expression variations. Despite recent advances in the field, achieving a high accuracy in face verification remains challenging, especially in scenarios involving occlusions or poor image quality. Improving the methods used to compare facial embeddings has become a key area of research for developing more robust and reliable face verification systems. Traditionally, metrics such as L1, L2, and cosine similarity have been employed to compare facial embeddings in computer vision. However, when used in isolation, each metric has inherent limitations, particularly in its ability to generalize across complex and diverse datasets. This study explores the effectiveness of combining various metrics to enhance the comparison of facial embeddings. We aim to improve accuracy by leveraging state-of-the-art CNN-based face verification methods, including AdaFace and ArcFace, as well as advanced vision transformer-based approaches such as Swin transformers. To achieve this, we developed a range of combinations of metrics using machine learning techniques, including Logistic Regression, k-Nearest Neighbors, Support Vector Machines, LightGBM, and XGBoost. The CASIA-WebFace dataset was used for training metric-combining models, and the BUPT-BalancedFace dataset was used for evaluation, ensuring balanced comparisons across demographic groups. The experimental results showed that while cosine similarity outperformed L1 and L2 metrics, the combination of multiple metrics was more effective than models relying on a single metric in both CNN-based facial verification and vision transformer-based methods. CNN-based models were more effective than transformer-based ones. The combined strategies resulted in models that achieved a better balance among recall, precision, and F1-score. In particular, the accuracy of these models increased by 1.1% compared to the best models that used a single metric.



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sciforum-104244: A Deep Learning-Based Framework for Enhanced Cyberattack Detection and Mitigation in Software Defined Networks

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The phenomenal advancements and vehement use of Software Defined Networks (SDNs) require robust cyberattack defense strategies. This arises from traditional intrusion detection systems (IDS), which often fail to solve the intricate security problems posed by SDNs. Defenses are challenged by substantial data volumes and the intricacies of changing network setups, resulting in inadequate attack detection and mitigation. Moreover, while advantageous for network administration, SDN's centralised architecture presents exploitable vulnerabilities. Therefore, to tackle these challenges, this paper introduces an innovative defence mechanism against cyberattacks in SDN. This leverages advanced deep learning techniques to enhance the precision and accuracy of detection and mitigation. This suggested model incorporates an Enhanced CenterNet architecture specifically designed for network traffic, supplemented with knowledge graphs to overcome traditional feature extraction restrictions. In this architecture, to enhance attack classification robustness, a hybrid DenseNet-201 model incorporating network topology, user behavior, and historical attack patterns is implemented. This is further augmented by adversarial training to counter sophisticated attacks. Especially, this dynamic defense mechanism, orchestrated by a remote SDN controller, reconfigures network resources in real-time for a prompt response to distributed denial-of-service (DDoS) attacks. To verify the effectiveness of the proposed model, an experimental analysis has been conducted on InSDN and DDoS-SDN datasets. This analysis is implemented in the Python/Mininet environment. From the results, it is observed that the proposed model achieved significant improvements in precision (4.5%), accuracy (5.9%), recall (4.5%), AUC (2.9%), and specificity (3.9%) of attack detection, reducing response delay by 10.4% when compared to conventional deep reinforcement learning (DRL) and hybrid quantum-classical convolution neural network (HQCNN). Additionally, it improves attack prevention precision (1.9%), accuracy (1.5%), recall (2.5%), AUC (3.5%), and specificity (2.9%), with a 3.5% delay reduction. Thus, this work significantly advances SDN cyberattack defense mechanisms and provides a robust solution to evolving security challenges.



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sciforum-105946: A Hybrid Feature Extraction Approach Using DenseNet and Local Binary Patterns for Alzheimer's Disease Classification

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Alzheimer's Disease (AD) is a prevalent neurodegenerative disorder that significantly impacts cognitive and functional abilities. Early and accurate diagnosis of AD and its associated cognitive impairments is critical for effective management and intervention. In this study, we propose a hybrid feature extraction method combining Local Binary Patterns (LBPs) and the DenseNet deep learning model to enhance the classification accuracy of AD and related cognitive conditions. The ADNI3 dataset, consisting of five distinct classes, Alzheimer's Disease (AD), Control, Early Mild Cognitive Impairment (EMCI), Late Mild Cognitive Impairment (LMCI), and Mild Cognitive Impairment (MCI), was employed in this analysis.

Images from the dataset were preprocessed by converting them to grayscale for LBP extraction and resized to 224x224 pixels for DenseNet processing. The extracted LBP and DenseNet features were concatenated to form a comprehensive feature set, which was then used to train a multi-class Support Vector Machine (SVM) classifier with Error-Correcting Output Codes (ECOCs).

The proposed method demonstrated a robust performance with an overall accuracy of 95.36%. The confusion matrix analysis revealed precision, recall, and F1 scores of 96.93%, 91.54%, and 93.96%, respectively, indicating high reliability in classifying the different stages of cognitive impairment. These findings suggest that the integration of LBP and DenseNet features provides a powerful approach for the early diagnosis and classification of Alzheimer's Disease, with potential applications in clinical settings for facilitating timely interventions and improving patient outcomes.



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sciforum-097580: A Hybrid Swarm Optimization Algorithm For Improving Feature Selection In Machine Learning

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In the era of big data, the sheer volume of information available for machine learning applications has grown exponentially. However, this increase in data often leads to a decrease in the quality of datasets due to issues such as noise, redundancy, and irrelevance, which can adversely affect the performance of predictive models. To address these challenges, dimensionality reduction techniques are employed, with feature selection being a prominent method. The objective of this research is to enhance machine learning prediction performance by developing a novel hybrid feature selection algorithm. This algorithm synergizes the strengths of cat swarm optimization (CSO) with those of the crow search algorithm (CSA), aiming to refine feature selection processes. The proposed hybrid algorithm was meticulously implemented and applied using the K-Nearest Neighbors (KNN) model on a diverse array of datasets. To rigorously evaluate its efficacy, the algorithm was tested on 12 carefully selected datasets, encompassing various domains and complexities. The performance was measured based on the accuracy of the machine learning predictions. Remarkably, the proposed hybrid algorithm achieved an average accuracy rate of 87%, which represents a significant improvement over previous approaches that had an average accuracy of 83%. These results underscore the potential of the proposed hybrid feature selection algorithm in enhancing the predictive capabilities of machine learning models by effectively reducing dimensionality and eliminating irrelevant features. The findings suggest that integrating CSO and CSA can lead to more robust feature selection mechanisms, thereby improving the overall quality and reliability of machine learning predictions.



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sciforum-104318: A low-cost solution to improve video projector management and connectivity using virtualization

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The video projector is an essential tool for various activities such as teaching, organizational tasks, and conferences. This article introduces a low-cost and effective architecture designed to enhance video projection resources, including older models, through the incorporation of virtualization for improved management and sharing capabilities. The proposed solution addresses prevalent connectivity issues caused by differing connector types, transmission protocols, and configuration incompatibilities (such as frequency and resolution) between video projectors and computers. These incompatibilities frequently lead to delays and challenges in effectively utilizing video projection resources.

The innovative architecture utilizes a Raspberry Pi combined with three virtualized applications to create a user-friendly system. This system not only facilitates the efficient management of video projection resources but also allows for seamless sharing and connectivity across various devices. By leveraging virtualization, the architecture ensures compatibility and adaptability, reducing the downtime typically associated with setup and configuration issues.

The implementation of this solution is aimed at enhancing the functionality and accessibility of video projectors, enabling new paradigms in working and teaching environments. The approach provides a low-cost and practical method to upgrade existing video projection infrastructure, thereby extending the lifespan and utility of older projectors while introducing modern capabilities and improving overall user experience.



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sciforum-103684: A New Approach for Improving Sentiment Analysis Using Multi-Dimensional Feature Reduction

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Sentiment Analysis is a sub-field within Natural Language Processing (NLP), concentrating on the extraction and interpretation of user sentiments or opinions from textual data. Despite significant advancements in the analysis of online content, a continuing challenge persists: the handling of sentiment datasets that are high-dimensional and frequently include substantial amounts of irrelevant or redundant features. Existing methods to address this issue typically rely on dimensionality reduction techniques; however, their effectiveness in removing irrelevant features and managing noisy or redundant data has been inconsistent.

This research seeks to overcome these challenges by introducing an innovative methodology that integrates ensemble Feature Selection techniques based on Information Gain with Feature Hashing. Our proposed approach aims to enhance the conventional feature selection process by synergistically combining these two strategies to more effectively tackle the issues of irrelevant features, noisy classes, and redundant data. The novel integration of Information Gain with Feature Hashing facilitates a more precise and strategic feature selection process, resulting in improved efficiency and effectiveness in sentiment analysis tasks.

Through comprehensive experimentation and evaluation, we demonstrate that our proposed method significantly outperforms baseline approaches and existing techniques across a wide range of scenarios. The results indicate that our method offers substantial advancements in managing high-dimensional sentiment data, thereby contributing to more accurate and reliable sentiment analysis outcomes.



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sciforum-103668: A New Glaucoma Detection Method Using A Swin Transformer And Image Segmentation

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Introduction

This study investigates the development and evaluation of an advanced automated system for glaucoma detection using deep learning techniques. Traditional diagnostic methods for glaucoma are often time-consuming and reliant on ophthalmologist expertise, leading to inconsistencies and delays in treatment. By utilizing state-of-the-art transformer-based models, this research aims to improve the accuracy and efficiency of glaucoma detection.

Methods

Five publicly available retinal fundus image datasets—ODIR-5K, ACRIMA, RIM-ONE, ORIGA, and REFUGE—were merged into one large dataset to ensure comprehensive model training and evaluation. The SegFormer model was employed for optic cup and disc segmentation, addressing the limitations of traditional CNNs in feature discrimination. This model captures both local and global contexts in fundus images, which is critical for accurate glaucoma detection. Segmented images were then classified using the Swin Transformer, known for its hierarchical architecture and ability to efficiently process high-resolution images through shifted window self-attention mechanisms. Data manipulation and preprocessing were conducted using Pandas and NumPy to optimize model performance.

Results

The combination of SegFormer for segmentation and Swin Transformer for classification resulted in superior performance compared to standalone models and other CNN-based approaches. The proposed model achieved an accuracy of 97.8%, precision of 97.5%, recall of 98.29%, and an F1-score of 98.33%. This significantly outperformed other state-of-the-art CNN models, demonstrating the effectiveness of transformer-based architectures in glaucoma detection.

Conclusions

This research showcases the potential of integrating SegFormer and Swin Transformer models for automated glaucoma detection. The high accuracy and scalability of this system suggest broader applications in medical diagnostics, offering a reliable and efficient solution for clinical settings.



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sciforum-107116: A novel approach for classifying gliomas from magnetic resonance images using image decomposition and texture analysis

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The accurate classification of gliomas from magnetic resonance (MR) imaging is vital for effective treatment planning. However, due to the irregular and diffuse boundaries of gliomas, manual classification is both difficult and time-consuming. To address these challenges, we present a novel methodology that combines image decomposition with local texture feature extraction to improve classification accuracy. The process begins by applying a Gaussian filter (GF) to the MR images to smooth them and reduce noise. Subsequently, Non-subsampled Laplacian Pyramid (NSLP) decomposition is used to capture multi-scale image details, which enhances the visibility of glioma boundaries. After decomposition, Total Variation-L1 (TV-L1) normalization is applied to reduce intensity inconsistencies, and Local Binary Patterns (LBPs) are utilized to extract key texture features from the processed images. These extracted texture features are then input into several supervised machine learning classifiers, including Support Vector Machines (SVMs), K-nearest Neighbors (KNNs), Decision Trees (DTs), AdaBoost, and LogitBoost. These models are trained to distinguish between low-grade (LG) and high-grade (HG) gliomas. Experimental results demonstrate that our proposed method consistently outperforms current state-of-the-art techniques in glioma classification, delivering superior accuracy in differentiating between LG and HG gliomas. This approach offers significant potential for improving diagnostic accuracy, thereby supporting clinicians in making informed and effective treatment decisions.



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sciforum-107466: A Novel Approach for Sketch Colorization Using Generative AI

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The colorization of sketches is a key aspect in computer vision, with applications ranging across the art, design and entertainment realms. True conversion of a monochromatic sketch into color is an invaluable skill for creative people and enthusiasts. Machine learning techniques, especially deep learning, have shown significantly better performance in various computer vision tasks, particularly for image segmentation, object classification, and other tasks. Although these methods are very promising, the literature still lacks concrete examples of GAN+autoencoder techniques and an in-depth discussion of their integration. Our research adopts a novel method, which integrates GANs and autoencoders to fill this gap. The intent of this integration is to improve the accuracy and effectiveness of color images generated from sketches. But our tests show that the proposed model is superior to existing techniques in terms of capturing fine details and creating a pleasing image. These results have significance in that they represent a breakthrough for state-of-the-art sketch colorization techniques, and enable artists and designers to create realistic images of their sketches. This research not only highlights the lack of integration among GANs and autoencoders; it also offers an entirely new approach that helps both to improve the accuracy and degree of realism in colorized images. This represents a major breakthrough for sketch colorization techniques overall.



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sciforum-107651: A novel machine learning approach for revolutionizing orthodontic care

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Anticipating the type of orthodontic treatment holds significant weight in patients' decision-making processes. Several deep learning techniques have shown impressive results in recent times in several computer vision tasks especially in image segmentation, image classification, image identification, etc., using convolutional neural networks. This study aimed to develop a model using convolutional neural networks for predicting orthodontic malocclusion types, which are very difficult to work on using traditional image processing techniques. Currently, proposals to use orthodontic software in dental clinics have been enacted , however they lack the ability to comprehensively analyze complex patient data, including genetic factors, craniofacial features, and treatment outcomes, potentially leading to sub-optimal treatment decisions. Therefore, the use of Machine Learning in orthodontics remains largely unexplored due it being a very vast field. In this study, dental images of three thousand six hundred (3600) patients were used to predict the malocclusion . It included the images both before and after the treatment. The results of this study demonstrate the effectiveness of convolutional neural networks in accurately classifying different types of orthodontic treatment. The findings reveal the potential for machine learning to assist orthodontists in treatment planning decisions, providing valuable decision support to orthodontists and improving patient outcomes, thus opening avenues for further advancements in orthodontic care.



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sciforum-107356: A recommender system approach for adaptive human-machine interfaces using deep learning techniques.

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As industrial environments progress from Industry 4.0 to Industry 5.0, intelligent and adaptive human-machine interfaces (HMIs) capable of dynamic response to changing operational conditions are becoming a tangible reality. This research proposes an advanced recommendation system designed to refine the layout and organization of HMI components by leveraging cutting-edge deep learning techniques. The primary objective of the system is to provide contextual recommendations that improve user interface design based on a wide range of factors, including process variables, user roles, and operational demands.

The proposed recommendation system will analyze a comprehensive set of data sources, including real-time process variables, role-specific requirements, and historical performance data, to generate the most effective and personalized configurations of user interface components. By applying deep learning methods, the system will learn from a vast array of existing HMI designs and interaction patterns, enabling it to suggest interfaces that are not only efficient but also tailored to the unique needs and capabilities of individual operators.

Moreover, the system will continuously adapt these recommendations as operational conditions evolve, ensuring that the HMI remains responsive, intuitive, and effective across various industrial scenarios. This adaptive approach is expected to significantly improve operator performance, reduce human error, enhance system resilience, and ultimately contribute to the overall optimization of industrial processes in complex environments.



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sciforum-099047: A Rule-Based Model For Stemming Hausa Words

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The increasing number of online communities has led to significant growth in digital data in multiple languages on the Internet. Consequently, language processing and information retrieval have become important fields in the era of the Internet. Stemming, a crucial preprocessing tool in natural language processing and information retrieval, has been extensively explored for high-resource languages like English, German, and French. However, more extensive studies regarding stemming in the context of the Hausa language, an international language that is widely spoken in West Africa and one of the fastest-growing languages globally, are required.

This paper presents a rule-based model for stemming Hausa words. The proposed model relies on a set of rules derived from the analysis of Hausa word morphology and the rules for extracting stem forms. The rules consider the syntactic constraints, e.g., affixation rules, and performs a morphological analysis of the properties of the Hausa language, such as word formation and distribution.

The proposed model's performance is evaluated against existing models using standard evaluation metrics. The evaluation method employed Sirstat's approach, and a language expert assessed the system's results. The model is evaluated using manual annotation of a set of 5,077 total words used in the algorithm, including 2,630 unique words and 3,766 correctly stemmed Hausa words. The model achieves an overall accuracy of 98.8%, demonstrating its suitability for use in applications such as natural language processing and information retrieval.



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sciforum-107673: Accessible Vision: Empowering the Visually Impaired through Voice-Assisted Object Recognition and Spatial Awareness

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This research paper introduces Accessible Vision as an innovative assistive technology meant to improve the independence and reliance of people with visual impairments on context-aware assistive technologies by employing intricate computer vision algorithms. This system is composed of the following functional components: YOLOv8 model for real-time object detection, MiDaS for distance measurement together with stereo vision, and a TTS for real-time audio feedback for the blind. Precisely, this helps visually impaired people to achieve an improved picture of their environment by giving them accurate information on the objects in the vicinity and their relative position in space. The main focus of Accessible Vision is to respond to the unique difficulties that people with vision impairment have to face in order to make it through daily environments. Many conventional assistive devices are not capable of delivering the processing of real-time features nor how accurate they are regarding the recognition of objects and space. Since YOLOv8 yields high performance, our approach enables the recognition of numerous objects with high speed and recall accuracy. Moreover, for estimating depth information for monocular cameras or for stereo vision, the applicability of MiDaS is again beneficial since distance measurements are critical for orientation. The working procedure of the system has been described in our methodology section, which outlines the following steps: Firstly, the YOLOv8 model\cite{lou2023dc} was trained and optimized on a broad dataset of objects in different settings to increase the algorithms' adaptability to various conditions. It also provides comparison between MiDaS and stereo vision as well as the geeks and ticks of both approaches under different context. The incorporation of the TTS model is explained in this paper's context, with a focus on its function of availing satisfactory and contextually relevant sound prompts to the user.



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sciforum-104436: Accurate Classification of Acute Lymphoblastic Leukemia Subtypes Using Stacked Ensemble Learning on Peripheral Blood Smear Images

Tiar Mohamed Lakhdar * and Terki Nadjiba

University Mohamed Khider Biskra

In this study, we leveraged a publicly available dataset containing 3256 peripheral blood smear (PBS) images, prepared in the bone marrow laboratory of Taleqani Hospital in Tehran, Iran. This dataset consists of blood samples from 89 patients suspected of Acute Lymphoblastic Leukemia (ALL). The images were captured using a Zeiss camera at 100x magnification and stored as JPG files. The dataset is divided into two primary classes: benign hematogones and malignant lymphoblasts. The malignant lymphoblasts are further categorized into three subtypes: Early Pre-B, Pre-B, and Pro-B ALL. The definitive classification of these cell types and subtypes was performed by a specialist using flow cytometry tools.

To classify these images into four distinct categories, we employed a stacked ensemble learning approach. Our model stack included three base models, DenseNet121, VGG16, and VGG19, with a K-Nearest Neighbors (KNN) classifier acting as the meta-model. This ensemble method capitalizes on the strengths of each individual model to improve overall classification performance. Our approach achieved a high accuracy of 94%, demonstrating its robustness and reliability in distinguishing between the various cell types and subtypes within the dataset.

The significant accuracy attained underscores the potential of advanced machine learning techniques in medical image analysis, particularly in the context of hematological malignancies. Our findings suggest that such methodologies could greatly enhance diagnostic precision and efficiency, leading to better patient outcomes. This study illustrates the promising application of deep learning models in the automated classification of ALL subtypes, paving the way for future advancements in the field.



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sciforum-103263: Acquiring News Texts about Public Security for the construction of Corpora in Portuguese

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The acquisition of texts for the purpose of composing corpora in specific domains from sources on the social web is a process that requires analyzing the structures of websites where the texts are published. This involves searching for specific fields to guide the access of responsible agents, known as scrapers. With these texts in hand, performing more refined analyses focused on tasks such as named entity recognition, text summarization, sentiment mining, and associated classifications (e.g., opinion polarities) becomes possible. This article aims to demonstrate the process of acquiring news texts in the domain of public safety in Brazil to build corpora in the Portuguese language. Since Portuguese still lacks dedicated corpora on this topic, scraping agents were developed for three initial news sources in the Northeast region, specifically in the states of Alagoas, Pernambuco, and Rio Grande do Norte. Based on these scraping agents, the corpora were stored in a cloud-based schema for use in an ongoing research project to analyze texts related to public safety to support decision-making processes. The constituted corpus enabled the execution of multiple preliminary analyses, including the identification of crime patterns, sentiment analysis in public security reports, and the mapping of risk areas. These analyses provided valuable information that can support the formulation of public policies and the development of more effective security strategies.



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sciforum-100568: AI-Driven Detection and Treatment of Tomato Plant Diseases Using Convolutional Neural Networks and OpenAI Language Models

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Plant diseases pose a significant threat to global food security, particularly affecting tomato crops that are vulnerable to various pathogens. Despite advancements in disease identification methods, farmers continue to experience substantial decreases in yield due to delayed and imprecise diagnoses, along with inadequate treatment recommendations. This research aims to address this critical issue by developing an innovative Artificial Intelligence (AI)-based system that can detect tomato plant diseases and provide effective treatment suggestions. To achieve this, a Convolutional Neural Network (CNN) based on the InceptionV3 architecture has been trained using a comprehensive dataset of 11,000 tomato leaf images representing nine different diseases and healthy samples. The approach combines deep learning techniques for accurate image classification with natural language processing, leveraging OpenAI's GPT-3.5 Turbo model to generate customized treatment recommendations. The results demonstrate the exceptional performance of the model, with a training accuracy of 99.85% and a validation accuracy of 88.75%. Rigorous evaluation using confusion matrices and assessment metrics further confirms the model's high precision and recall rates for different disease categories, showcasing its robust generalization capabilities. Furthermore, the inclusion of an intuitive Streamlit interface enhances user experience and ensures practical applicability in real-world scenarios. This study makes a significant contribution to agricultural technology by providing a comprehensive solution that integrates precise disease detection with actionable treatment guidance. The developed system holds immense potential to revolutionize tomato crop management practices, potentially minimizing financial losses and promoting sustainable agriculture through targeted disease management strategies.



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sciforum-104122: An data engineering architecture for analyzing the Zone of Proximal Development of public school students in Brazil

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In the didactic approach, Lev Bygotsky developed what he would classify as ZDP: Zone of Proximal Development, whose main objective would be to measure student learning. This demonstrate how data engineering can facilitate the classification of ZDP for use in brazilian public schools.

Therefore, the use of mining tools, like Scrapy or Beautiful Soup, was essential for collecting students' pedagogical data from the platforms of the Alagoas state government. With the data in hand, it was up to the teacher to define the student's learning zones, based on teaching goals under the subject syllabus: assessments, activities and playful moments for the student's understanding of the subject studied. Thus, with the influence of the teacher and the information collected from the student, it was possible to create a machine learning model, specifically a supervised classification model, which evaluates the student's performance and returns the current learning level, taking into account their pedagogical needs to be delivered to the teacher. With the application, public school teachers were able to diagnose students according to their pedagogical needs, directly influencing student performance when these needs were met. This data architecture was able to directly meet a need that is still evident in public schools in the state of Alagoas in Brazil.



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sciforum-104274: An Effective Heart Disease Prediction Model Using Hybrid Machine Learning

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Heart disease is becoming one of the critical diseases day by day in the current global scenario. Clinical data analysis faces huge challenges in heart disease prediction due to the increased number of cases and common symptoms across multiple diseases. Thus, this work attempts to improve the early detection of heart failure to save lives. It employs machine learning algorithms, including logistic regression, Decision Tree, Random Forest, K-nearest neighbors Algorithms, Support Vector Machine, Stochastic Gradient Decent, Multi-layer perceptron (MLP), XGBoost, Ada Boosting, Extra Tree, Gaussian Naïve Bayes, and Gradient Boosting Algorithm (GBA), to compare their performance to achieve this task. Further, this paper proposes an enhancement to the proposed hybrid Multi-layer perceptron (MLP) model with the Gradient Boosting Algorithm (GBA) by developing a novel feature set that achieves the highest possible accuracy scores. All methods have been successfully validated using the cross-validation method. The efficacy of the proposed model was evaluated by using evaluation metrics such as accuracy, precision, recall, and F1 score. The hybrid proposed model predicts early heart disease with a 98% accuracy rate, according to the results, demonstrating extraordinary accuracy. This grouping combination leads to enhanced accuracy, robust feature selection, better treatment of high-dimensional and unnecessary data, and improved simplification and interpretability. This proposed work has important scientific value in the medical field for improving cardiovascular risk assessment.



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sciform-106421: An Investigation on the Most Used Programming Language for Developing Applications in Software Development Industries (Case study of Kano State Nigeria)

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The software development industry in Kano State, Nigeria, has seen rapid growth in recent years, driven by increasing demand for mobile and web applications. With the availability of various programming languages, understanding the most commonly used language is essential for developers to enhance their skill sets, allocate resources more efficiently, and drive industry growth. This study aimed to identify the most widely used programming language in Kano's application development sector and to explore the factors influencing its adoption. The research employed a mixed-methods approach, including surveys, interviews, and observations, to gather data from software development companies operating in Kano. Stratified sampling was used to select ten companies, representing a range of sizes and specializations within the industry. Questionnaires were designed to collect information on programming language usage, the factors influencing language adoption, and the demographic details of the developers. In addition to this, interviews with industry experts and experienced developers provided further qualitative insights. The results indicate that Java is the most commonly used programming language in Kano's application development industry, accounting for 40% of usage. Python follows with 30%, while JavaScript is used in 20% of projects. Other languages, including C++, C#, and PHP, make up the remaining portion. The primary factors driving programming language adoption in Kano include the specific requirements of projects, the skill levels of developers, and industry trends. These findings have important implications for developers and companies looking to optimize their development processes and stay competitive in a fast-evolving market.



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sciforum-105411: Application of quantum computing algorithms in the synthesis of control systems for dynamic objects

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Currently, the main focus in the automation of technological processes is on developing control systems that enhance the quality of the control process. Because the systems being controlled are often complex, multidimensional, and nonlinear, quantum computing algorithms offer an effective solution. Although there are several intelligent control methods available to improve the quality of technological processes, each has certain drawbacks. Quantum algorithms, which rely on the principles of quantum correlation and superposition, are designed to optimize control while minimizing energy and resource consumption. This article discusses the diesel fuel hydrotreating process, a critical step in oil refining. The primary goal of hydrotreating is to enhance fuel quality by removing sulfur, nitrogen, and oxygen compounds. To accurately model this process, it is essential to consider not only the external factors affecting it but also its physical characteristics. By doing so, the mathematical model becomes more precise. Based on this approach, a quantum fuzzy control system for the diesel fuel hydrotreating process was developed using quantum algorithms. These algorithms can rapidly analyze large amounts of data and make decisions. At the same time, a computer model of a fuzzy quantum control system for the process of hydrotreating diesel fuel was constructed, and a number of computational experiments were carried out. As a result, a 1.8% reduction in energy costs for the diesel fuel hydrotreating process was achieved.



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sciforum-104192: Artificial Intelligence in the Pharmaceutical Sector: Revolutionizing Drug Discovery and Research

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Artificial Intelligence (AI) has come a long way in healthcare, having played significant roles in data and information storage and management—such as in patients' medical histories, medicine stocks, sale records, and so on; automated machines; and software and computer applications like diagnostic tools, including MRI radiation technology, CT diagnosis, and many more—all of which have been created to facilitate and simplify healthcare measures. Without a doubt, artificial intelligence (AI) has transformed healthcare over the past few decades to become more effective and efficient, and the pharmaceutical industry is not an exception. AI has had several implications for the pharmaceutical industry. The first sector is Drug Development and Discovery: businesses such as Atomwise accelerate the early phases of drug discovery by using AI for virtual screening, which predicts the behavior of various compounds. The second sector is clinical studies; by identifying suitable participants, forecasting results, and continuously monitoring patient data, artificial intelligence (AI) assists in the design of more effective clinical studies. AI is used, for instance, by IBM Watson Health to match patients with suitable clinical trials by analyzing patient data. The third sector is personalized medicines; AI is used in personalized medicine to customize care based on each patient's unique genetic profile. Businesses like Tempus help doctors tailor cancer treatment regimens by using AI to evaluate clinical and molecular data. The fourth sector is Supply Chain Management; AI makes the supply chain more efficient by forecasting demand, controlling inventories, and guaranteeing that medications are delivered on time. This lowers expenses and boosts productivity in the pharmaceutical sector. This analysis highlights the advantages and disadvantages of the many AI-based techniques used in pharmaceutical technology.



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sciforum-104385: Artificial intelligence-supported intuitive Inherent irrigation approach employing Zigbee and Arduino in wireless sensor networks

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An inventive use of technology in agriculture is an artificial intelligence-supported intuitive irrigation system that makes use of Arduino and Zigbee in a wireless sensor network. This system makes use of wireless connection, microcontrollers, sensors, and AI. An open-source microcontroller framework serves as the system's brain, gathering information from detectors and managing irrigation equipment. A variety of sensors are positioned across the field to measure various parameters, including relative humidity and air temperature. One of the most crucial issues that needs to be taken into consideration while creating wireless sensor networks is energy conservation. The goal of this research is to figure out how to automate irrigation. This system creates a smart and fully-automated watering arrangement. In order to establish the ideal watering needs of plants, this system first uses artificial intelligence to evaluate a range of environmental characteristics, including soil moisture, the temperature, and the weather. This makes it possible to precisely and strategically water plants, lowering the possibility of stress on plants and production losses brought on by either exceeding or under-watering. Second, using microcontrollers such as Arduino offers a flexible and robust environment for processing, controlling, and gathering data. Thirdly, the system's numerous components, such as detectors, Arduino circuits, and actuators, can communicate with one another more efficiently through the Zigbee wireless sensor network. Zigbee is perfect for large-scale installations because to its low power consumption and strong mesh networking capabilities, which makes it easier to create a decentralized and networked irrigation system.



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sciforum-103972: Asymmetric logistic model applied as an activation function in artificial neural networks

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In recent years, Artificial Neural Networks (ANNs) have stood out among machine learning algorithms, being successful in a huge range of applications, especially in recognizing image, audio and video patterns, as well as in natural language analysis. The use of activation functions plays a crucial role in the operation of these algorithms, directly influencing the representation capacity and training effectiveness of ANNs. The logistic (or sigmoid) function is often used as a standard activation function in many neural network models due to its favorable properties of non-linearity and smooth derivatives. However, the existing literature lacks in-depth investigations into the potential of the Skew-Logistic (SL) function as a viable alternative, especially in scenarios where asymmetry in the data is a common reality. This work aims to investigate the SL function as an activation function in ANNs, exploring its ability to deal with asymmetric data. To achieve this, the SL function was implemented computationally in different neural network architectures. The models were trained on various databases selected for the experiments, and their performance was evaluated using standard metrics such as accuracy, precision, recall and F1-score. This procedure was carried out in each experiment with the SL and sigmoid activation functions in order to compare them. The results indicate that SL can bring improvements to the models in some asymmetric data sets, in which a significant increase in performance metrics was observed compared to the traditional logistic function. It was also noted that in binary classification tasks, SL can improve accuracy or sensitivity, depending on the sign of the asymmetry factor selected, predicting fewer false positives or fewer false negatives. It is concluded that the SL function offers a viable and promising alternative to conventional activation functions, providing better adaptation to asymmetric datasets.



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sciforum-106128: Ausculmate: Neural Networks for Better Patient Care

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A crucial part of examining patients suspected of having respiratory diseases is auscultation. Doctors use a stethoscope to listen to breath sounds to diagnose lung conditions. These noises, such as wheezes and crackles, indicate different respiratory conditions. Nevertheless, distinguishing these sounds is frequently reliant on the doctor's expertise and is subject to interpretation, underscoring the necessity for a more impartial method. This research presents a method that utilizes deep learning to examine lung sounds. The setup includes an electronic stethoscope for collecting chest noises, a smartphone application for recording and tracking patient information, and a sophisticated artificial intelligence model for categorizing chest sounds. Data preprocessing for audio involves normalization, temporal segmentation, applying Short-Term Fourier Transform (STFT), and converting data into spectrograms suitable for CNN input. The CNN is trained using multilabel classification methods, utilizing categorical cross-entropy as the loss function and assessing metrics like accuracy, precision, recall, F1-score, and ROC curve examination. The mobile app, which is easy to use, utilizes Flutter for the frontend and MongoDB and Django for the backend and database, respectively, guaranteeing compatibility across platforms, as well as speed and scalability.

This study suggests a practical categorization of lung noises as wheezes, crackles, and normal states. The performance metrics of the model indicate its potential value in clinical environments, with a validation precision of 96.42%, a recall of 94.75%, and a validation loss of 0.15. The combination of an e-stethoscope, mobile app, and DL model in the automated analysis system for lung sounds shows great potential in enhancing the accuracy of diagnosing respiratory diseases. This approach has the potential to improve patient outcomes by reducing the subjectivity of traditional auscultation, leading to more accurate and timely intervention.



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sciforum-106452: Automated Detection and Classification of Malaria Parasites in Microscopic Images Using Deep Learning Techniques

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Malaria, a life-threatening disease caused by Plasmodium parasites, remains a major global health challenge, particularly in regions with limited access to medical resources. Traditional diagnostic methods, such as microscopic examination of blood smears, are labor-intensive, time-consuming, and susceptible to human error, leading to delays in diagnosis and treatment. To overcome these challenges, we propose an automated system leveraging advanced computer vision and deep learning techniques, specifically utilizing the region-based fully convolutional neural network (R-FCN) object detection model. The R-FCN model is particularly adept at identifying and localizing objects within images, making it highly suitable for the accurate detection and classification of malaria parasites. Our system is trained on a labeled dataset of approximately 1,328 images, each annotated with bounding boxes to highlight the presence of malaria parasites. Through rigorous experimentation, our proposed system has demonstrated superior performance to baseline methods, achieving higher accuracy and efficiency in parasite detection. By automating the diagnostic process, our system significantly reduces the need for human intervention, thereby minimizing errors, accelerating diagnosis, and improving patient outcomes. Moreover, this approach holds great promise for streamlining the malaria diagnosis and treatment process globally, contributing to a broader effort to combat this devastating disease and enhance public health outcomes in affected regions.



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sciforum-104475: Automated Digital Modeling of Corrugated Board Structures Using Image Processing and Metaheuristic Techniques

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Corrugated board is widely used as an eco-friendly and robust material in the packaging sector. Ensuring the proper mechanical properties of such composite materials is crucial. Therefore, designing packaging made of corrugated board often involves various numerical techniques to analyze the mechanical behavior of the structure under specified loads. To expedite the process of creating digital models of corrugated board, this study introduces an algorithm that leverages image processing techniques.

The proposed algorithm consists of two stages. The first stage utilizes basic image processing methods to extract geometrical parameters of the corrugated board, including layer and overall board thickness, as well as flute height. It also determines the locations of the center lines of each layer. In the second stage, it is assumed that the flutes can be modeled as a sinusoidal function. An objective function is defined based on the sum of the distances between the points of the potential sinusoidal function and the corresponding points on the binary image obtained in the first stage.

This study compares the effectiveness of four metaheuristics—genetic algorithms, particle swarm optimization, simulated annealing, and surrogate optimization—in refining the sinusoidal model of the flutes. The algorithm was successfully applied to three- and five-layered corrugated boards, demonstrating its capability to accurately model the geometric structure and support the design of packaging with optimized mechanical properties.



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sciforum-107405: Can Benford's Law Serve As A Data Science Tool?

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Making meanings out of the huge amounts of data that are generated almost every second across the globe is becoming an important data science concern. Discovering a unique feature(s) that can aid in the classification, prediction, and general analysis of a particular system under consideration could be considered a major task of data science. Data science tools are desperately needed to draw insights from the vast amounts of data that are generated for critical decision-making and planning for the government, businesses, military, politics, and academia, amongst several other critical organizations. In this paper, our motivation is to investigate whether Benford's law can serve as a data science tool. For this, experiments were performed on Point of Sale (POS) datasets. POS key features such as TranTime (Transaction time in seconds), BreakTime (Break time including idle time in seconds), ArtNum (Number of items, i.e., basket size), and Amount (Transaction value) served as inputs into Benford's law. Results obtained showed that the Amount feature of the POS system perfectly conforms to Benford's law based on its plots and chi-square divergence. The results showed that normal Amount transactions on POS systems followed Benford's law, whereas fraudulent/tampered POS Amount transactions deviated from this law. We found that Benford's law can actually serve as a data science tool by giving us insights into POS operations.



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sciforum-104110: Can Virtual Worlds be used as Intelligent Tutoring Systems to innovate teaching and learning methods? Future challenges for Metaverse and Artificial Intelligence in education.

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The continuous evolution of digital technologies enriches the panorama of possible opportunities that digital transformation offers to the advantage of the educational system in reference to new ecological systems and sustainable teaching methodologies for the benefit of increasingly interactive, personalized and effective learning.

Among the different types of interactive learning environments, there is a growing expanse of literature on virtual worlds as risk-free educational contexts capable of enhancing today's critical life skills such as critical thinking, creativity, communication and collaboration, of increasing new digital skills and of supporting students in their learning process.

At the same time, we are witnessing an increase in the use of Artificial Intelligence in education and, in particular, among the Adaptive Learning Systems, Intelligent Tutoring Systems are configured as valid solutions to support students in an increasingly personalized and student-centered learning process.

Based on recent studies in the literature on the use of virtual worlds in the processes that accompany students in effective learning and that offer collaborative learning spaces in which to co-construct knowledge, this paper aims to point out the characteristics of virtual worlds, through the analysis of recent case studies, and those of Intelligent Tutoring Systems in order to outline similarities between the two learning systems, defining the possible future challenges that affect the combined use of the Metaverse and Artificial Intelligence in education.



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sciforum-104795: Comparative Analysis of LSTM and GRU Models for Chicken Egg Fertility Classification using Deep Learning

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This study explores the application of advanced Recurrent Neural Network (RNN) architectures—specifically Long Short-Term Memory (LSTM) and Gated Recurrent Unit (GRU)—for classifying chicken egg fertility based on embryonic development detected in egg images. Traditional methods, such as candling, are labor-intensive and often inaccurate, making them unsuitable for large-scale poultry operations. By leveraging the capabilities of LSTM and GRU models, this research aims to automate and enhance the accuracy of egg fertility classification, thereby contributing to agricultural automation. A dataset comprising 240 high-resolution egg images was employed, resized to 255x255 pixels for optimal processing efficiency. LSTM and GRU models were trained to discern fertile from infertile eggs by analyzing the sequential data represented by the pixel rows in these images. The LSTM model demonstrated superior performance, achieving a validation accuracy of 89.58% with a loss of 1.1691, outperforming the GRU model, which recorded a lower accuracy of 66.67% and a significantly higher loss of 12.6634. The LSTM's complex gating mechanisms were more effective in capturing long-range dependencies within the data, leading to more reliable predictions. The findings suggest that LSTM models are better suited for precision-critical applications in poultry farming, where accurate fertility classification is paramount. In contrast, GRU models, while more computationally efficient, may struggle with generalization under constrained data conditions. This study underscores the potential of advanced RNNs in enhancing the efficiency and accuracy of automated farming systems, paving the way for future research to further optimize these models for real-world agricultural applications.



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sciforum-101559: Computing Discrete Simulations for Efficient Queuing Management of Financial Aid Services

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Introduction

Managing bank queues efficiently is crucial for maintaining customer satisfaction, operational efficiency, and compliance with regulations. Nevertheless, it involves overcoming significant challenges related to demand variability, resource constraints, and the need for technological and procedural adaptations. During emergency crises such as the COVID-19 pandemic, offering robust measures for discrete simulations becomes challenging due to significant and unexpected variations in customer arrival rates. This study proposes computing discrete event simulations based on queuing theory and tests of the empirical probability distribution for each particularity to support improvements in waiting times for segments of *Caixa Econômica Federal* (CEF) responsible for financial aid services (Express, Tellers, and Gov-Social sectors).

Methods

The methodology involves conducting discrete event simulations (DES) using real-time data collection to accurately model customer arrival and service rates. Key parameters included the expected queue length, waiting time, and number of arrivals per unit time, based on service time, the number of servers, the number of clients, and the average waiting time per month. We apply the Kolmogorov-Smirnov test to identify the most fitting probability distributions for these rates, adjusting them as needed on each scenario.

Results

The computing simulations indicated a potential reduction in queue size by approximately 45%. Specifically, hiring at least one more employee for the Express sector in some specific production scenarios could decrease the average waiting time from 36 minutes to 17 minutes, thereby increasing the capacity to serve more customers. In extreme pandemic scenarios, six more employees are necessary to maintain reasonable service times.

Conclusions

The study's findings suggest that strategic employee allocation can significantly improve service efficiency in high-demand sectors at CEF. By implementing the recommended staffing changes, financial institutions can offer satisfactory service, enhance business profitability, and better manage the effects of the pandemic or similar public emergency contexts.



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sciforum-104327: Conflicts management of users comfort preferences in a smart environment, a case of study

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Managing user comfort preferences in a smart environment presents unique challenges due to conflicting requirements and expectations. This paper explores innovative strategies to harmonize diverse user preferences within shared smart spaces. As smart environments become increasingly prevalent in homes, offices, and public buildings, the need to accommodate individual comfort settings for temperature, lighting, and noise while minimizing conflicts among users becomes critical.

This study investigates a specific case within a multi-occupant smart building, analyzing how conflicts in comfort preferences are identified, addressed, and resolved. By implementing a dynamic preference management system, which utilizes machine learning algorithms and real-time data analytics, the proposed solution aims to balance and optimize individual comfort levels. The system considers historical data, context-aware adjustments, and predictive modeling to preemptively address potential conflicts.

The findings demonstrate that integrating advanced computational techniques with user feedback mechanisms significantly enhances the overall comfort experience. The research highlights the importance of adaptive systems that can learn and evolve with user preferences, ultimately leading to more harmonious coexistence in shared smart environments.

This paper contributes to the field of smart environment management by providing a comprehensive framework for conflict resolution and offering practical insights into the deployment of user-centric comfort management systems. The case study underscores the potential of technology to create more responsive and personalized smart environments that cater to the diverse needs of their occupants.



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sciforum-107458: Customized Learning for ADHD: An AI-Driven Assistive Study App

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In this paper, we discuss and address the significant educational disparity and academic challenges encountered by students diagnosed with Attention Deficit Hyperactivity Disorder (ADHD). Traditional learning environments often fail to accommodate the unique cognitive needs and attention deficits of these students, leading to difficulties in focusing, retaining information, and managing study schedules effectively. Consequently, lower academic performance, increased stress levels, and diminished self-esteem are common consequences.

The goal of this study is to provide a solution that caters to the diverse learning needs of students with Attention Deficit Hyperactivity Disorder. Our project introduces an innovative educational app specifically designed for this demographic. The app utilizes a personalized learning system that adapts to individual preferences, integrating Artificial Intelligence to provide intelligent responses. Key features include screen-time monitoring, daily schedule management, group study jams, and study reminders. Moreover, this solution emphasizes affordability and accessibility, particularly targeting students with limited resources. By addressing the key challenges faced by students with Attention Deficit Hyperactivity Disorder in traditional learning environments, our educational app aims to empower them with the tools necessary to thrive academically and mitigate the negative consequences associated with their condition. We propose a novel way to address Attention Deficit Hyperactivity Disorder by using a smart Artificial Intelligence-based application.



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sciforum-104112: Data architecture to facilitate the diagnosis of arboviruses.

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Arboviruses are diseases caused by viruses transmitted by mosquitoes, with dengue, chikungunya, and Zika being the most common in urban environments, transmitted by *Aedes aegypti*. In Brazil, dengue poses a constant threat, with over 3 million cases reported in 2024. Arboviruses share similar characteristics, complicating accurate diagnosis and treatment, and under-reporting remains a significant challenge. To improve diagnosis and treatment, a system is proposed that integrates and standardizes data collected at health posts. This system utilizes artificial intelligence algorithms to diagnose and suggest treatments.

Challenges include collecting relevant patient data, such as temperature, symptoms, and travel history, through electronic medical records (EMRs), which avoid paper waste and ensure information security and organization. Additionally, ensuring the accuracy and completeness of data collection is crucial for the effectiveness of the proposed system. After collection, the data must be stored in appropriate database systems, depending on whether they are structured or unstructured.

Subsequently, the ETL (extraction, transformation, and loading) process is necessary to move the data to suitable repositories, enabling the use of machine learning algorithms. These measures aim to improve diagnostic accuracy and treatment effectiveness for arboviruses, contributing to saving lives.

Furthermore, continuous monitoring and updating of the system are required to adapt to new strains of arboviruses and emerging health threats. Public health education and awareness campaigns are also essential to encourage the public to participate in prevention measures, such as eliminating mosquito breeding sites. By addressing these challenges, the proposed system can significantly enhance public health responses to arboviruses outbreaks, ultimately reducing the burden of these diseases and saving lives.



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sciforum-104516: Data-Driven Insights: Leveraging machine learning in house price prediction

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Accurate and efficient prediction of house prices is a critical challenge in the real estate market. This research aims to develop a robust machine learning model capable of estimating property values. By systematically analyzing key determinants of house prices, including location, square footage, and number of bedrooms, this study seeks to contribute to the advancement of property valuation methodologies. Our research investigated the complex interplay between house features and their corresponding prices. The study involved the meticulous examination of a comprehensive dataset, allowing for a thorough understanding of market trends and patterns. Various machine learning algorithms were rigorously tested and compared to identify the most effective model for predicting house prices. The findings of this research demonstrated that linear regression emerges as the superior algorithm for estimating property values within the given dataset. Furthermore, the study highlights the significant influence of specific features, such as bathroom and bedroom numbers, on predicted prices. These insights underscore the importance of considering a holistic range of factors when evaluating property values. The developed model holds the potential to revolutionize the real estate industry by providing stakeholders with a reliable tool for informed decision-making. By accurately predicting house prices, this research contributes to enhancing market efficiency, optimizing investment strategies, and supporting equitable property valuations.



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sciforum-100506: Detection Of Students' Emotions In An Online Learning Environment Using The Cnn-Lstm Model

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Abstract: Emotion recognition, particularly through facial expressions, has become vital across diverse domains like healthcare, entertainment, and education, providing insights into user experiences and guiding decision-making processes. However, the realm of education, particularly in online learning environments, presents distinct challenges. Traditional emotion recognition approaches are insufficient to capture the emotional states expressed by students during the learning process. This research addresses this gap by introducing the concept of learning emotions, specifically emotions like interest, boredom, and confusion, exhibited by learners during online lectures. This research presents a novel approach for recognizing learners' emotions in online learning environments using a deep learning architecture combining convolutional neural networks (CNNs) and long short-term memory (LSTM) networks. The proposed model aims to improve emotion recognition accuracy and enhance the online learning experience. A custom dataset was created by mapping action units from existing emotions in the FER2013 dataset to new emotion categories (interested, confused, and bored). The model was trained and evaluated on this dataset, achieving an accuracy of 98.0%, precision of 97%, recall of 98%, and F1-score of 98%. These results surpass existing approaches for emotion recognition, demonstrating the effectiveness of the CNN-LSTM model in recognizing learners' emotions. This research contributes to the development of affective computing in online learning environments, enabling personalized support and improved learning outcomes. The proposed model has potential applications in various fields, including education, psychology, and human-computer interaction.



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sciforum-101688: Digital Semantics for Enterprise Information Systems Development

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Introduction: Artificial Intelligence (AI) is the most important paradigm shift of our time. Its purpose is to simulate human intelligence inside a machine, and it's already affecting many aspects of our life. The core of AI research concerns defining solutions to get, understand, store and elaborate digital inputs in order to return results: solutions to think like a human being. Our contribution is a position paper about our vision and ideas on this topic. Our proposal is additional to current AI approaches: it aims to integrate the path of knowledge and development of AI. **Methods:** the literature on AI regarding proposals, approaches and models is vast and encompasses an enormous number of application domains. Our research goal is to propose a paradigm to simulate human intelligence within a computer, limited to the Enterprise Information System (EIS) domain, by means of automata and ontologies. Nowadays automata are used in Software Engineering to manage decision-making processes and control the information flow within a software system. The term "ontology" has several meanings, depending on the discipline and domain. In the EIS domain, by "ontology" we mean a set of concepts and relationships that represent a knowledge area. We propose the Digital Semantics (DS), a novel paradigm and definition to our knowledge. DS is the proposed solution to define ontologies, which in turn will have to be implemented through automata. To reach this goal, we answer 3 Research Questions (RQs): (RQ1) Is it possible to define Digital Semantics as a metamodel based on the semantics of natural languages? (RQ2) Is it possible to define ontologies with Digital Semantics? (RQ3) Can automata be the solution to implement ontologies defined with Digital Semantics? **Conclusions:** the aim of the paper is to answer to the RQs and obtain feedback from the international scientific community.



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sciforum-104309: Emulation of manufacturing equipment through the dynamic generation of graphic and interactive environments

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The work presented in this paper is part of an Industry 4.0—Factories of the Future project, which explores the use of intelligent multi-agent architectures to control flexible manufacturing units. The concept of flexibility results from the ability to adapt manufacturing processes in an agile way to context variations, whether these result from changes in the references under production, the priority and quantity of orders, limitations to or unavailability of equipment, or a lack of components. Studying control solutions for such diverse environments and with such different contexts is a complex task, particularly with regard to validating and evaluating the control solutions. Mass application in a real context is impractical, at least in the initial stages, so the only option is to resort to simulation, which is perfectly suitable for scientific validation but not flexible and practical enough to be used as proofs of a more practical nature or for demonstrations. It is in this context that the work presented here was developed. The result is a framework that is used to generate virtual manufacturing equipment. Assuming that the behavior of the equipment is described according to a code routine, this framework allows for annotating the state, input, and output variables, and based on this, it generates a virtual version of the equipment with a graphical and interactive interface that can be interconnected with other virtual and real equipment. In this way, it is possible to replicate a manufacturing unit with real and virtual equipment and test the practical behavior of the control solutions, allowing us to interact with the equipment (for example, turning off the equipment, injecting faults, conditioning the production rate, etc.) and, thus, pragmatically and visually assess the behavior of the entire solution.



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sciforum-106092: Enhancing High-Resolution MRI for Precise Diagnosis and Treatment of Atypical Teratoid Rhabdoid Tumor

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Atypical Teratoid Rhabdoid Tumor (ATRT) is an aggressive brain tumor in children, requiring precise imaging for accurate diagnosis and effective treatment planning. High-resolution Magnetic Resonance Imaging (MRI) is essential for visualizing ATRT, but traditional imaging methods face challenges in detecting and analyzing such rare tumors. This study examines the use of advanced machine learning models to improve MRI analysis for ATRT, aiming to enhance diagnostic accuracy and treatment outcomes. The study utilizes cutting-edge deep learning models, including Vision Transformers (ViTs), ResNet-based Convolutional Neural Networks (CNNs), and Generative Adversarial Networks (GANs). These models were customized for specific tasks such as tumor detection, segmentation, and classification. To overcome the issue of limited data for rare tumors, techniques like transfer learning, multi-scale image processing, and synthetic data augmentation were applied. These deep learning approaches led to enhanced tumor segmentation, providing more detailed visual analysis, which is crucial for developing precise treatment strategies. By optimizing high-resolution MRI scans with these technologies, the study seeks to assist clinicians in making better-informed decisions for ATRT treatment. The integration of these advanced techniques shows promise for improving diagnostic precision and tailoring treatment plans, representing a notable advancement in pediatric neuro-oncology. Ongoing refinement of these methods is key to furthering progress in ATRT diagnosis and management.



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sciforum-101354: Enhancing Spam Email Detection with an Optimized Soft Voting Ensemble Classifier

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Spam email detection is essential for maintaining cybersecurity, protecting user privacy, and reducing security risks. The persistent activity of spammers necessitates continuous advancements in spam filtering methods. This study introduces an automated spam filtering system using an optimized soft voting ensemble classifier to address this challenge. Initially, the process employs the Grid Search Optimizer to fine-tune the parameters of four distinct classifiers: Support Vector Machine (SVM), Random Forest (RF), Naive Bayes (NB), and XGBoost. Subsequently, the final classification is performed using a soft voting ensemble method, combining the optimised classifiers' outputs to enhance overall accuracy in detecting and classifying spam emails. This study evaluates the proposed model using the Spam_Mails Dataset and Enron1 Dataset. The experimental results demonstrate that the proposed ensemble model, which integrates hyperparameter tuning with soft voting, significantly outperforms existing approaches. Specifically, the model achieved accuracies of 99.22% and 99.12% on the Spam_Mails and Enron1 datasets, respectively. Additionally, the ensemble model attained an AUC of 1.00 on both datasets, indicating its high effectiveness in distinguishing between spam and legitimate emails (ham). The ensemble model exhibits superior accuracy, generalization, and robustness compared to individual classifiers. This innovative combination of Grid Search and soft voting results in a highly effective and efficient spam email detection model. The findings underscore the importance of hyperparameter tuning and ensemble learning in enhancing the performance of spam detection systems, setting a new benchmark for future research in this domain.



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sciforum-104093: Ethical Data Engineering for AI in Crime Analysis: Strategies to Minimize Bias and Enhance Fairness

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This research addresses the development of strategies for ethical data engineering in crime analysis, emphasizing the minimization of ethical and racial biases. The focus is on structured datasets, specifically those on hate crimes and police shootings in the United States, sourced from Kaggle. These datasets include both categorical and numerical features, making them appropriate for evaluating diverse techniques before expanding to more complex data types, such as images.

The data engineering process employs various methods to ensure fair representation and reduce bias. For data quality, techniques such as outlier detection, correlation analysis, and feature scaling are utilized to balance the distribution of sensitive attributes and minimize distortions. In the preprocessing stage, issues like missing values, incorrect labels, and potentially biased correlations are addressed. Dataset balancing is achieved through methods including SMOTE, Adaptive Synthetic Sampling, and NearMiss to manage class imbalances and ensure proportional representation. These steps are supported by fairness metrics such as disparate impact and equalized odds to continuously evaluate and refine the model outputs.

Preliminary tests were structured to evaluate the effects of different data engineering strategies on bias reduction. The application of various preprocessing and balancing methods demonstrated that systematic handling of class imbalances and feature distributions resulted in a significant decrease in model bias. Consequently, models showed improved fairness and reduced disparities across sensitive attributes, such as race and gender. These findings indicate that a robust data engineering process can positively impact the ethical performance of AI systems, mitigating issues such as discrimination and underrepresentation.

The results suggest that these strategies effectively enhance both technical and ethical standards in AI systems. Future research will expand this framework to non-categorical datasets, allowing broader applications in public security and beyond.



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sciforum-104037: Evaluating TPUs and GPUs in a Two-Views EfficientNet-based architecture for cancer classification on mammograms: performance and speed analysis

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Introduction

Breast cancer is the most prevalent cancer among women worldwide. Mammography is the primary exam used to detect this disease in its early stages. Currently, radiologists interpret these radiological images, but CAD (Computer-Aided Detection and Diagnosis) systems have been developed to assist in this process. While GPUs have traditionally been used for training these systems, newer hardware like TPUs (Tensor Processing Units) were designed specifically for machine learning tasks, and offer advantages over GPUs that can be explored, such as having more memory.

Methods

This work compared the performance of a two-view mammogram classifier proposed by Daniel Petrini et al. in "Breast Cancer Diagnosis in Two-View Mammography Using End-to-End Trained EfficientNet-Based Convolutional Network" and its components (the one-view classifier and patch classifier) on the public dataset CBIS-DDSM (Curated Breast Imaging Subset of the Digital Database for Screening Mammography). The comparison was made using both a GPUs and TPUs, leveraging the extra memory and specialized architecture of TPUs.

Results

Training on TPUs was up to 18 times faster than on GPUs, a significant increase in training speed, potentially leading to better models in future work. However, no conclusive evidence showed that using higher resolution images with TPUs improved model performance. Metrics (accuracy and ROC-AUC) were similar at 1152x896 (GPU) and at 2304x1792 (TPU).

Conclusions

Despite the classification performance did not improve when increasing exam resolution, the use of TPU is justifiable due to the increase in training speed, opening up possibilities to train with more data and using more complex architectures, which could lead to better classification results.



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sciforum-098286: Evaluation of different filtering strategies for ICESat-2 ATL08 data for evaluation of DEMs for Madurai Region

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A large number of studies over different experimental sites globally has successfully shown the utility of ICESat-2 LIDAR sensor-based datasets for the evaluation of topography (elevation) and water level. The current study evaluates the different filtering strategies for the selection of ATL08 footprints from the Advanced Topographic Laser Altimeter System (ATLAS) instrument based on the terrain uncertainty available in the ATL08 data. The openly accessible digital elevation models (DEMs), namely ASTER GDEM V003, CartoDEM V3 R1, TanDEM-X EDEM Global 30m, and SRTM 1 Arc Second Global, were evaluated for the Madurai Region. The footprints with unknown (null) uncertainties were removed first, and thereafter different datasets were generated for DEM assessment based on uncertainties of 10m, 5m, 2.5, 1, 0.75, 0.5m, 0.25m, and 0.1m. It is observed that the CartoDEM performance is better than ASTER among the optical photogrammetrically derived DEMs, whereas TanDEM-X is better than the SRTM among the SAR Interferometry (InSAR)-based DEMs. Overall, the accuracy of TanDEM-X EDEM was found to be best upon comparison of RMSE among the four openly accessible DEMs used in the analysis. For example, with the filtering strategy of footprints selected with 0.75m uncertainty, the RMSE values for ASTER GDEM V003, CartoDEM V3 R1, TanDEM-X EDEM Global 30m, and SRTM 1 Arc Second Global were 7.14m, 3.68m, 1.52m, and 3.16m, respectively. It is also observed that reducing the uncertainties beyond an uncertainty level does not provide clear estimates due to inherent qualities and errors in different DEMs as well as techniques employed in DEM generation. The results may vary from one DEM to another, thus indicating that a careful selection of DEMs shall be performed before using in any application.



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sciforum-104760: Exploration of Key components in wireless sensor networks utilizing Artificial Intelligence and virtualized security

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Introduction: The future wireless sensor network (WSN) has to be able to autonomously handle a large number of IoT gadgets in actual time, in extremely dynamic circumstances and offer extremely reliable, minimal latency connectivity. In order for wireless sensor networks to behave intelligently and become adaptable to changes in a range of operating environments, artificial intelligence competency must be included. Numerous difficulties arise from the features of WSNs, including a huge number of detector nodes, dense dispersion, dynamic topological structure, storage capacity, and communication proficiency.

Methodology: The use of artificial network approaches to advance wireless sensor networks' adaptation and smart computation capabilities will increase those networks' functioning and persistence rate. In business applications including production automation and health services, wireless sensor networks are becoming increasingly important. In sensor networks, virtualization may offer scalability, economical solutions, and increased management. This article showcases a broad range of cutting-edge virtual sensor network projects. Through the proposed framework, which leverages tiered architecture and distributed agent systems to facilitate cognitive ability, it is feasible to contrive an outcome that allows a sensor network to function as an distributed agent system.

Results: The suggested model highlights how WSN functions and how to make it clever. In situations like smart home automation, medical monitoring, combat surveillance, rock falls, and animal crossings in hilly terrain, a virtual environment in sensor networks may be possible.

Conclusions: An architecture for a multi-source sensor network might be set up to make effective use of the physical organization of sensors. The virtual infrastructure of sensor networks may provide a new business model by enabling a variety of wireless sensor network topologies to coexist on the same hardware substrate. In order to do this, we are developing a virtual machine that will allow for the real virtual environment of WSNs.



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sciforum-104604: Facial Expression Recognition for Identifying Customer satisfaction on Products utilizing Hybrid Deep Learning Models

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Facial expression recognition for identifying customer satisfaction with products is one of the most powerful and challenging research tasks in social communication. AI-based emotion recognition harnesses the collective strength of machine learning, deep learning, and computer vision to decipher the subtleties of human emotions. By intricately analyzing facial expression, including the nuanced movements of the mouth, eyes, and eyebrows. Recent innovations have driven notable progress in face detection and recognition, which enhance performance and reliability. This study focuses on leveraging AI-based facial expression recognition to identify customer satisfaction with products. The objective of this research is to develop a robust and accurate facial expression recognition system capable of analyzing customer emotions and determining their satisfaction levels based on their facial expressions. The proposed study used a hybrid CNN-GRU deep learning model to extract meaningful features from facial images and classify them into different emotional states. The trained model is evaluated using a separate test dataset to measure its performance in accurately recognizing customer emotions and assessing satisfaction levels. The evaluation metrics include accuracy, precision, recall, and F1-score. Experimental results demonstrate the effectiveness of the proposed AI-based facial expression recognition system in identifying customer satisfaction with products. The proposed experiment achieved excellent results with a real-time image-based dataset.



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sciforum-096043: Facial Recognition Of Tribal Marks Using Machine Learning

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Tribal marking is an African cultural practice which is carried out for the purpose of identifying a person's tribe or family. In facial recognition systems, tribal marks are considered soft biometrics, which have been used to improve the performance of facial recognition systems. Facial mark recognition (FMR) refers to the ability of a system to determine whether a small skin patch taken from a facial image contains a facial mark. Although there have been significant improvements in detecting facial marks using Convolutional Neural Networks, a system integrating African facial marks has not been implemented yet. In this thesis, we implemented a facial recognition system for African tribal marks using a one-shot learning model which employed a collected dataset consisting of images of people with tribal marks. Due to limited sources of data, we adopted Data Augmentation techniques to increase the size and balance of our dataset. Face detection and extraction was carried out by a mtcnn model, after which embedding points were created using a pre-trained (Facenet) model. After the points were created, we employed a classifier which matched the faces to their appropriate classes based on the training dataset. We evaluated our model using various evaluation metrics, and we obtained an accuracy of 100% for training and 88% for testing for the first experiment and 99% and 83% for the second experiment. We evaluated the model's performance further using F1 score and MCC, and we reported a score of 0.887 and 0.757, respectively, for the first experiment and 83% and 0.733 for the second experiment. This study can prove useful in areas such as twin identification, profiling, forensic analysis, etc.



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sciforum-107299: Farm Forecast: An AI-Powered predictive system for stabilizing Agricultural council prices.

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The high price volatility of agri-horticultural commodities, especially essential ones like pulses, onions, and potatoes, poses formidable economic challenges to consumers, producers, and government bodies. The Department of Consumer Affairs is under constant pressure to stabilize markets, address inflation, and support sustainable agriculture. Farm Forecast solves this by providing a predictive analytics platform that combines artificial intelligence with cutting-edge algorithms to predict the future price movement of major agricultural commodities.

The Aurelius Market Intelligence System utilizes the ARIMA (Autoregressive Integrated Moving Average) model to examine past data and factors like weather, political affairs, supply chain bottlenecks, and trade scenarios globally. Farm Forecast is able to deliver an out-of-the-box forecast, stretching up to a full year ahead, on expected prices for maize, thus empowering different stakeholders like farmers, policy makers, and retailers to take informed decisions pertaining to production schedules, buffer stock management, pricing strategies, etc.

This user-friendly web dashboard offers interactive real-time insights and predictive analytics. This provides a chance for farmers to select crops as per the market demand, while government agencies can act before they are outsold due to sudden price changes. It also allows for automatic alerts to the Department of Consumer Affairs when market prices anticipate a shock (and hence increase uncertainty and price volatility).

In the future, Farm Forecast will be upgraded to include real-time data streams and operate in other crop markets. We plan to experiment with more advanced models like neural networks as the system matures to enhance prediction quality even further. Farm Forecast combines this mash-up of machine learning and economic modelling to provide a transformative tool for stabilizing commodity prices that benefits consumers as much as it does the agriculture industry.



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sciforum-107452: Feature Engineering for Lung Cancer Classification Using Next-Generation Sequencing Data

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Next-generation sequencing (NGS) has profoundly transformed the field of genomics with its ability to detect molecular findings on a large scale, particularly for the somatic genome. Research on complex diseases such as lung cancer has shifted significantly as NGS technology provides an efficient method to unravel the genetic fingerprint of this extensively studied disorder. This advancement has opened new pathways for understanding the molecular underpinnings of lung cancer, facilitating more targeted approaches in diagnosis, treatment, and research. While NGS data are highly dimensional and complex, they pose a significant challenge for data analysis and classification tasks. In this paper, we investigated feature engineering to improve the classification accuracy of lung cancer using NGS data. The goal of all these methods of dimensionality reduction, feature selection, and transformation techniques is to improve machine learning's predictive power. In this work, the dimensionality reduction method Principal Component Analysis (PCA) is used to optimize feature selection. Advanced transformation techniques like normalization and scaling are applied to optimize the data for better model performance. The efficacy of these techniques is evaluated through a comprehensive comparison of various machine learning classifiers, including Support Vector Machines (SVMs). The results demonstrate that efficient feature engineering enhances the classification accuracy and robustness of lung cancer prediction models, providing valuable insights for the development of precision medicine approaches in oncology.



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sciforum-104384: Fitting Hysteresis Arctangent Model using Particle Swarm Optimization Method

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Abstract– This article is devoted to the identification of an arctangent hysteresis model, using the particle swarm optimization method. Results obtained from simulated and measured curves are compared and analyzed.

Introduction

Swarm intelligence-based algorithms are widely used to solve difficult optimization problems. Scientists and researchers are particularly interested in the PSO approach, as it needs few parameters, it is adapted to nonlinear functions, and it is easy to implement.

Describing mathematical hysteresis loops is one of the most challenging aspects of ferromagnetism. Mathematical models are characterized by their simplicity of implementation.

This paper suggests the use of PSO method in order to identify the parameters of the arctangent hysteresis model that will be presented in the coming section.

Methodology

For a given magnetic field H , the magnetic induction B in the arctangent model hysteresis curve is represented by the following equations.

For the upward curve:

$$B = \arctan(b(H-d)cH) \quad (1)$$

For the downward curve:

$$B = \arctan(b(H+d)cH) \quad (2)$$

Generally, the parameters a , b , c , and d are calculated from analytical expressions. The particle swarm optimization method is used to identify them too. This method is based on the definition of a search space, which includes a set number of particles and the function to be optimized. Each particle is identified by its present location, speed, and best position.

Results

It is obvious that the hysteresis curve generated by the PSO method leads to a better fit of the measured loop than the one obtained using the analytical approach. The convergence of the PSO method is very fast and can be reached in a few iterations.

Conclusion

From the obtained results, it is evident that the identification of the set of parameters (a , b , c , and d) using the PSO method gives a better approximation of the measured curve than those obtained when they are analytically identified.



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sciforum-107417: Free Public Transportation on Market Days: Enhancing Urban Mobility and Sustainability in Mid-Sized Cities

Winicius Carlos da Silva *, Antonio de Lima, Jean Turet, Thyago Nepomuceno and Lucimario Gois de Oliveira Silva

UFPE

Public transportation plays a vital role in the development of mid-sized cities, significantly impacting urban mobility, economic growth, and overall quality of life. This article explores the potential benefits of implementing a free public transport system on designated market days, focusing on its economic, social, and environmental advantages. The proposed initiative aims to improve access to markets, encourage the use of public transportation, and reduce reliance on private vehicles, contributing to the reduction of traffic congestion and CO2 emissions. The study incorporates data science and machine learning methodologies, with an emphasis on time series analysis, to forecast key metrics such as passenger demand, vehicle circulation, and pollutant emissions. These predictive models also evaluate the financial implications of the initiative, accounting for operational expenses including depreciation, staffing, fuel consumption, and maintenance costs. By assessing both the short-term and long-term impacts, we demonstrate that free transport policies can optimize the efficiency of the transportation system, lower operational costs over time, and contribute to improved air quality. In addition to the environmental and economic benefits, this initiative has the potential to provide significant social value by increasing accessibility to commercial areas, services, and public spaces. It can stimulate local economies by enhancing consumer access to markets and promoting local business activities.



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sciforum-107635: Fruit and Vegetable Recognition Using MobileNetV2: An Image Classification Approach

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Automated food item recognition and recipe recommendation systems have gained increasing importance in dietary management and culinary applications. Recent advancements in Computer Vision, particularly in object detection, classification, and image segmentation, have facilitated progress in these areas. However, many existing systems remain inefficient and lack seamless integration, resulting in limited solutions capable of both identifying food items and providing relevant recipe recommendations. Furthermore, modern neural network architectures have yet to be extensively applied to food recognition and recipe recommendation tasks. This study aims to address these limitations by developing a system based on the MobileNetV2 architecture for accurate food item recognition, paired with a recipe recommendation module. The system was trained on a diverse dataset of fruits and vegetables, achieving high classification accuracy (97.2%) and demonstrating robustness under various conditions. Our findings indicate that the modified model, the MobileNetV2 model, can effectively recognize different food items, making it suitable for real-time applications. The significance of this research lies in its potential to improve dietary tracking, offer valuable culinary insights, and serve as a practical tool for both personal and professional use. Ultimately, this work advances food recognition technology, contributing to enhanced health management and fostering culinary creativity. Some potential applications of this work include personalized dietary management, automated meal logging for fitness apps, smart kitchen assistants, restaurant ordering systems, and enhanced food analysis for nutrition tracking.



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sciforum-107463: Harnessing Vision-Language Models for Improved X-ray Interpretation and Diagnosis

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As AI and transformers make progress, Vision Language Models (VLMs) are set to have a big impact on medical diagnostics when it comes to understanding picture-based data. X-rays play a key role in radio diagnosis helping doctors spot many different illnesses. This research aims to train a Vision Language model Visual BERT, to diagnose diseases by using both written patient info and X-ray images. In the past few years, researchers around the world have tried out various AI models to identify different health problems however, since Vision Language Models are pretty new, people use them for general stuff like chatbots. But these models could be useful for automating the process of diagnosing diseases from X-rays. Proposed methodology involves merging three separate datasets to build a full dataset that covers many diseases that X-ray images can spot. By bringing together different datasets, the model can figure out how to spot a wide range of conditions, which makes it better at diagnosing and more useful. This method shows how VLMs can change medical diagnostics for the better giving doctors a smart way to spot diseases faster and more. Visual BERT is trained on dataset to diagnose diseases using visual as well as textual data. For Evaluation matrix Accuracy score is used and after fine tuning model on combined dataset we obtained 60% accuracy score. To test model Front end app with Streamlit is made to make it easier to use for end users.



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sciforum-093834: HauBert: A transformer Model for Aspect-based Sentiment Analysis of Hausa-Language movie reviews

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In this study, we present a groundbreaking approach to aspect-based sentiment analysis (ABSA) using transformer-based models. ABSA is essential for understanding the intricate nuances of sentiment expressed in text, particularly across diverse linguistic and cultural contexts. Focusing on movie reviews in Hausa, a language under-represented in sentiment analysis research, we propose HauBert, a bidirectional transformer-based approach tailored for aspect and polarity classification, by fine-tuning a pre-trained mBert model. Our work addresses the scarcity of resources for sentiment analysis in under-represented languages by creating a comprehensive Hausa ABSA dataset. Leveraging this dataset, we preprocess the text using state-of-the-art transformer techniques for feature extraction, enhancing the model's ability to capture nuanced aspects of sentiment. Furthermore, we manually annotate aspect-level feature ontology words and sentiment polarity assignments within the reviewed text, enriching the dataset with valuable semantic information. Our proposed transformer-based model utilizes self-attention mechanisms to capture long-range dependencies and contextual information, enabling it to effectively analyze sentiment in Hausa movie reviews. The proposed model achieves significant accuracy in aspect term extraction and sentiment polarity classification, with scores of 96% and 94%, respectively, outperforming traditional machine models. This demonstrates the transformer's efficacy in capturing complex linguistic patterns and sentiment nuances. Our study not only advances ABSA research but also contributes to a more inclusive sentiment analysis landscape by providing resources and models tailored for under-represented languages.



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sciforum-107200: Heart Disease Prediction Using IoT Sensors and Explainable AI: Machine Learning Integration for Health Monitoring[†]

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Context: Heart disease is considered to be the leading cause of death around the world. Accurately predicting heart disease early is one of the most challenging tasks of the 21st century. Not only is accurate prediction important, but taking necessary precautions is also crucial. In this era, heart disease is regarded as the most prominent source of illness and death globally.

Objectives: The objective of this article is to predict heart disease early using IoT sensory data and an XAI framework. In this article, we have developed a framework that includes the integration of IoT sensors for real-time monitoring of patient data. The machine learning models used to analyze the sensory data utilize XAI to ensure the interpretability and transparency of these models' predictions.

Materials/Methods: This article aims to predict heart disease early using IoT sensory data and an XAI framework. We developed a framework integrating IoT sensors for real-time patient data monitoring. To analyze and predict these data, we used machine learning and deep learning algorithms. XAI techniques such as SHAP and LIME were applied to ensure model prediction interpretability and transparency.

Results: In this article, we employed machine learning and deep learning algorithms to predict heart disease early. The ML algorithms used were LOGR and SVM, while the DL algorithms were RNN and LSTM. It was observed that Support Vector Machine achieved a high accuracy rate of 97%, compared to other classifiers.



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sciforum-107603: Image Enhancement Using Generative Adversarial Networks in Computer Vision

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Image enhancement serves as a critical function in the field of computer vision, improving the quality and clarity of images for various applications. In this study, we present an advanced approach to image enhancement by leveraging the power of Generative Adversarial Networks (GANs). Our method employs a sophisticated GAN architecture, specifically tailored for image enhancement tasks. The GAN model comprises two primary components: a generator and a discriminator. The generator is responsible for producing enhanced images from the input data, while the discriminator evaluates the authenticity of these images, distinguishing between real, high-quality images and the ones generated by the model. Initially, the generator utilizes a deep convolutional neural network (DCNN) to process the input image. It aims to enhance the image by reducing noise, improving resolution, and refining details. The generator is trained to learn the mapping from low-quality images to high-quality counterparts through a series of convolutional and deconvolutional layers, incorporating techniques such as residual learning and attention mechanisms to optimize the enhancement process. Parallely, the discriminator functions as a binary classifier, assessing the quality of the generated images against real, high-resolution images. The discriminator's feedback is crucial, as it guides the generator to produce more realistic and high-quality images through an adversarial learning process. This dynamic interplay between the generator and discriminator forms the crux of the GAN framework, driving continuous improvement in image quality. Our approach was rigorously evaluated on several challenging datasets, including medical and low-light image datasets. The results underscore the superior performance of our GAN-based method compared to traditional image enhancement techniques. Key achievements include significant improvements in image clarity, reductions in artifacts, and enhanced resolution, all achieved with efficient computational performance. These compelling findings not only validate the effectiveness of our proposed method but also highlight its potential applications in various fields.



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sciforum-088204: Influence of Two-Step Verification Technique Over Privacy Security Threat on Social Networks

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The rapid adoption of Online Social Networks (OSNs) has redefined how people interact, share information, and collaborate. Yet, these platforms also introduce notable privacy and security concerns. This study investigates the inherent vulnerabilities of OSNs and evaluates the role of Two-Step Verification (2SV) as a countermeasure to strengthen user security.

Our research utilizes a multi-faceted approach, including a comprehensive literature review and an analysis of data breaches, privacy policy infractions, and user experiences within OSNs. The surveys capture user insights, and the case studies of security incidents highlight specific technical vulnerabilities. To assess 2SV, we examine its effectiveness in blocking unauthorized access, its impact on user experience, adoption trends, and its performance in comparison to alternative security measures such as strong passwords and biometrics.

The findings show that common OSN vulnerabilities include data breaches, phishing attempts, and weak privacy safeguards. User insights reveal varying levels of privacy risk awareness, with many being unclear about the available security options, including 2SV. Our evaluation finds that 2SV is effective in reducing unauthorized access and has achieved moderate user adoption due to its balance between security and usability. However, comparisons with options like biometrics point to 2SV's limitations in both convenience and security resilience.

This study offers valuable perspectives on OSN security challenges and the potential of 2SV as a mitigation strategy. These insights contribute to ongoing efforts to enhance privacy and security across online social platforms.



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sciforum-104019: Integração e Padronização de Dados Heterogêneos de Autismo

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Autism Spectrum Disorder (ASD) affects a significant portion of the population, with approximately 636,000 students diagnosed with autism enrolled in schools in Brazil, reflecting a 48% increase compared to previous years, according to the 2023 School Census. However, the joint analysis of ASD-related data presents a challenge due to the heterogeneity of sources, including medical records, monitoring devices, clinical evaluations, and questionnaires. This project aims to address these challenges by developing an automated pipeline to collect, clean, transform, and integrate heterogeneous ASD data. Using tools such as Pandas, Amazon S3, Google BigQuery, Tableau, Scikit-learn, and TensorFlow, the pipeline ensures data quality and standardizes its formats and terminologies. Automation was managed by Apache Airflow, ensuring the continuous and efficient execution of the process. The integrated data enabled advanced analyses, such as identifying behavioral patterns, correlating clinical and monitoring data, and performing sentiment analysis in questionnaires. The findings provided valuable insights into ASD, surpassing the state of the art by offering more accurate predictive models and clear visualizations that support decision-making by healthcare professionals. The project resulted in the creation of a robust infrastructure that improves the quality and usability of available ASD data, contributing to the development of more effective interventions and targeted public policies.



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sciforum-107298: Integrated Crop Recommendation and Soil Nutrient Analysis using IoT Sensors and Machine Learning

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Context: The productivity of agriculture is fully depending on the health and nutrient status of the soil. As the global population is increasing, the demand for food is increasing simultaneously. Traditional Farming practices always rely on general recommendation for soil management and crop selections. This may not be sufficient for different soil types and environmental conditions.

Objective: In this paper, we used the concept of the oversampling and under sampling techniques to balance the data. By using Machine Learning techniques, We analysed different types of soil nutrients for crops. We collected data on various attributes, like pH, Potassium(K), Rainfall, humidity, labels (different crops like rice, maize, etc.), temperature, etc. We used various Supervised Learning Algorithms in this project to predict the most efficient crop for different types of soil and environments like Decision Tree, Logistic Regression, SVM, Naive Byes, Random Forest, etc.

Method / Materials: We collected data from different sources and IoT sensors, like soil moisture sensors, pH sensors, temperature sensors, EC (Electrical Conductivity) sensors, nutrient sensors, etc). The collected dataset was converted into a .csv file. Further, we sent these data to the cloud over Wi-Fi. After analysing our data, we found that our dataset was unbalanced. So, we applied many data balancing techniques to balance our data for crop prediction. We have applied under sampling (counter) and oversampling (SMOTE) to our dataset.

Result: We have compared both under sampling and oversampling algorithms. After applying each of the algorithms, we obtained the best accuracy for Gaussian Naïve Bayes, which was 99.77% for crop recommendation and soil nutrient analysis. We estimated the performance metrics for all the classifiers and found that an accuracy of GNB 99.77% in comparison to the others.



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sciforum-100554: Investigating the Availability and Key Features of Dental Health Applications in the Google Play Store

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Amidst the rapid proliferation of mHealth applications, questions persist regarding their efficacy, usability, and integration into oral health practice. This review aims to inform practitioners and stakeholders in the field of oral health on the potential of digital technologies to transform healthcare delivery and promote healthy behaviours. Key terms included "dental", "dentistry", "oral health", "dental treatment", and "tooth care". The Google Play Store search identified 130 applications, out of which 17 met our study objectives. Most applications (n=13) focused on providing dental appointments, oral health education, and promotion. Mobile Application Rating Scale (MARS) quality rating revealed that only 50% of these applications were high quality. Engagement and information were the least-scored subscales. The review highlights the many benefits that these digital tools provide, including online appointments, teleconsultations, and oral health educational resource access. Nevertheless, despite their potential, the current state of dental health applications leaves substantial room for development, especially in the areas of user involvement and information quality. The lack of reliable and accurate information in many applications may be harmful to users' health. To fully realize the potential of these digital technologies and enhance oral health outcomes on a larger scale, coordinated actions involving stakeholders from the technology and dentistry sectors are imperative.



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sciforum-107678: IoT-Based Smart Irrigation System Using Hybrid Ensemble Models for Water Usage Prediction

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Background: According to Earth.org's report 600 million people in India faced an acute water shortage, which also significantly affects agricultural productivity as the country's agricultural sector heavily relies on groundwater for irrigation. According to UN News in Breadbasket of India Punjab, groundwater levels have dropped significantly. India's annual groundwater consumption is 90%. Global Citizen reported groundwater loss in India threatens millions of farmer's ability to grow. Also, Environmental changes have strained India's water resources. IoT-based smart irrigation systems can help minimize these challenges by optimizing water usage in agriculture.

Objective: This System's objective is to optimize the irrigation system for maximum water efficiency and less water wastage and to enhance crop yields. This system helps to save costs by lowering water bills and energy consumption. This system provides Remote monitoring and control for farmers' convenience. This system is scalable, configurable, and adaptive to another system by real-time data.

Methods/Materials: Soil Moisture Sensors, Temperature and Humidity Sensors, Rain Sensors, and Other Weather data collection sensors are used to collect the data so the system will provide the water when needed. Arduino or Raspberry Pi-like microcontrollers are used to process the data from sensors and control the irrigation valves based on parameters. We have used different machine learning models like SVM, Linear Regression, Decision Tree, Random Forest, Boosting, Bagging, and two hybrid ensemble models LRBoost(linear regression and boosting) and LR²F (linear regression and random forest)to predict the water usage.

Results: So after using different kinds of regression models, we have found that among all the models that we have used Ensemble Liner regression and Random Forest model outperformed the other models by acquiring an accuracy of 96.34% MSE score of 0.0016 and RMSE score of 0.040. So we have chosen the respected model.



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sciforum-105491: Machine Learning Approach for Evaluating water Safety for human consumption in Dili city, Timor-Leste

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Drinking water is essential for human survival and the sustainability of all life on Earth. In developing countries like Timor-Leste, government-provided water services are severely limited and face numerous challenges, including low service standards, poor water quality, and insufficient funding. In Timor-Leste, 80% of the population is dependent on agriculture. In Dili, 70% of the water supply comes from groundwater and 30% from surface water. As the population grows, the demand for water increases, affecting both its availability and quality. Efforts are underway to address these issues and improve the safety of water for drinking and other domestic uses. In Dili, 46 boreholes are used for water supply, has been used in this study, but ten are over-exploited and fifteen are unfit due to microbiological contamination, manganese, iron, TDS and hardness of water. Machine learning (ML) has shown promise in solving real-world challenges, including water quality assessment. In this paper, three ML algorithms-K-Nearest Neighbors (KNN), Decision Trees, and Naive Bayes (NB)-are applied to assess the potability of water. Performance evaluation and k-fold cross-validation were used to assess the effectiveness of the models. The KNN algorithm showed the highest accuracy, reaching 97%. Thus, in the future water quality prediction in Timor-Leste is necessary to incorporate environmental data and sewage systems.



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sciforum-107709: Machine learning for early diagnosis of autism spectrum disorder

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Context: Autism Spectrum Disorder (ASD) is a developmental disorder that affects communication, social interaction and behaviour. By building a machine learning model that predicts the probability of ASD through certain behaviours, demographic information and clinical history. We will be able to contribute to moving forward with getting a diagnosis for individuals with ASD even earlier. The study and resulting neural network that exists were created to be a universally available, scalable approach that can help with early diagnosis in both clinical and non-clinical situations. **Objective:** The main objective of this project is to build a comprehensive AI-based model for the early detection of ASD. Our approach is designed to augment early intervention efforts using a cloud-based web interface and machine learning techniques that deliver insights in an easy-to-use manner. **Methods:** The dataset used for the study was the "Autism Dataset for Toddlers". High-dimensional assessment of ASD traits was done using several machine learning techniques, like K-Nearest Neighbors (KNN), Decision Trees (DT), Random Forests (RF), Support Vector Machines (SVM), XGBoost and LightGBM. We created and evaluated the performance of the models using accuracy, precision, recall, F1-score and ROC AUC after feature selection-based techniques such as ANOVA-SVM. **Results:** XGBoost was the best classifier as it had 99.6% accuracy and ROC AUC was even better than the Decision Tree, and Random Forest even though they achieved an accuracy of 98.8%. With a close 98.10% with Support Vector Machine followed up, with K-Nearest Neighbors at 96.68%. Because the system runs on a cloud-based interface, this processing occurs in real time and enables early ASD screening. Altogether, our XGBoost model holds great potential for early autism screening as it provides a viable option for both clinicians and families.



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sciforum-095924: Machine learning model for Hausa part-of-speech tagging

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Part-of-speech (POS) tagging involves tagging each word in a text with the appropriate part of speech. POS tagging is regarded as one of the fundamental technologies required in Natural Language Processing (NLP) applications. For many natural language processing jobs, this procedure is regarded as one of the pre-processing processes. Recently, with the development of machine learning-based algorithms, the process of part-of-speech tagging improved, and there are now a respectable number of taggers accessible for high-resource languages like English. However, low-resource languages like Hausa continue to lack accurate and effective computational approaches for part-of-speech tagging. Despite the recent exponential expansion of Hausa online content on websites like BBC.com/Hausa, Freedomradio.com.ng, Hausa Leadership.ng, Aminiya and dailytrust.com.ng, part-of-speech tagging on such Hausa web content has not been investigated by the research community. Therefore, part-of-speech tagging on Hausa-based web contents is a new topic that can be researched. This research work proposed a machine learning-based method for Hausa part-of-speech tagging. We implement three architectures, namely, long short-term memory (LSTM), bi-directional long short-term memory (BLSTM) and gated recurrent unit (GRU), to perform part-of-speech tagging on a Hausa data set. The labeled data are transformed into a one-hot-vector encoding and then sent through a deep neural network using LSTM, BLSTM and GRU hidden layers. We obtain precision, recall, accuracy and f1-score as the evaluation matrix of the three architectures. In conclusion, the system achieves an overall result of 99%, and this shows that the proposed approach outperforms the previous approach (with a result of 79.14%) in terms of precision, recall, accuracy and f1-score.



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sciforum-104453: Missing data imputation using machine learning techniques applied to IoT air quality sensors: A case study in Amazonia

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The problem of poor air quality in the Amazon is a serious issue, as air pollution in the region negatively affects public health, resulting in thousands of premature deaths and severe damage to the environment. Monitoring emissions is crucial for enforcing laws that restrict these emissions and for preventing fires and their devastating consequences. For this reason, an air quality monitoring network has been implemented in the Amazon region, currently with several sensors distributed throughout the state of Acre/Brazil. However, many sensors have significant data gaps, in some cases with more than 80% loss. This is due to power failures, internet connection problems and device defects, thus compromising the consistency and accuracy of air quality measurements. This paper investigates the use of imputation techniques applied to estimate missing data from Amazon sensors collected from January 1, 2020 to December 31, 2023. Simple imputation techniques (Mean, Median) and those based on machine learning (MICE, KNN and MissForest) were selected. In the experiments, missing data was randomly introduced into the complete dataset (from 10% to 50%), and the techniques were compared using the following evaluation metrics: Mean Square Error (MSE), Root Mean Square Error (RMSE) and coefficient of determination (R^2). The results showed that advanced techniques such as KNN and MICE are superior to simpler techniques, with lower MSE and RMSE, as well as a higher R^2 . Even for the most critical case (50% missing data), KNN achieved an MSE of 0.0013 and an R^2 of 0.85, and MICE presented an MSE of 0.0013 and an R^2 of 0.93, standing out as effective methods for data imputation.



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sciforum-107334: Modelling the Quantitative Structure–Activity Relationship of 1,2,4-Triazolo[1,5-a]pyrimidine Analogues in the Inhibition of *Plasmodium falciparum*

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Triazolopyrimidine and its analogues represent important lead structures in anti-malarial research. This study modelled the quantitative structure–activity relationship (QSAR) of 125 congeners of 1,2,4-triazolo[1,5-a]pyrimidine from the ChEMBL database in the inhibition of *Plasmodium falciparum* using six machine learning algorithms. Recursive feature elimination was used to select the most significant of 306 molecular descriptors with 1 molecular outlier. A split ratio of 20 % was used to split the x and y matrices into 99 training and 24 test compounds. The regression models were built using machine learning scikit-learn algorithms (multiple linear regression (MLR), k-nearest neighbours (kNN), support vector regressor (SVR), random forest regressor (RFR), RIDGE regression and LASSO). Model performance was evaluated using the coefficient of determination (R^2), mean squared error (MSE), mean absolute error (MAE) and root mean squared error (RMSE) p-values, F-statistic and variance inflation factor (VIF). The number of significant variables considered to build the model was 5 ($p < 0.05$) with the regression equation $\text{pIC}_{50} = 5.90 - 0.71\text{np}1 - 1.52\text{pmi}3 + 0.88\text{slogP} - 0.57\text{vsurf-CW2} + 1.11\text{vsurf-W2}$. On 5-fold cross validation, three algorithms, KNN (MSE=0.46, $R^2=0.54$, MAE=0.54, RMSE=0.68), SVR (MSE=0.33, $R^2=0.67$, MAE=0.46, RMSE=0.57) and RFR (MSE=0.43, $R^2=0.58$, MAE=0.51, RMSE=0.66) showed robustness, high efficiency, and reliability in predicting the pIC_{50} of 1,2,4-triazolo[1,5-a]pyrimidine. The models provided useful data on the functionalities necessary for developing more potent 1,2,4-triazolo[1,5-a]pyrimidine analogues as anti-malarial agents.



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sciforum-107300: Natural Language Interface for Database Querying: A Multilingual Chatbot

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In the age of data-driven decision-making, database access is crucial for both non-technical and technical users. This study presents a powerful database chatbot that facilitates interaction with databases in human language and which does not require advanced SQL knowledge. It features chatbot-specific processes like handling user input, interpreting natural language, and presenting SQL queries; under the hood, this layer operates via Lang chain, where we leverage advanced language models. The chatbot can respond in a range of languages, catering to users who speak different languages.

Its multilingual support is one of the key reasons why this chatbot stands out, as it encourages users to engage in both regional and international languages, thereby including the entire spectrum of the population. Other important features are the inclusion of Google Text-to-Speech (GTTS), which makes this software text-to-speech- accessible, especially for users who have disabilities and want audio output. The app also allows users to copy responses to the clipboard and download all responses for greater flexibility and convenience.

Another advantage is session persistence. The chatbot can store session information so that it remembers the context of the conversation (i.e., I have been chatting with you and keep track of my previous messages, etc.). This is also powered by SQL and database semantic queries, as well as context-aware responses to give better solutions. Future work will require further database compatibility, more query optimization, and advanced contextual conversation management to provide an even richer user experience.

As it bridges the gap between users and database systems using natural language processing, this project simplifies the way a database is handled by everyone over the globe, thereby making access to data easier through enhancing its usability for every kind of audience.



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sciforum-107357: Numerical stability of phase-shifting digital holography

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Abstract—As a non-destructive and fast imaging technique, phase shifting digital holography (PSDH) has been widely applied in many optical imaging problems including measuring the surface morphology and cell refractive index. In this paper, it was found that PSDH is not stable w.r.t interference intensity in the noisy setting. Moreover, it was unveiled that PSDH is a linear problem w.r.t the intensity difference.

Based on this, for the first time we establish the numerical stability w.r.t the intensity difference. It should be noted that the used phase shiftings are nonuniform, which brings great flexibility for the phase-shifting. Numerical simulations are conducted to verify the stability result. For the traditional PSDH, the phase shifting must be calibrated and controlled with a high level of accuracy since the calibration error serves as the measurement error. Unlike this, PSDH from nonuniform phase-shiftings does not require such a high level of calibration accuracy and provides great flexibility for the phase-shiftings. Incidentally, the nonuniform phase shiftings are commonly utilized in transmission electron imaging. To the best of our knowledge, the numerical stability remains unexplored in the literature especially for generalized PSDH from nonuniform phase shiftings. Finally, we check the stability result by numerical simulations. We verified that Phase-shifting digital holography has good stability.



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sciforum-104142: Optimization Of Hydroponic Strawberry Growth Using Spectral Manipulation Machine Learning And Deep Learning Analysis

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New technologies solve complex problems in agricultural production, enabling both food security and the optimization of the use of natural resources. In this paper, we will cover hydroponic agriculture, advanced monitoring, and data analysis. Plants interact with light, humidity, and temperature environmental factors. Light is one of the most important environmental factors for photosynthesis and growth. Various wavelengths have contrasting impacts on plant development and physiological traits. Artificial manipulation of light conditions may allow for an improvement in crop production and quality. Thus, the present study deals with the influence of diverse light wavelengths on the growth of strawberry plants cultivated in a hydroponic system. The growing processes of strawberry plants (*Fragaria × ananassa*) have been taken into consideration due to their importance as food and the sensitivity of their cultivation. It tests the influence of specific wavelengths on plant growth and development. State-of-the-art technologies include Arduino-based temperature and light sensors to monitor the cultivation conditions in real-time, while Convolutional Neural Networks trace the growth patterns and pests of the crops by images taken. This work models and predicts behaviors of plants under different light conditions using Machine Learning techniques, thus optimizing cultivar development with a view of maximum yield production. The results obtained show that red light promotes growth through enhanced flower and fruit development. Blue light is favored by robust leaf and stem growth since it is most effective in photosynthesis. Green lights, which help inner light penetration inside the leaf canopy, have less of an effect on photosynthesis. Yellow light also has some advantages in general growth but is inefficient compared with blue and red light. Result using CNN architecture, accuracy 89%. This work contributes to precision agriculture, sensor technology, and sustainable farming practices.



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sciforum-104283: Optimizing Ensemble Performance with Condorcet Voting: A Study on Weak Learners for Image Classification

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Introduction:

Convolutional neural networks (CNNs) are a primary tool for image classification. This study proposes a novel approach to enhance ensemble learning by modifying the voting rule for aggregating results from individual classifiers. Typically, simple and weighted majority rules are used, but recent literature suggests other rules may be more efficient for specific tasks, particularly in multi-classification. This project tests the Condorcet voting rule for image classification.

Methods:

Ensemble learning combines predictions from multiple classifiers into a single result based on voting. Traditional voting rules often limit the potential of these ensembles, especially with weak learners whose accuracy is below 50% in multi-classification tasks. By exploring the Condorcet voting rule, this study aims to improve accuracy without domain-specific knowledge, efficiently balancing the classifiers' achievements and weights. This approach may benefit weak learners, which consume less energy and achieve peak performance faster than traditional methods.

Classical networks such as VGG, ResNet, EfficientNet, and other CNNs were employed. Condorcet rule was compared against traditional simple and weighted majority rules. The CIFAR-100 dataset was used for a balanced and comprehensive evaluation of the models' performance. The models were limited to 35 layers, with average accuracy across individual models being no more than 28% (random guessing yields 1% accuracy in a 100-class setup).

Results:

The ensemble model using the Condorcet rule showed a minimum of 4% accuracy improvement compared to simple and weighted majority rules, and over 15% improvement relative to the average accuracy of individual models.

Conclusions:

This study suggests that alternative voting rules, such as the Condorcet, can improve the performance of ensemble in image classification without domain-specific knowledge, and without altering the energy spent or training time of individual classifiers. Further study on even weaker learners to optimize the balance between energy consumption and accuracy is promising for the field.



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sciforum-104952: Optimizing Network Traffic Classification Through a Novel BAT-ANN Model: An Empirical investigation in Improved Accuracy and Scalability in Network Security

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The modern network has expanded significantly due to the rapid rise of network usage, making it a big, dynamic, and complicated system. The management of modern network traffic has now become a major challenge as a result of large-scale network-based applications. Consequently, the smart traffic analysis-based monitoring of networks has become an urgent need. Network traffic classification is an important approach used in network management, as well as in network security. Traditional methods often require ongoing maintenance, struggle with dynamic ports, and lack the granularity needed for precise classification. They can also be resource-intensive and have scalability issues for large networks. To overcome these limitations, many organizations are turning to more advanced techniques like machine learning and behavior analysis for better network traffic classification and security. Accurate classification is crucial for network traffic due to its multifaceted importance. It serves as the foundation of network security by enabling the rapid detection of security threats and illegal activity, which is critical for protecting against cyberattacks. This study suggests a smart, intelligent system based on a BAT artificial network for network traffic classification. The proposed system makes use of a publicly available NIMS dataset. Furthermore, we have applied some preprocessing and feature selection techniques before feeding the data into the classifier. The experimental outcomes reveal that the proposed approach achieved high accuracy and low computation time, and performed better than the previous approaches used for network traffic classification.



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sciforum-104303: Optimizing Urban Traffic and Enhancing Mobility in Brazilian Cities: A Study on Simulation and Real-Time Data Analysis

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The simulation of routes and the optimization of urban traffic are crucial research areas for improving mobility in contemporary cities, particularly in Brazil. With population growth and a rapidly expanding vehicle fleet, urban areas face increasing challenges such as traffic congestion, pollution, and extended travel times. This study centers on an initial traffic analysis using computational models to predict and optimize road and public transport flows. The methodology integrates real-time traffic data from public agencies and georeferenced information from bus fleets to analyze congestion patterns and vehicle behavior. Various scenarios are examined, including modifications to road infrastructure, the use of intelligent traffic light systems, and the promotion of alternative transportation modes like bike lanes and enhanced public transport. These scenarios are tested to assess their potential impact on reducing congestion and improving public transit usage. Optimization tools like genetic algorithms and linear programming are employed to determine the most effective traffic management strategies. Using simulation software as BEAM— Behavior, Energy, Autonomy, and Mobility, together with exact models such as Traveling Salesman Problem (TSP) and The K-Rural Postman Problem(K-RPP) allow us to archive these goals. Preliminary results showed the critical parts of traffic and the pollution caused by it. With this data we can simulate changes in bus routes and schedules, and also make interventions. This way we can increase traffic speed, reduce congestion and improve the functioning of public transport. This study supports sustainable urban planning by providing a data-driven foundation for decision-making on urban mobility. By using real-world data from Brazil, we can test which models perform best in more complex environments like Pernambuco, where disorganized growth presents significant challenges for maintaining efficient transit flow.



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sciforum-104339: Parametric Middleware Routing and Management Services Platform Model for Smart Cities

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Smart cities are made to provide services, including software services, for citizens.. There are many services that these cities provide, and the number of active users and connected devices may vary. Traditional approaches to software design and development do not take into account both the high-level and low-level management of complex services, which include IoT devices, real-time applications, and AI-related processing frameworks. Some of the most important components of software system management are internal task routing and services management. Smart city systems are developed and implemented for real-world cities using real-world data. For example, Kyiv city is the largest city in Ukraine in terms of population and total area. In this study, data on Kyiv city are used as a foundation of the proposed smart city system model. We provide a generalized software service model that is based on control parameters, benchmarks, and weights. These services are provided in an algorithmic and software model version that allows for their implementation in already existing services or when developing new smart city solutions. The smart city platform is based on the integration of various components; in turn, each individual component consists of its own set of software and hardware services and components. The tasks of sub-services and module management are as crucial as they are complex. The system manager module is a middleware/core-layer software system. Event handling, routing, and service/process activation are determined by the appropriate mathematical calculation mechanism. This role can be filled by special routing and management services, each being platform- and deployment-agnostic. While routing services are designed following standard protocols, APIs, and middleware-layer services, sub-service management systems are low-layer data/process processing- and computation-first systems.



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sciforum-104039: Performance Evaluation of Machine Learning Algorithms for Predicting Flow rate in Pipeline Maintenance Optimization.

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Abstract

Using machine learning to predict maintenance schedules for crude oil pipelines is crucial for enhancing efficiency and minimizing disruptions in the oil and gas sector. Our research explores the effectiveness of machine learning algorithms in this context, with a specific focus on using oil flow rate as a primary predictor. Machine learning models, when trained with a variety of inspection data, can accurately predict flow rate, thus improving maintenance planning. Several pipeline scenarios were analysed, and Python library was used for dataset augmentation. The study shows a correlation between variations in the buildup deposits and flow rate in the pipeline, indicating that the flow rate gives an indication for determining the needs for maintenance. Specifically, higher flow rate aloud longer intervals between maintenance activities like pigging, while lower flow rate could indicate there is accumulation of deposit which necessitating intervention. Ensembled machine learning models was train, variation in performance were observed. Gradient Boosting and XGBoost Regressor show best performers with lower values for MSE, RMSE, and MAE, and higher R^2 scores compare to the Support Vector Regressor. The result shows Gradient Boosting has MSE of 0.000005, RMSE of 0.002259, MAE of 0.000968, and an R^2 of 0.997259, follow by XGBoost Regressor with MSE of 0.000005, an RMSE of 0.002269, an MAE of 0.000922, and an R^2 of 0.997234. while Support Vector Regressor indicate the least performance, with MSE of 0.002868, RMSE of 0.053554, MAE of 0.046311, and an R^2 of -0.540765. The findings of the study emphasize the necessity of choosing machine learning algorithms that are appropriately suited to the features of the dataset and the task. The findings highlight the importance of selecting machine learning algorithms that are more suitable to the features of the dataset and the task.



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sciforum-107410: Predicting Crop Yield Sale Prices with Computer Vision and Machine Learning Techniques

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Introduction: All are interested in the estimation of the sale price of crop yield beforehand. Crop yield is dependent on the growth rate of the plant. Plant growth rate depends on factors like soil, water, sunlight, and season. Due to this multi-factor dependency, it is not easy to estimate the sale price of the crop yield or predict the timeline beforehand. **Objective:** By advancing AI technology, we can leverage and eliminate the challenges and predict crop yield, timeline, and sale price. We use computer vision, Deep Learning, and regression to predict the estimation of the sales price of the crop yield. **Materials/Methods:** By using computer vision YOLO algorithms, we detect plants in the field and categorize the plants using the CNN classification algorithm. We use IOT devices to monitor the growth of the plant from time to time and collect the data. The collected data are used to predict time, crop yield, and sale price beforehand. The prediction is derived based on historical data of sales prices in different sessions and a plant growth data set using regression algorithms. **Result:** The experimental results demonstrate the effectiveness of the proposed approach, where we detect the plant using computer vision; categorize the plant using CNN; and accurately predict yield, timeline, and sale price using regression. To evaluate the proposed framework, we conducted experiments using sample data. Through hypothesis testing using the "T Test" and "chi-square" test, we failed to reject the null hypothesis, and the evaluation metrics show that the accuracy of plant detection is 92.5; the categorization of plants using CNN is 96.31; and the accuracy score obtained using regression to predict yield, timeline, and sale price is 91.57. The Precision, Recall, and F1 scores also look good.



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sciforum-104056: Predicting Infrared stellar flux densities: teaching WISE to detect like Spitzer

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Astrophysics is an ideal field in which to take advantage of machine learning (ML) techniques due to the great amount of astronomical data and its peculiar characteristics. The space satellite WISE is considered the current best infrared all-sky survey in both quality and coverage. In contrast, the space satellite Spitzer, with smaller coverage, has better spatial resolution (3x-2x, depending on the band) and sensitivity in the same spectral region. Some studies have claimed to find some kind of noise or contamination in WISE, resulting in discrepancies when comparing the measurements of both satellites. In this communication [1], we intend to overcome these discrepancies and report an ML approach to predict mid-infrared fluxes at two specific bands from WISE variables.

We have tested several ML regression models in a large sample of confirmed members (stars) from open clusters (groups of stars physically related) with both WISE and high-quality Spitzer data. In our particular case, Extremely Randomized Trees gave the best performance with values of $R^2 > 0.95$ in both bands. Importantly, we have been able to improve the results at lower fluxes (the ones with the largest discrepancies) and to prove the good correspondence between the predicted fluxes and the real Spitzer ones when available.

The use of ML allows us to bring the best characteristics of both satellites together without the loss of data other approaches could cause. We believe a similar strategy could be useful in other studies when dealing with similar discrepancies.

[1] Fonseca-Bonilla et al. 2024, under review.



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sciforum-103759: Prediction model for classification of 5G network slicing

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5G networks have had a major impact on the communication industry in recent years. With its high data transfer rates and improved latency, 5G networks have enabled a range of services such as autonomous vehicles, virtual reality, and the Internet of Things (IoT). As a result of these applications, a massive amount of data is generated every minute. This has created significant issues and considerably impacted network slicing performance. To provide end users with customized network services and improved user experience of 5G network slicing technology, an efficient prediction model is needed for the classification of different types of 5G network slicing. In this paper, we propose a model for predicting the different classes of 5G network slicing. The model utilizes machine algorithms to classify the 5G network into four different slices, eMBB (enhanced mobile broadband), mMTC (massive machine type communications), URLLC (ultra-reliable low-latency communication) and V2X (vehicle-to-everything) slicing. The results obtained indicate that the proposed model is capable of accurately classifying the 5G network slices with an average precision of 0.94% and an average recall of 0.96%. This showcases the effectiveness of our approach. The experimental results indicated that the proposed model could significantly influence the delivery of accurate 5G network slicing services.



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sciforum-106118: PSO-Based Algorithm for Constrained Flow Shop Scheduling

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Introduction

Motivated by the practical relevance in manufacturing systems, this research investigates the two machines flow shop scheduling problem (FSSP) with a single transport robot and raw materials constraints. This problem is a new extension of the FSSP. The objective of this research is to develop an effective scheduling approach that minimizes makespan, while addressing the complexities arising from the movement of jobs between the two machines and the limited availability of raw materials that are supplied from external suppliers at different time moments.

Methodology

To address the computational complexity of the proposed problem, a customized Particle Swarm Optimization (PSO) approach is suggested for resolution. Since we are in the context of solving a FSSP, i.e., we are looking for the permutation of jobs that minimizes the makespan under constraints imposed by transport robots and raw material availability. Hence, in order to customize PSO for a discrete problem, we maintain the job-permutation-based encoding scheme. The swarm is initialized randomly, and particles positions and velocities are updated using crossover and mutation operators borrowed from Genetic Algorithms (GA), and guided by personnel and global best positions with mutations applied to prevent stagnation. The approach refines solutions iteratively, optimizing job scheduling performance under considered constraints.

Results

The proposed approach was examined on a series of newly developed benchmark included various configurations of resource availability and transportation times between machines. Results show that the approach achieves makespans close to the optimal values reported by a develop ILP model for small instances and reduces makespans by 5-10% on medium-to-large instances compared to standard GA.

Conclusion

This study proposed a customized PSO approach that addressees two machines FSSP with transport robot and raw materials constraints. The results demonstrated that proposed approach is capable to provide good performance, particularly in challenging scenarios with multiple constraints.



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sciforum-102203: Quadruped robot locomotion based on deep learning rules

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Terrestrial locomotion of robots employs two main methods: the use of wheels or tracks, and the use of articulated joints. Articulated locomotion offers advantages over wheels, such as lower energy consumption, access to irregular and rough terrains, better maneuverability in homes by climbing and descending stairs, and improved planning. Additionally, articulated robots are lighter, can be produced and prototyped with 3D printers, and offer greater flexibility in various environments. However, they also present some disadvantages, including complex mechanical structures, increased control complexity, and expensive actuators. This work presents the design and implementation of a reinforcement learning model based on Proximal Policy Optimization (PPO) for the locomotion of a 12-degrees-of-freedom quadruped robot that ensures stable trajectory. For this purpose, a reinforcement learning model based on TensorFlow and Gym was implemented and tested in the Pybullet simulation environment. With the correct adjustment of the model's hyperparameters, maximum stability in the robot's walking trajectory is achieved. During walking, the robot attains a smooth response curve when measuring its center of gravity. The application of reinforcement learning in this context shows the potential for advanced control techniques to address the complexities of articulated robots. By optimizing control strategies and leveraging modern simulation tools, this study demonstrates improvements in the stability and performance of quadruped robots, contributing to the development of more efficient and versatile robotic systems.



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sciforum-107832: Quantum-inspired Multi-objective Optimization of ESN using SRG for Nonlinear Time Series Prediction

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This paper introduces a novel method for time series forecasting by leveraging Quantum-inspired Non-dominated Sorting Genetic Algorithm II (QNSGA-II) to optimize Echo State Networks (ESN), complemented by the evaluation of reservoir dynamics through the Separation Ratio Graph (SRG). The integration of QNSGA-II enables the simultaneous optimization of multiple ESN hyperparameters, aiming to reduce forecast error while enhancing the diversity and performance of the reservoir. SRG is employed as a metric to assess the quality of the reservoir's internal states, allowing for the identification of configurations that improve the model's ability to capture the complex dynamics inherent in time series data.

The proposed approach is validated using the Mackey-Glass time series dataset, a benchmark known for its nonlinear dynamics. Results show that the QNSGA-II optimized ESN with SRG evaluation significantly outperforms traditional ESN models, yielding a lower Mean Squared Error (MSE) in predictive performance. Additionally, the use of SRG offers deeper insights into reservoir behavior, facilitating more informed decision-making in the selection of optimal configurations.

The combination of QNSGA-II and SRG not only enhances the robustness of the ESN but also provides a comprehensive framework for improving the accuracy and reliability of time series forecasting. This method represents a step forward in leveraging quantum-inspired optimization techniques for neural networks, demonstrating the potential of hybrid approaches in addressing the challenges of nonlinear and chaotic time series prediction.



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sciforum-107736: Recognizing Human Emotions Through Body Posture Dynamics Using Deep Neural Networks

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Body posture dynamics have garnered significant attention in recent years due to their critical role in understanding the emotional states conveyed through human movements during social interactions. Emotions are typically expressed through facial expressions, voice, gait, posture, and overall body dynamics. Among these, body posture provides subtle yet essential cues about emotional states. However, predicting an individual's gait and posture dynamics poses challenges, given the complexity of human body movement, which involves numerous degrees of freedom compared to facial expressions. Moreover, unlike static facial expressions, body dynamics are inherently fluid and continuously evolving. This paper presents an effective method for recognizing 17 micro-emotions by analyzing kinematic features from the GEMEP dataset using video-based motion capture. We specifically focus on upper body posture dynamics (skeleton points and angle), capturing movement patterns and their dynamic range over time. Our approach addresses the complexity of recognizing emotions from posture and gait by focusing on key elements of kinematic gesture analysis. The experimental results demonstrate the effectiveness of the proposed model, achieving a high accuracy rate of 96.34% on the GEMEP dataset using a deep neural network (DNN). These findings highlight the potential for our model to advance posture-based emotion recognition, particularly in applications where human body dynamics are key indicators of emotional states.



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sciforum-104020: Revolutionizing Stock Market Forecasting: A Cutting-Edge Analysis of Machine Learning Models (CNN, ARIMA, LR, GB, and LSTM)

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This comprehensive research delves into the burgeoning field of stock market forecasting, emphasizing the use of advanced artificial intelligence (AI) and machine learning (ML) technologies. The primary objective is to develop a robust model capable of predicting short-term stock market movements for major US-listed companies across various sectors. The predictive algorithm relies heavily on historical price data, technical indicators, and sentiment analysis derived from news sources to generate directional forecasts.

This study investigates several critical components of stock market analysis, including pattern recognition, risk assessment, and the use of machine learning algorithms to predict investment returns. A thorough examination of the Efficient Market Hypothesis (EMH) is conducted to understand its implications on forecasting stock prices using historical data. Additionally, the research evaluates a range of approaches and models pertinent to financial prediction. These include the Generalized AutoRegressive Conditional Heteroskedasticity (GARCH) model, the AutoRegressive Integrated Moving Average (ARIMA) model, and Long Short-Term Memory (LSTM) networks.

Furthermore, this study addresses the inherent data limitations, the risks of overfitting, and the ethical considerations associated with the application of AI and ML in stock market forecasting. By examining these factors, this research aims to highlight the potential and challenges of employing technology-driven methods in financial markets. The ultimate goal is to enhance the accuracy and reliability of stock market predictions, thereby providing valuable insights for investors and stakeholders. Through this rigorous exploration, this study contributes to the ongoing development of more sophisticated and effective forecasting models in the financial industry.



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sciforum-104343: Self-diagnosis of Applications – Architectural Solution and Ontology

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Software package management tools have become common and are available for practically all SDKs. They allow for the definition of dependencies between packages, ensuring consistent use of their respective versions, especially during installation, updating, configuration, and removal. These tools are primarily used in the software development phase by programmers. While the utility of software package managers and the added value they provide to programmers during the development stage are unquestionable, there are still many gaps concerning the remaining phases of the software lifecycle—commonly referred to as the maintenance stage. The need for maintenance arises from the outdatedness of packages, resulting from incompatibilities with other packages, the introduction of improvements and optimizations, the correction of errors, the elimination of vulnerabilities, and so on. Although it is usually possible to identify packages that are deprecated or obsolete, updating is still a manual process initiated by the programmer. In this paper, authors propose a solution, still in its prototype stage, aimed at equipping applications with the means to report their status concerning update needs, particularly for critical updates. The solution consists of a background service that processes technical reports published by various sources, an ontology used to standardize information and concepts from responsibility disclosure reports, a REST service used by applications to obtain a self-diagnosis of their condition and a REST client that is automatically installed in the application.



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sciforum-107750: Semi-supervised facial beauty prediction using contrastive pretraining with SimCLR

Djamel Eddine Boukhari

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Facial beauty prediction is a complex task that relies on subjective human perceptions, making it a challenging area of study within computer vision. In this paper, we propose a semi-supervised approach that using contrastive pre-training with SimCLR (simple framework for contrastive learning of visual representations) to predict facial beauty scores. By utilizing contrastive learning, our model learns robust representations through the self-supervised task of distinguishing between different views of the same image and between different images. We leverage a diverse dataset, SCUT-FBP5500, which comprises 5,500 annotated facial images, to develop a model capable of accurately predicting beauty scores. Our proposed method involves two primary phases: first, we pre-train the model using contrastive learning to acquire robust visual representations from a larger set of unlabeled images, and then we fine-tune it on the labeled SCUT-FBP5500 dataset. The results demonstrate that our model achieves a Pearson correlation coefficient of 0.9267, surpassing state-of-the-art methods in beauty prediction. These findings indicate the effectiveness of using contrastive pre-training for this application, as our model not only enhances prediction accuracy but also aligns more closely with human judgments of beauty. This study contributes to ongoing research in aesthetic assessment and highlights the potential of semi-supervised learning to improve performance in subjective evaluation tasks.



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sciforum-104715: Spatial Pattern Recognition for Precise Water Body Extraction: Integrating PRISMA Hyperspectral Data with Evolutionary Machine Learning Algorithms

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Features Extraction (FE) plays a crucial role in image classification by reducing the dimensionality of the raw hyperspectral Remote Sensing (RS) data while retaining discriminative information. This technique helps to simplify complex hyperspectral data, which contain hundreds of spectral bands, to make them more manageable by identifying the most important information for classification. Reducing the number of dimensions, this helps to overcome the problem of the "curse of dimensionality", improves classification accuracy, and speeds up data processing. This study proposed an innovative approach to improve the accuracy of water body extraction from hyperspectral RS data by combining FE and Convolutional Extreme Learning Machine (CELM) with evolutionary algorithms. This method integrates several advanced techniques to optimize water surface extraction. FE allows us to select the most relevant information from hyperspectral data, reducing complexity while preserving essential details. The addition of evolutionary algorithms allows us to automatically optimize the model parameters, improving its performance. CELM is trained in a supervised manner directly on raw data to learn discriminative features for classification steps. Then, these extracted features are used for the final classification using the CELM with the hybridization of evolutionary algorithms (EAs) such as Genetic Algorithms (GAs). This hybrid approach aims to overcome the challenges related to the spectral variability of water bodies and the presence of mixed pixels, thus offering a more robust and accurate solution for water resource mapping from hyperspectral images. In order to validate the effectiveness of our approach, we conducted experiments on hyperspectral data acquired by the RISMA (PRecursore IperSpettrale della Missione Applicativa) satellite. The obtained results were then compared with the existing methods documented in the scientific literature using recognized evaluation metrics such as precision, accuracy, recall, Intersection Over Union (IOU), and F1 score.



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sciforum-106525: SpectoResNet: Advancing Speech Emotion Recognition through Deep Learning and Data Augmentation on the CREMA-D Dataset

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Speech emotion recognition (SER) is a particularly challenging task due to the intricate and non-linear features of emotional expressions in audio signals. In this work, we introduce SpectoResNet, an improved version of ResNet architecture that was tuned for classifying emotions using audio features from the CREMA-D dataset. CREMA-D, provided by the Speech and Emotion Research Group from New York University (NYU), is a crowdsourced dataset consisting of 7,442 audio-visual recordings from 91 actors, which displays happiness, sadness, anger, and neutrality, among other emotions. While this dataset tries to provide opportunities for research into emotional recognition, its intrinsic variety and subtle differences due to individual traits and contextual environments pose significant obstacles to precise classification. To do this, we converted voice signals into 2D spectrograms to enable the deep CNN of ResNet to analyze and classify the emotions. ResNet was initially developed for image recognition and relies on residual connections in order to be able to train very deep networks effectively. Advanced data augmentation—adding noise and changing pitch—was used to simulate the variability found in real-time speech and make the model robust for different acoustic environments. Our model, trained on augmented spectrogram data, achieved 65.20% classification accuracy—a state-of-the-art breakthrough in vocal emotion recognition using deep learning. Success with SpectoResNet emphasizes the prowess of deep CNNs in extracting detailed patterns and subtleties within emotional audio expressions, thus paving the path toward more advanced model developments for multimodal emotion recognition.



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sciforum-105954: Stock Market Prediction Using Machine Learning: A Comprehensive Approach to Data Collection, Model Selection, and Performance Evaluation

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Stock market prediction using machine learning (ML) is a complex yet important area of financial research aimed at forecasting future stock prices based on historical and real-time data. Accurate predictions are crucial for investors, financial analysts, and policymakers to develop better investment strategies and risk management practices. However, stock prices are highly volatile and influenced by various factors, such as geopolitical events, economic indicators, and investor sentiment, making accurate prediction challenging.

This study examines different ML techniques for stock market prediction, focusing on data collection, feature engineering, model selection, and performance evaluation. Effective data collection involves gathering diverse data types, including historical prices, trading volumes, economic indicators, sentiment data, and company-specific information. Feature engineering enhances model inputs with relevant variables like moving averages, RSI, sentiment scores, and volatility measures.

The research evaluates both traditional models (linear regression, decision trees) and advanced techniques (neural networks, ensemble methods). Traditional models are effective for linear trends but less so for complex market behaviors, whereas advanced methods like Long Short-Term Memory (LSTM) networks excel in modeling sequential data and time-series forecasting. Ensemble methods, such as stacking and boosting, improve predictive performance by combining multiple models to reduce bias and variance.

The study also emphasizes backtesting models through simulated trading strategies to assess their real-world applicability and robustness. Challenges such as market efficiency, data quality, and overfitting are highlighted, with solutions including reinforcement learning and anomaly detection to enhance model adaptability and robustness.

Overall, the study provides a framework for developing robust stock prediction models, integrating various ML techniques while addressing ethical and regulatory considerations. Continuous evaluation and adaptation of models are essential to ensure their reliability and effectiveness in the ever-changing financial markets.



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sciforum-098252: The Assessment of Machine Learning Algorithms for Predicting Irrigation Water Quality : A Comparative Study

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The growing world population is increasing the demand for food, and climate change is causing erratic rainfall patterns. This has led to greater reliance on irrigation, especially in the Sahel and arid regions, to sustain food production. As freshwater resources become scarce, farmers are utilizing various water sources to keep their crops irrigated, aiming to ensure food availability and profitability. However, the rise in industrial activity is increasing pollution, which affects water quality, making its monitoring time-consuming and extensive. The aim of this study is to develop a machine learning approach for predicting irrigation water quality. To achieve this, a large dataset consisting of 1750 water samples was curated. The data were preprocessed, and Sodium Adsorption Ratio (SAR) and Irrigation Water Quality Index (IWQI) were computed. Five machine learning models (XGBoost, K-Nearest Neighbors, Support Vector Machine and Random Forest) were trained using the following parameters: Sodium(Na), Calcium(Ca^{2+}), Bicarbonate (HCO_3^-), Electrical Conductivity (EC), and SAR. The results revealed that XGBoost outperformed the other algorithms, achieving a mean absolute error (MAE) of 0.90, a mean squared error (MSE) of 3.26, a root mean squared error (RMSE) of 1.81, and an R^2 of 0.96. The use of machine learning algorithms in predicting irrigation water quality is essential for farmers and crop planning, as it can save costs and time while ensuring healthy food production.



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sciforum-107838: The Development of a Classifier Based on Neural Networks and K-Neighbors for Pediatric Pneumonia Diagnosis through X-Ray Images

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This research focuses on the classification of pediatric pneumonia diagnosis through X-ray images. The database utilized in this study consists of anteroposterior chest X-ray images obtained from retrospective cohorts of pediatric patients aged one to five years at the Guangzhou Women and Children's Medical Center. These images were selected based on their relevance to the study of pneumonia, specifically concerning the identification of bacterial infections.

Using a MATLAB program, seven relevant characteristics were extracted from each X-ray image. These features were essential in determining whether the patient exhibited signs of a bacterial infection associated with pneumonia or if the diagnosis was normal. The classification process was carried out using two distinct methodologies: neural networks and the k-nearest neighbors (K-NN) algorithm. A comparison of these classifiers was performed to evaluate their effectiveness in diagnosing pediatric pneumonia.

The dataset included a total of 49 images diagnosed as normal and 48 images indicating the presence of the bacteria linked to pneumonia. The characteristics considered for analysis included mean, standard deviation, entropy, contrast, correlation, energy, and homogeneity, which play a critical role in image analysis. The results demonstrated an impressive efficiency of 89% for the k-nearest neighbors algorithm and over 96.9% for the neural-network-based classifier, indicating the potential for these methodologies to aid in accurate pediatric pneumonia diagnosis through X-ray imaging.



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sciforum-107461: The Impact of Boosting Algorithms on the Classification Accuracy of Skin Cancer Types

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Skin Cancer is one of the most growing type of cancer due to pollution and many other factors. Early diagnosing of the Skin cancer and it's types can cause to stop this rapid growth of skin cancer disease and for this purpose AI can be utilized. Skin cancer is one of the most researched topics, with various methods used to diagnose it; however, there is always room for improvement and new technologies to perform this task more effectively. This study aimed to utilise a dataset containing skin cancer types, known as PAD-UFES-20, to classify different types of skin cancers using advanced data pre-processing and a combination of deep learning and machine learning techniques and finally those features will be analysed who impact most on disease to be classified as skin cancer. Proposed methodology includes detailed pre-processing of the data set, custom Convolutional Neural Network model for feature extraction, training Boosting models on pre-processed data and finally finding features that impact the most on model to identify disease to be a skin cancer's type. CatBoost Classifier, XGBoost Classifier and LGBM Classifier are trained on PAD-UFES-20 data set to diagnose Skin cancer and it's six different types. With better pre-processing techniques we get more accurate results compare to previous studies XGBoost classifier produced highest accuracy then CatBoost and LGBM classifiers. In addition this study also includes research on the features of data set which effect most on the prediction of model. In summary proposed method more focused on best pre-processing and feature extraction techniques to get most possible predictions from Boosting models.



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sciforum-107674: Towards a More Natural Urdu: A Comprehensive Approach to Text-to-Speech and Voice Cloning

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This work focuses on the centrality of NLP and TTS in promoting communication for the Urdu speaking population where there is a dearth of language assets in the regional languages. While English and other languages of European origin have reliable computational assets available, Urdu is still considered relatively unlitrate in this aspect, and hence restricted. To address this problem, therefore, we collected our own dataset using audio from a YouTube playlist that contains an Urdu novel reader for more than 100 hours. This dataset was carefully preprocessed for our use and different errors were corrected to provide high quality input for our TTS models. Our work constitutes one of the first research attempts at creating a large-scale Urdu speech dataset and at employing unique techniques of Automatic Speech Analysis. To achieve this purpose, the linguistic and cultural characteristics of the Urdu language are incorporated in this approach to guarantee that the voices generated are sincere. In view of this, our project was aimed at developing TTS systems for creating natural voice outputs that takes into consideration cultural differences and youthful Appeal by building upon well-established neural network models in speech synthesis and by incorporating new techniques. The results of our work are promising: We also managed to create a TTS model for accurately reading Urdu text and also it was marked to have perfect native speaker like pronunciation. These are the practical implications of our research across education, digital accessibility and media possibly shifting popular culture. What we are trying to achieve is more friendly and natural biometrics for speech interfacing for Urdu users.



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sciforum-105000: Transformer-based Purchase Intention Mining: A Comparative Study Using A Novel Dataset

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The scarcity of high-quality, contextually relevant datasets is a significant impediment to progress in the field of purchase intention mining. The absence of comprehensive datasets that capture the subtleties of consumer intentions across various contexts often hinders the development of robust and accurate predictive models. This research addresses this critical gap by developing a novel dataset specifically designed to encapsulate the intricacies of consumer purchase intentions. The primary aim of this research is to develop and evaluate a new dataset tailored for purchase intention mining and to assess the effectiveness of transformer-based models in this domain. To achieve this, we collected, preprocessed and analyzed a new dataset and fine-tuned advanced transformer models, including RoBERTa, ALBERT, and DistilBERT, on the newly created dataset. These models were then rigorously compared against traditional machine learning algorithms and deep learning architectures, such as Logistic Regression, Support Vector Machines, LightGBM, and Convolutional Neural Networks (CNN) with and without LSTM layers. The results of our comprehensive evaluation demonstrate that transformer models significantly outperform traditional approaches, achieving near-perfect accuracy, precision, recall, and F1-scores across different purchase intention categories (Positive, Negative, and Neutral). This superior performance was consistent across both undersampled and oversampled versions of the dataset, underscoring the robustness of our proposed dataset in facilitating high-precision sentiment analysis tasks. In conclusion, this research not only highlights the effectiveness of transformer models in understanding and predicting consumer purchase intentions but also emphasizes the importance of developing specialized datasets to overcome the challenges posed by dataset scarcity. Our findings align with existing literature, reinforcing the dominance of transformer-based approaches in natural language processing applications and setting a new standard in the field of purchase intention mining.



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sciforum-107206: Use of AI and Federated Learning for accurate software estimation.

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Introduction: Software estimation plays a crucial role in predicting the budget and duration of software projects, and thus in their success. To estimate software, historical data are generally used, and machine learning is leveraged to predict software estimation. Vendors and companies share their past historical estimations with a central server, where a model is trained to evaluate and predict the estimation. However, all companies maintain confidential past estimations on their local servers. **Objective:** To eliminate this challenge, we use a federated learning framework to leverage AI and keep vendors' past estimates private in their local servers without sharing them with the central server. We also use machine learning to predict the software cost and duration. **Material/Methods:** In this framework, we train and evaluate the model in local servers and share their encrypted weights, bias, and accuracy score with a central server while ensuring past estimations are kept private. The central server will aggregate and average the weights and bias and share them back with the local server for retraining. This process will continue until it reaches the accuracy score necessary to predict and share the size of the new requirement with the central server and return the cost and duration. In the central server, we use a federated averaging algorithm for model aggregation, where the global model is updated by averaging the local model updates.

Result: The experimental results demonstrate the effectiveness of the proposed approach in accurate cost estimation and duration prediction by FLML. To evaluate the proposed framework, we conduct experiments using sample data. We compare the performance of the FL-based models with centralized models in terms of evaluation metrics. The performance will need to be improved (because of distributed/parallel data processing), but the FL framework provides privacy guarantees.



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sciforum-103638: Use of Time or Frequency Domain in ECG Analysis

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Machine learning techniques have been widely applied in the medical field, with electrocardiogram (ECG) signals being pivotal for detecting arrhythmias and other applications such as sleep analysis and biometric identity recognition. Traditionally, selecting the right features was essential for achieving good performance in classification. However, with the advent of deep learning, particularly convolutional neural networks (CNNs), the classifier itself extracts and selects the relevant features. This development raises the question of whether it is necessary to represent ECG data in different domains, such as the frequency domain, for optimal performance.

This study aims to evaluate the performance of CNNs in three tasks: classification of rhythm, apnea detection and identity recognition, using three input formats: time sequence, Fourier frequency components and spectrogram. The databases used for this analysis were MIT-BIH Arrhythmia, ECG-ID and Apnea-ECG from PhysioNet. Customized CNN networks were employed for time series and Fast Fourier Transform (FFT) components, while transfer learning with EfficientNet, pre-trained on the ImageNet database, was utilized for spectrograms. The results were validated using N-fold cross-validation, with N being 10 for the arrhythmia and apnea databases, and 4 for the identity database.

The mean accuracy obtained for each task was consistently higher when using the time domain compared to the frequency domain, with differences ranging from 1.4% to 5.4%. Consequently, there is no advantage in transforming time-series data into the frequency domain for these tasks.



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sciforum-102260: Using a virtual assistant for interactive student engagement at universities

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This project introduces the development and implementation of a virtual assistant tailored specifically for student interaction in a higher education institution. With the increasing demand for personalized support and efficient communication channels in educational settings, virtual assistants have emerged as a promising technology to enhance student engagement, support academic success, and streamline administrative processes. The virtual assistant presented in this project leverages natural language processing, machine learning, and artificial intelligence techniques to provide an intuitive and interactive platform for students to seek information, access resources, and receive personalized assistance. Some functionalities of the virtual assistant include the following: Information Retrieval: the virtual assistant serves as a knowledge repository, allowing students to obtain quick and accurate answers to frequently asked questions regarding academic programs, course offerings, campus facilities, and administrative procedures; Personalized Guidance: by analyzing student profiles and historical data, the virtual assistant offers tailored guidance on academic planning, course selection, and career pathways, ensuring that students receive relevant and timely advice based on their individual needs and goals; Task Automation: the virtual assistant automates routine administrative tasks, such as registration, scheduling, and grade tracking, reducing administrative burden and allowing students to focus more on their learning experience; and Interactive Support: through natural language processing capabilities, the virtual assistant engages in dynamic conversations, allowing students to ask questions, seek clarifications, and receive real-time feedback on their academic progress. Throughout the project's development, a user-centered approach is followed, with continuous feedback from students, faculty, and administrators. Rigorous testing and quality assurance measures are implemented to ensure the accuracy, reliability, and usability of the virtual assistant.



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sciforum-107459: Using clustering of biometric data in evaluating virtual reality experiences

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Virtual reality (VR) has the potential to offer an excellent opportunity for truly immersive experiences.

However, it can sometimes be challenging to discern changes in emotional state during immersive scenarios. It might be helpful to consider the use of a stress device to detect changes during the VR experience. This study investigates the potential effectiveness of an entirely in-house developed VR roller coaster simulation, consisting of a moving chair and a visor, providing a 3D scenario with adjustable speed and level of realism. During the ride, the participants kindly agreed to use a wearable stress detection device developed in-house, which is designed to collect biometric data using heartbeat and galvanic skin (i.e. sweat level) sensors. A comparative analysis of different clustering techniques (K-means, Agglomerative, Mean Shift and Gaussian Mixture Model) has been conducted using the biometric data with the aim of identifying the various levels of stress experienced by participants during the ride. At the conclusion of the VR experience, the participants were respectfully invited to complete a brief questionnaire to share their perceptions. These data were then cross-referenced with the stress levels obtained by the clustering to check for potential correspondences, crucial to assess the effectiveness of the VR experience. This will provide insight into whether VR experiences can have an impact on emotional states and consider the potential for VR to provide a comparable experience to reality.



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sciforum-107666: Using Convolutional Neural Networks for Enhanced Pneumonia Detection via Chest X-Rays

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As a deadly lung disease, pneumonia remains a leading cause of child mortality under five years old. Machine learning, especially deep learning have played a significant role in the improved performance for detection and identification of various diseases in the field of healthcare. Neural networks, especially the recent development of newer architectures, have revolutionized the object identification, and classification applications in clinical diagnosis of various diseases. This study presents the application of Convolutional Neural Networks (CNN) for the timely and accurate detection of pneumonia using chest X-rays, a development with considerable potential in aiding clinical diagnosis. The research deployed dropout regularization in model design to mitigate overfitting and relied on recall and F1 scores for thorough model evaluation. Although comparable studies achieved higher overall accuracy, our models registered a recall rate of 98%, crucial in reducing false negatives and enhancing patient safety. This suggests the potential of our CNN model as a vital tool for healthcare professionals in early pneumonia detection in children and adults, with the capacity to process a high volume of X-ray images rapidly and accurately. The successful model construction was enabled through various parameter tuning techniques, thus enhancing patient care efficiency and the potential to decrease mortality rates.



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sciforum-103742: Using Real-ESRGAN to Apply to Low-Resolution Natural Landscape Images

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Super-resolution is essential for improving images in computer vision and image processing. When using super-resolution for images of natural landscapes, some challenges are encountered, related to factors such as degradation present in the real world with different levels of illumination and the presence of small details and noise that make the process of applying and reconstructing super-resolution more difficult. With the advances in Deep Learning techniques, Real-ESRGAN has stood out in the transformation of images from low to high resolution, and can be used to elucidate the challenges encountered in the super-resolution of natural landscapes. In this sense, this research applies Real-ESRGAN to images of natural landscapes with realistic degradation, with the aim of generating super-resolution images of real scenarios. Using the DIV2K, Landscape Pictures and Landscape Classification datasets, four training sessions were carried out, varying the iterations and adjusting hyperparameters. The inclusion of datasets focused on landscapes, in addition to DIV2K, and enriched the database, optimizing the model. A quantitative analysis was carried out, using MSE, PSNR, SSIM and NIQE to evaluate performance. The best experimental results achieved high-quality images with an MSE of 0.029, an NIQE of 2.5566, a PSNR of 22.43 and an SSIM of 0.525, preserving original details and structures. A qualitative analysis was also carried out to assess the visual characteristics of the images, confirming that the results generated achieved an improvement in visual quality. The results indicate that the Real-ESRGAN methodology, based on landscape-oriented datasets, is effective in improving image quality in a consistent and robust manner.



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sciforum-107464: VigilantAI: Real-time detection of anomalous activity from a video stream using deep learning

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In an era where artificial intelligence (AI) solutions are increasingly integrated into various sectors, this research delves into leveraging AI for enhancing public safety through real-time detection of illegal activities such as robberies and threats at gunpoint using CCTV footage. With the advancement in deep learning in object detection, the study focuses on deploying the YoloV5 model, trained on a custom dataset compiled from diverse CCTV sources and movies, to identify specific criminal actions. This dataset, enriched through augmentation techniques and annotated with bounding boxes, allows for the precise detection of threats, achieving an accuracy rate of 85%. Our system stands out by not only spotting robbery and gun point activities but also by instantly alerting security personnel, facilitating a rapid response to potentially dangerous situations. This capability is important for law enforcement agencies worldwide, offering them an advanced tool to act swiftly and prevent crimes, thereby enhancing public security. The essence of our work demonstrates the practical application and significant impact of AI in strengthening security measures, providing a solid foundation for future enhancements in the field. Through this initiative, we aim to foster a safer environment in public spaces, reducing crime rates and increasing the general public's sense of safety.



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sciforum-105512: Hybrid Association Rule Mining and Clustering for Enhanced Market Basket Analysis

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Introduction

Product recommendation systems are very important in enhancing customer behavior and experiences by suggesting relevant products based on records and preferences. Data mining plays a crucial role in recommending products. Apriori algorithm and clustering techniques are two powerful algorithms of data mining that help enhance the effectiveness and accuracy of these recommendations.

Objectives

The main objective of this paper is to develop enhanced product recommendation systems by using Apriori algorithms, FP-Growth, K-Means, K-Medoids, and Agglomerative Hierarchical Clustering approaches. The robust framework can identify frequent itemsets and discover association rules. It not only generates associations but also creates meaningful clusters to enhance recommendation accuracy.

Materials/Methods

This paper analyzes a transactional dataset using various algorithms including Apriori, FP-Growth, K-Means Clustering, K-Medoids, and Agglomerative Hierarchical Clustering. We also used hybridization among these to make association rules stronger. Association rules are generated based on the metrics (support, confidence, and lift). The Apriori algorithm identified key itemsets such as "Bread," "Cheese," "Milk," "Soda," and "Yogurt" with high support values, which were further clustered into distinct groups. FP-Growth confirmed these findings with additional rules. K-Medoids and Agglomerative Clustering revealed clear cluster formations, with items like "Chips" and "Eggs" forming separate groups due to lower support values.

Conclusion

The hybridization of FP-Growth algorithms with clustering techniques like K-Medoids and Agglomerative Hierarchical Clustering provides effective product recommendations. Frequent itemsets such as "Bread," "Cheese," "Milk," "Soda," and "Yogurt" form Cluster 1 with higher support values, while "Chips" and "Eggs" form Cluster 2 with relatively lower support values. Significant association rules included: [Cheese] → [Bread] with support 0.24, confidence 0.46, and lift 0.88 in Cluster 1. [Eggs] → [Bread] with support 0.30, confidence 0.60, and lift 1.15 in Cluster 2. Not only does it provide recommendations, but it also groups similar items, improving the accuracy and relevance of recommendations.



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sciforum-105420: Practical Evaluation and Performance Analysis for Deepfake Detection using Advanced AI Models

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Introduction

In the 21st century of digital technology, deepfakes are increasingly becoming a serious cause for the nation. Deepfake technology, which can generate extremely realistic fake images and movies, can be used for both creative and harmful objectives..Nowadays it is very difficult to identify which image/video/media is original or fake.

Objective

Our objective of this paper is to create a robust and reliable model that recognizes the Deepfake media using some of the advanced artificial intelligence techniques like:- Machine Learning and Deep learning classifiers

Material/methods

In our research work we have used digital tools and advanced technologies that capture real-time images, and videos as well as cameras, and microphones that are used to monitor. The data we have collected from the Kaggle repository and as well as a real-time environment for training as well as testing purposes. The Edge Devices is used for video processing and analysis purposes. Deep learning algorithms like CNN, RNN, VGG16, MTCNN, InceptionResnetV1, and the Facenet_pytorch are used to identify which one is real or fake. The extensive feature selection algorithms(Recursive Feature Elimination, PCA, CORR) are used to improve the effectiveness of the model

Results

For the effectiveness of our model, we compare the training and testing accuracy of the algorithms. The performance metrics (Accuracy, precision, recall, and F1-score) are used for unseen environment data. Our experimental work gave an excellent result with an accuracy of 95% by MTCNN, 98% by InceptionResnetV1 98% by the Facenet_pytorch, and 92% by CNN.



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sciforum-104402: Control of the spread of infectious diseases in cows on farms

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Controlling infectious diseases in animals on farming holdings plays an important role in ensuring livestock health and productivity. Infectious diseases can spread rapidly among animals, leading to severe consequences such as reduced productivity, increased mortality, and substantial economic losses. Therefore, implementing effective disease control measures is crucial for safeguarding animal welfare and farmers' livelihoods. When animals are kept outdoors in large areas, identifying diseases and their sources of contamination can be particularly challenging. The vastness of these environments makes it difficult to monitor every animal closely and detect early signs of illness. Additionally, the mingling of animals from different areas can facilitate the spread of diseases, making it harder to pinpoint and control outbreaks. This paper presents an architecture designed to mitigate these challenges. To sum up, this solution uses a set of IoT sensors that try to identify the proximity of healthy animals to animals with disease to stop transmission. The IoT sensors will provide farmers with real-time data, enabling them to swiftly isolate infected animals and implement targeted interventions. By improving disease detection and monitoring, this technology will help farmers maintain healthier herds and reduce the risk of widespread outbreaks, thereby enhancing both animal welfare and agricultural productivity significantly.



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sciforum-101778: Data Protection in Brazil: Applying Text Mining in Court documents

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With the intensification of information technology usage and the emergence of artificial intelligence, data protection has become a topic of debate in academia, spanning from the business context to the political sphere. In Brazil, from a legal perspective, data protection is not a new topic; it has been the subject of court rulings and jurisprudence long before the enactment of the Brazilian General Data Protection Law (GDPL). This work aims to present the analytical process and the outcomes of analyzing jurisprudence regarding data protection and relates issues. To achieve this, search strings and data acquisition agents were developed for use on a portal dedicated to Brazilian legal texts, creating a corpus containing 10,009 documents. Through this, an exploratory analysis of the texts from Courts of Justice was conducted considering the types of jurisprudence and case summaries. The main results in the current research phase demonstrate the evolution of associated texts before and after GDPL, based on the date of promulgation of the law. It is also possible to visualize how the cases are distributed among each state court, highlighting the states of the southeast and south regions, as well as the main occurrences within each Brazilian state. By analyzing the legal levels at which decisions have been made, we can also understand the extent of these cases that have been aggravated.



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sciform-102259: Integration of Sakai LMS using a multi platform mobile application

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In the age of mobile technology, the demand for seamless access to educational resources has become essential. This abstract presents a project proposal for developing a mobile application aimed at integrating with the Sakai Learning Management System (LMS). The application seeks to enhance the learning experience by providing students, instructors, and administrators with anytime, anywhere access to Sakai's core functionalities. The proposed mobile application will serve as a comprehensive extension to the Sakai LMS, extending its capabilities to mobile devices such as smartphones and tablets. Leveraging the ubiquity and convenience of mobile devices, students will be empowered to engage in learning activities beyond the traditional classrooms. As principal features we identify the following: Seamless Access, users will be able to log in securely to the Sakai LMS from their mobile devices, accessing their course materials, assignments, discussion boards, and grades effortlessly; Course Notifications, push notifications will alert students to new announcements, upcoming assignments, and other important events reducing the risk of missed deadlines; Content Consumption, students will have the ability to access diverse learning materials, including documents, multimedia files, and interactive content, optimizing their learning experience on mobile devices and Progress Tracking, the mobile application will provide students with a comprehensive overview of their academic progress, including grades, attendance records, and completion status for assignments, empowering them to stay organized and motivated. The development process was done with continuous feedback from educators and students. With different testing and quality assurance measures implemented to ensure the security, reliability, and performance.



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sciforum-100798: Optimizing Brain Tumor Classification: Integrating Deep Learning and Machine Learning with Hyperparameter Tuning

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Brain tumors significantly impact global health, posing serious challenges for accurate diagnosis due to their diverse nature and complex characteristics. Effective diagnosis and classification are essential for selecting the best treatment strategies and forecasting patient outcomes. Presently, histopathological examination of biopsy samples is the established method for brain tumor identification and classification. However, this method is invasive, time-consuming, and susceptible to human error. To address these limitations, we required a fully automated approach to classify brain tumors. Recent advancements in deep learning, particularly convolutional neural networks (CNNs), have shown promise in enhancing the accuracy and efficiency of brain tumor classification from magnetic resonance imaging (MRI) scans. In response, we developed a model integrating machine learning (ML) and deep learning (DL) techniques. The process started by splitting the data into training, testing, and validation sets before resizing the images and then performing cropping to enhance model quality and efficiency. Further, the relevant texture features are extracted using a modified Visual Geometry Group (VGG) architecture. These features were fed to various supervised ML models, including support vector machine (SVM), k-nearest neighbors (KNN), logistic regression (LR), stochastic gradient descent (SGD), random forest (RF), and AdaBoost, with GridSearchCV-based hyperparameter tuning. The evaluation of the model's performance was conducted using several key metrics, including accuracy, precision, recall, F1-score, and specificity. The experimental results demonstrate that the presented approach offers a robust, automated solution for brain tumor classification, achieving the highest accuracy of 94.02% with VGG19 and 96.30% with VGG16. The proposed model can significantly assist healthcare professionals in early detection of tumors and improving diagnosis accuracy.



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sciforum-104444: Optimizing product/service recommendations and marketing strategies using market trends

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This paper proposes a solution aimed at optimizing recommendation systems for online commerce. Taking an ordered list of products to recommend as input, the proposed solution optimizes this list by considering trends in web searches. The solution collects data on web search trends, filters the data to retain only searches related to products and services, identifies the relevant characteristics of these products, and subsequently reorders the recommendation list based on the similarity of these characteristics with the characteristics of the products on the recommendation list. This establishes a relationship between market search trends and the most recommendable products/services from the existing offer. The solution adopts the power of Google Trends to capture consumer interest across various topics, products, and services—it is assumed that web search trends reflect market trends. Second, ChatGPT is added to refine the gathered raw trend data by removing noise, contextualizing information and matching it with the attributes of products or services in the recommendation list, ensuring that the trend insights are relevant and actionable. Finally, it integrates these insights with the user preferences to dynamically reorder the recommendation lists, prioritizing items that are most representative. Initial results show its effectiveness in improving the relevance of recommendations by demonstrating its potential as a scalable and automated framework for optimizing digital marketing campaigns to build adaptive recommendation engines. This approach provides a robust foundation for future innovations by aligning user preferences with external market signals.



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sciforum-106831: Strengthening Data Security through AES Encryption and Image Steganography

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Steganography, a technique of concealing data within shared information, plays a crucial role in addressing the imperative of safeguarding data within computer networks. While encryption serves as a vital process for encoding both text and images to ensure data security, its susceptibility lies in the potential exposure of encryption keys, which can lead to decryption by unauthorized parties. Cryptography, on the other hand, employs mathematical techniques to secure communication and information, ensuring confidentiality, integrity, authentication, and nonrepudiation of data. By fortifying cybersecurity, cryptography serves as a pivotal tool in protecting sensitive information across various applications.

The objective of this project is to develop a robust Advanced Encryption Standard (AES) algorithm capable of encrypting text before embedding the resulting ciphertext within an image through steganography. The Advanced Encryption Standard (AES) is widely used for securing sensitive data. This approach ensures that decoding the concealed information necessitates the correct encryption key, thereby ensuring protection for both the image and the embedded text. By integrating AES encryption with steganography, the project aims to enhance data security through layered measures, mitigating conventional encryption risks by hiding ciphertext within the pixels of an image. This fusion of encryption and steganography presents a promising strategy for bolstering data confidentiality and security within communication channels.



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sciforum-100346: The role of a user in a smart space: concepts, challenges, and trends

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This paper explores the evolving role of a user within the context of a smart space, focusing on the concepts, challenges, and emerging trends in this rapidly advancing field. As technology continues to surround us, transforming traditional spaces into intelligent environments, it becomes crucial to understand the dynamics between users and these smart spaces. This work delves into the foundational concepts of a smart space, which encompasses an environment enriched with sensors, actuators, and interconnected devices capable of perceiving, analyzing, and responding to user needs and preferences. Smart spaces are designed to enhance user experiences, optimize resource utilization, and improve overall efficiency. However, the introduction of smart spaces brings forth diverse challenges that impact the user's. These challenges include privacy concerns, security risks, ethical considerations, and the potential for information overload. Understanding and addressing these challenges are vital to ensuring the successful integration and acceptance of smart spaces in different domains, such as homes, offices, healthcare facilities, and cities. This paper also explores emerging trends that shape the role of users in smart spaces. These trends encompass novel interaction paradigms, personalized experiences, context-awareness, adaptive automation, and the integration of artificial intelligence and machine learning techniques. Additionally, we examine the influence of user-centered design principles, emphasizing the importance of involving users in the development and evaluation of smart space technologies. By studying the concepts, challenges, and trends in the user's role within smart spaces, this work aims to shed light on the transformative potential of these environments. Understanding how users interact with and adapt to smart spaces can guide the design, implementation, and future development of intelligent systems that prioritize user needs, preferences, and well-being. Also we have defined a strategy to evaluate the performance of this concept, namely by accessing the user feedback on the different moments.



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sciforum-104052: Two-Stage Detection of Diseases and Pests in Coffee Leaves Using Deep Learning

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Coffee cultivation is of extreme economic importance in many regions of the world. However, diseases and pests pose serious challenges, significantly affecting productivity. To solve this problem, deep neural network techniques are emerging as promising solutions, offering precision and efficiency in identifying plant leaf pathologies under different environmental conditions. This study proposes the analysis of a two-stage methodology, detecting the diseased regions of coffee leaves and classifying the diseases into Miner, Rust, Cercospora and Phoma. The experiments were conducted using two public datasets with a total of 1747 images of Arabica coffee leaves. The complete dataset was used for the detection stage and a subset of data with 4104 cropped images of the diseased region of the leaves was generated for the classification stage. The early stopping technique was used to train the models with a patience of 20 and a total of 300 epochs. The YOLOv8 model was chosen to detect the affected regions on the leaves due to its established real-time detection capability and low computational cost. After detection, the clipped regions of interest were submitted to the InceptionResNetv2, DenseNet169 and Resnet50 models, which are state-of-the-art methodologies used for disease classification. The results show that YOLOv8 obtained an mAP of 85.1% and, for classification, the InceptionResNetv2 model obtained the highest average accuracy with 98.18%, which can be seen in the robustness of this architecture compared to the others. The use of the two-stage methodology makes it possible to optimize each stage separately, making it easier to adjust other architectures for new types of diseases or plants.



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sciforum-107829: Using bioinformatic predictions to identify key bacterial strains for bioremediation of wildfire-affected soils

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Microbiome management is becoming an increasingly interesting strategy for soil bioremediation and the substitution of chemical fertilizers. However, variations between in-lab experimentation and field testing have demonstrated that understanding interactions within the microbiome is crucial for the success of synthetic consortia applications.

Current approaches to restoring soil properties in our local environment are limited to reforestation and traditional soil retention practices. To integrate microbiome management and harness beneficial dynamics for soil restoration, this study aims to dissect interactions among the soil microbial community from a forest area in the south of Nuevo León, Mexico, affected by wildfire.

In this study, we evaluated a bioinformatic pipeline to identify, characterize, and select key taxa within the bacterial communities of soil samples from burned and unburned areas. Using QIIME2, the workflow employs sequences of the molecular marker 16S to identify community taxonomic composition. Subsequently, with PICRUST2, we integrated abundances with genetic and enzymatic information from publicly available data to predict metabolic pathways in the community. We then used a statistical method for sparse data to infer the ecological network. We expect that identifying core species of the post-fire microbiome will allow us to harness their metabolic potential for bioremediation.

Finding simplified and accurate pipelines for the analysis of soil microbial communities is essential to accelerate ecological characterizations and optimize expenses in strain isolation, which represents an advantage for budget-limited research. This work also establishes a foundation for harnessing key members of the local soil microbiome, which is crucial for future investigations into soil bioremediation and reforestation.



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sciforum-107634: Using machine learning (ML) algorithms based on voice disorders to identify Parkinson's disease

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Parkinson's disease, described by James Parkinson, is a neurological syndrome affecting the central nervous system, leading to issues such as speech difficulties, tremors, and impaired movement. It is a prevalent neurological condition characterized by motor and cognitive impairments, affecting approximately 10 million people globally, according to WHO. Early diagnosis is critical, as delayed detection may lead to irreversible damage. Speech, being affected by motor control depletion, serves as a valuable tool for diagnosing Parkinson's disease. This work presents a machine learning-based approach for the systematic detection of Parkinson's disease using speech features. The dataset, obtained from the UCI Machine Learning Repository, consisting of biomedical voice measurements derived from speech recordings, and including data from 195 individuals (147 with Parkinson's and 48 healthy controls), was analyzed, incorporating 21 features derived from speech recordings. In this work, several classification algorithms in machine learning were utilized. Specifically, K-Nearest Neighbors (KNN), Support Vector Machine (SVM), Logistic Regression, AdaBoost, and Random Forest were implemented and evaluated using metrics such as accuracy, precision, recall, F1-score, and ROC-AUC curves. From the experiment results, K-Nearest Neighbors (KNN) emerged as the best performer, achieving 98.31% accuracy, ideal precision for the normal class (1.00), and ideal recall for Parkinson's cases (1.00), ensuring no missed diagnoses. Its F1-score of 0.98 highlights a strong balance between precision and recall. While AdaBoost matched KNN in accuracy, its slightly lower recall for Parkinson's cases (0.97) makes K-Nearest Neighbors (KNN) the preferred choice. Consequently, K-Nearest Neighbors (KNN) is proposed as the most reliable model for robust and accurate Parkinson's disease classification, showing outstanding performance compared to other models.



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Session 4. Electrical, Electronics and Communications Engineering

sciforum-101691: AI-Driven Digital Twin for Vehicular Networks: Leveraging Enhanced Deep Q-Learning and Transfer Learning

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The rapid development of intelligent transportation systems (ITSs) has made vehicular networks (VNs) indispensable, particularly through vehicle-to-everything (V2X) communication. This study proposes an advanced framework for the construction and migration of digital twins (DTs) in vehicular networks to improve decision-making and predictive maintenance. The construction phase utilizes a large model-driven framework enhanced by an advanced deep reinforcement learning (DRL) algorithm, specifically an Enhanced Deep Q-Network (EDQN). This framework processes complex and dynamic vehicular data, supporting EDQN in optimizing decision-making processes. EDQN adapts dynamically to vehicular environments, ensuring high decision accuracy and efficiency. In the migration phase, due to limited base station coverage, transfer learning techniques are employed to enable the seamless migration of DTs across different base stations. This method minimizes computational overhead compared to traditional approaches by adapting pre-trained models to new environments with minimal retraining. Experimental simulations demonstrate that the integration of the large model architecture with EDQN significantly enhances decision-making processes. The transfer learning strategy effectively extends the operational coverage, maintaining high performance and service continuity during DT migration. This research underscores the potential of leveraging advanced AI techniques to improve the management and operational efficiency of vehicular networks, providing a robust foundation for future advancements in ITS.



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sciforum-096298: Design and Implementation IoT-Driven Distribution Transformer health monitoring system for smart power grid.

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A power distribution company, along with any other company that consumes a significant amount of energy, has a substantial demand for dependable power to earn income and produce goods. According to the research findings, transformers are precious assets for businesses; hence, the maintenance and replacement of transformers are considered a luxurious activity for every business institution. Considering the factors above, this work develops an IoT-Driven Distribution Transformer health monitoring system for smart power grid. Remotely monitoring the health of distribution transformers at predetermined intervals is the objective of this system. Changes in current values on phases, phase failure, overvoltages, overcurrent, earth fault, undervoltages, oil temperature, body temperature, and load ability are just a few of the factors that are used to calculate the health index. Sensors detect these factors. It has been decided that Arduino will serve as the processor for transferring the data that has been sensed, and that the Blynk App will serve as the Internet of Things platform for presenting the data that has been received. The installation process occurs in the physical vicinity of the distribution transformer. After being processed, the values output by the sensors are stored in the system's memory. The system has predefined instructions to detect abnormal situations, which are automatically updated via serial communication on the internet. It is possible to put this low-cost technology in transformers anywhere so they can be monitored remotely. This not only helps assess the health state of the transformers but also assists in projecting their anticipated lifespan. The Internet of Things (IoT) can optimize transformer usage and detect potential issues before catastrophic collapse. An online-measuring system collects and analyzes data on oil temperature, body temperature, voltage, and current, enabling Transformer Health Measuring to identify unforeseen circumstances, resulting in increased reliability and cost savings.



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sciforum-107696: Improving the accuracy of loss point detection in optical fibers using double-slope BOCDR

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The aging of infrastructure has become a significant social issue, drawing attention to distributed optical fiber sensors for monitoring structural defects. Among these, Brillouin optical correlation domain reflectometry (BOCDR), which uses continuous light correlation control for spatial resolution, has been advanced to improve performance. BOCDR measures the distribution of Brillouin gain spectra in the fiber under test, allowing the extraction of Brillouin frequency shift distributions, which can be related to strain and temperature. However, traditional slope-assisted (SA-) BOCDR techniques have limited accuracy in real-time operation due to the slow frequency sweep of the electrical spectrum analyzer. To address this, double-slope-assisted (DSA-) BOCDR has been proposed, utilizing power ratios of two different frequencies for enhanced loss point detection accuracy. In this study, we experimentally demonstrated improved localization accuracy of loss points using DSA-BOCDR. We applied two distinct strains and a bending loss at different positions on a silica single-mode fiber and measured power variations at two frequencies (10.815 and 10.865 GHz). The results showed that the DSA-BOCDR could accurately detect strain and loss locations, with the power ratio method yielding sharper indications of loss compared to single-frequency measurements. The differential analysis further quantified the loss range, showing higher positional accuracy for loss detection using the power ratio. These findings confirm that using distinct power ratios of two frequencies in DSA-BOCDR significantly enhances the precision of loss point detection, offering a promising advancement for real-time structural health monitoring in aging infrastructures.



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sciforum-102214: Unmanned Amphibious Robot in Aiding Post-typhoon Heavy Flooding Response Using LoRa-based Communication and YOLOv5

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In the Philippines, about twenty (20) typhoons occur annually, causing heavy flooding which poses risks that lead to injuries and casualties despite preparedness measures. This study addresses the problem of hindered rescue efforts due to limited resources, dangerous access to flooded areas, and damaged communication infrastructures by introducing an innovative solution: an unmanned amphibious robot for search and monitoring tasks. The developed robot is capable of locating human presence and help needed while providing a live video feed. Evaluations demonstrated the capabilities of the robot to navigate both on land and water with respective speeds of 1.2 m/s and 0.205 m/s over a 120-m LoRa communication. The live video feed quality highlights the feasibility of a 4G LTE network for real-time display. The trained YOLOv5 model had high accuracy in detecting human presence and help needed over 3.5m and 7m distances with 90% and 93.33%, respectively. GPS coordinate reception yields good results in open areas only. There was also a seamless integration of data from the robot to the local website, offering accessible data. Limitations arose when live video feed streaming and YOLOv5 processing were performed simultaneously. This research contributes to aiding post-typhoon heavy flooding response by developing an unmanned amphibious robot, offering insights into its performance and potential for real-world applications in disaster response scenarios.



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sciforum-107781: A Certain Investigation On Non-Isolated Two Phase-Three Device And Three Phase-Two Device Interleaved Boost Dc-Dc Converters

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Abstract : This paper analyses the Interleaving technique applied to Boost DC-DC Converter. It is achieved by interconnection of multiple switching cells in series with diode and parallel with inductors, hence it will increase the effective pulse frequency by synchronizing several smaller sources and operating them with relative phase shift. Energy can be saved and power conversion can be increased without affecting conversion efficiency by interleaving technique. In this , two phases are used and three devices are connected per phase, three phases are used and two devices are connected per phase. The converters are tested at constant input voltage and variable duty cycle using simulation by Matlab/simulink. The ripple content of the output voltage and input current of the converter are obtained from design calculation and compared with simulated results

Introduction: With the increased need of renewable energy sources and energy storage, high-voltage-gain dc-dc power electronic converters used in green energy systems. The step-up converter provides low current ripple, high efficiency.

Methods & Results: The Multi device interleaved boost dc-dc converters are tested by simulation at duty cycle of 0.25 and 0.375 respectively . These duty cycles are selected based on the output voltage (Vo). Considering Vo is known. Fixed as 200V for both the converters

Conclusion: These Converters are analyzed, designed and simulated. Two Phase Three Device per phase boost dc-dc Converter provides 87.9 % of efficiency of power and provides ripple of 0.0106 % volts of output voltage .Three Phase Two Device per phase boost dc-dc Converter provides 92.8 % of efficiency of power provides ripple of 0.125 % volts of output voltage. By comparing these, Two phase Three Device Converters provides Low Output Voltage gain, Low efficiency of Power, Low Ripple Output Voltage and Three phase Two device Converter provides High Output Voltage gain, High efficiency of Power, High Ripple Output Voltage.



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sciforum-107743: A modified electrostatic cleaning system for dust removal from solar panels to improve energy efficiency

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The increasing adoption of solar photovoltaic (PV) systems as a renewable energy source is driven by their ability to provide clean, sustainable power. However, dust accumulation on solar panels significantly impacts their efficiency by reducing the amount of sunlight reaching the photovoltaic cells, leading to a decrease in energy output. This project aims to develop an automated cleaning system to address the efficiency losses caused by soiling on solar PV panels. The system employs a rotating brush mechanism driven by a DC motor and controlled by an Arduino microcontroller, which automates the cleaning process while minimizing water usage and manual intervention. The experimental results demonstrate that the automated cleaning system can restore solar panel efficiency by up to 18% under optimal conditions, thereby enhancing power output and reducing the operational costs associated with manual cleaning. This improvement not only increases energy yield but also extends the operational life of the solar PV systems by preventing potential damage caused by dirt buildup. The system's cost-effectiveness, scalability, and reduced reliance on manual labor make it particularly suitable for large-scale solar installations where regular cleaning is both labor-intensive and hazardous. Moreover, this work highlights the importance of optimizing water usage in the cleaning process, making the system more sustainable, especially in arid regions. By focusing on a dry-brush mechanism, the design minimizes water consumption while maintaining effective cleaning performance. This study's findings underscore the importance of regular, efficient, and cost-effective cleaning methods to maintain solar PV system performance.



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sciforum-107813: Advanced IoT Solutions for Plant Growth Monitoring: A Comparative Analysis of Machine Learning Approaches

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Background : Advanced IoT Agriculture presents a transparent review of emerging technologies like IoT-based smart Agriculture. Today's Agriculture industry is data-centered, advanced, and smarter than ever. Smart Agriculture moved the industry from a statistical to a quantitative approach.

Objective: The objective of this paper is to monitor the plant growth using machine learning technique, as well as predicting the plant growth patterns; to integrate and analyze machine learning models for assessing data obtained from IoT devices in order to predict plant health and growth; and to assess the performance of several IoT communication protocol LoRa in terms of data transmission, dependability, and energy efficiency in agricultural settings.

Material/Methods : In this paper , we have collected the real-time data through the different IoT sensors, namely soil moisture, temperature, and humidity, that are crucial for plant health. The collected data are transmitted to a cloud-based platform, where they undergo preprocessing and analysis. Advanced IoT devices generally automate environmental responses, requiring control systems. The key feature of this system is the deployment of the smart devices and sensors for the collection of data like average wet growth, plant height rate, average leaf area of the plant, average root length, and decisions based on the monitoring of trees. In this paper, our objective is to estimate the effectiveness of various machine-learning approaches for predicting plant growth outcomes based on the collected data.

Result We used several machine learning classifiers including Decision Trees, Naïve Bayes, and K-Nearest Neighbors. It has been observed that out of all the classifiers, the Support Vector Machine (SVM) performs well as comparison to other classifiers, i.e., by 99.96%. Other models also performed well, with Naïve Bayes and Decision Trees, both achieving 99.91% accuracy, and K-Nearest Neighbors achieving 98.99%. The result reveals the efficacy of integrating IoT solutions with advanced machine-learning techniques to enhance plant growth monitoring.



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sciforum-104058: Advanced power management algorithm for PV-EV charging stations using a real-time model predictive control

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In the context of grid-connected PV-EV charging stations, efficient power management is a crucial issue. However, existing approaches often rely on the stability of the electrical grid, which can be disrupted by grid faults, causing EV charging interruptions. Moreover, neglecting real-time adjustments and battery electric vehicle (BEV) state of charge can lead to battery damage due to over-current or overvoltage situations, regardless of weather conditions. To address these limitations, a novel station manager algorithm is proposed, which dynamically adjusts power flow among the PV system, EV power demand, and the grid based on real-time measurements of system powers, grid availability, and BEV state of charge. This dynamic adjustment ensures an uninterrupted power supply to the EV while maintaining its battery safe during the charging operation. The proposed station manager introduces multiple operating modes, including adaptive charging mode and fast charging mode, each integrated with a dedicated model predictive controller (MPC) to achieve its specific control objective. Through a semi-experimental simulation using a process-in-the-loop (PIL) test approach on an embedded board, the eZdsp TMS320F28335, the results demonstrate the effectiveness of the algorithm in balancing power flow between the PV power and the BEV, optimizing energy utilization, and ensuring uninterrupted and reliable power supply to the EV.



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sciforum-107397: Advanced quadrotor cooperation: PSO-enhanced backstepping and PID-based inter-distance control.

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This study introduces a sophisticated control framework for managing a pair of quadrotor drones in a leader-follower configuration, leveraging a combination of backstepping control optimized through Particle Swarm Optimization (PSO) and Proportional-Integral-Derivative (PID) control for maintaining inter-drone distance. The mathematical model of quadrotor is presented as a first step then the leader drone's trajectory is governed by a backstepping approach, which is fine-tuned using PSO to achieve optimal performance. This optimization enhances the backstepping controller's ability to manage complex trajectory tracking tasks, ensuring the leader drone follows its designated path with precision, robustness and minimal deviation. Simultaneously, the follower drone's position relative to the leader is managed by a PID control system, specifically designed to maintain a constant distance between the two drones. The PID controller adjusts the follower drone's position dynamically, responding in real-time to any variations in the leader's trajectory and ensuring that the desired separation distance is consistently maintained. Simulation experiments validate the effectiveness of the proposed control strategy. Results demonstrate that the leader drone adheres to its trajectory with exceptional accuracy, facilitated by the PSO-optimized backstepping control. The follower drone, in turn, effectively maintains the desired distance from the leader, showcasing the robustness and adaptability of the PID control system. The proposed approach significantly improves both trajectory tracking and distance maintenance, providing a reliable solution for coordinated multi-drone operations. This strategy not only enhances precision in trajectory adherence but also ensures stable and robust distance control, making it highly effective for complex and dynamic flying scenarios.



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sciforum-107485: AI-Driven Optimization of Hybrid Energy Systems: Integrating Wind Turbines, Batteries, and the Grid

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This project explores the development of an Energy Management System (EMS) designed to optimize power generation from wind turbines, battery storage, and load management using Reinforcement Learning (RL). By leveraging load profile and wind speed data, we create an RL agent that makes optimal decisions in a fluctuating energy landscape. The EMS incorporates key cost parameters, including USD 0.20 per kWh for imported energy, USD 0.05 per kWh for exported energy, and USD 0.10 per kWh for battery usage. The main objective of the agent is to maximize rewards by minimizing costs associated with energy consumption while improving the efficiency of both energy generation and storage.

Through extensive training and simulation, the RL agent adapts to varying conditions, effectively balancing energy supply and demand in response to changes in wind energy generation. Preliminary results indicate that the EMS not only enhances cost efficiency but also improves overall energy utilization. This demonstrates the viability of applying RL techniques in the management of renewable energy resources.

The findings of this research significantly contribute to the advancement of smart energy systems and the integration of sustainable energy sources, providing a framework for developing more efficient and resilient energy networks. By showcasing the potential of RL in optimizing energy management, this project paves the way for future innovations in renewable energy applications.



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sciforum-103733: An Optimized Wireless Image Transmission for achieving a Semantic Wireless Communication System for Smart Agriculture Monitoring Purposes.

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Smart agriculture systems have several applications and features that aim to provide an automated agriculture process with zero human intervention. Monitoring is one of the most demanding applications of the smart agriculture system. Image and video processing are very important features in the application of smart agriculture monitoring. However, the transmission of video and images requires a large bandwidth, stable connectivity, and noiseless transmission. Notably, high-quality images usually require more bandwidth. On the other hand, the smart agriculture system usually adopts wireless communication among its elements. However, the wireless communication channel generally has some noise which inversely affects the transmission system bandwidth. There are several research efforts found in the literature to address this issue. Some of the distinguished research efforts found address that by either compressing the image or correcting the image errors. However, the smart agriculture system elements are limited in the hardware capabilities. The limitation of the system's hardware configuration is a permanent constraint for this type of solution. This paper proposes an optimization technique to mitigate the issues encountered within the wireless channel while considering the limitation of the hardware resources. The paper jointly optimizes the resources by compressing the image and encoding it using the reed Solomon encoding technique. The results provided a 98% efficiency against the traditional unlimited resources system, along with better BER.



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sciforum-101943: Application of Quantum Key Distribution to Enhance Data Security in Agrotechnical Monitoring Systems Using UAVs

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Ensuring the security of data transmission in agrotechnical activities is crucial, especially when using advanced monitoring systems based on UAVs and AI methods. Traditional encryption methods face significant threats due to the emergence of quantum computing. This study explores the application of Quantum Key Distribution (QKD) to secure data transmission in UAV-based geographic information systems (GISs) used for monitoring both forest fires and agricultural fields. By leveraging the BB84 protocol with polarization of weak coherent pulses, quantum keys are distributed between UAVs and ground stations, ensuring data integrity and security. The hardware requirements for integrating QKD in UAVs and ground stations include compact lasers, polarization modulators, microlenses, polarization filters, and single-photon detectors. Simulation results indicate that the key generation speeds are sufficient for real-time secure data transmission, even under the constraints of UAVs such as limited power and size. Furthermore, this study examines the influence of atmospheric conditions, geometric losses, and receiver characteristics on the communication range and stability. The proposed QKD method enhances the efficiency of data security in GISs for agricultural production monitoring. Future research will focus on practical implementation, optimization of the QKD system for UAVs, and integrating QKD with existing communication systems and data transfer protocols. This integration aims to provide robust support system for agrotechnical activities, leveraging advanced AI methods and monitoring systems to increase the efficiency and security of agricultural production.



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sciforum-097998: Applying automation techniques in the preparation of railway signaling control tables

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Railway signaling is a critical component of ensuring the safe and efficient operation of train systems. The preparation of signaling control (interlocking) tables, which outline a specific signaling logic for controlling signals, switches, and track section vacancy, can be a complex and time-consuming task. These tables involve intricate logic, considering train positions, speeds, and potential conflicts within each possible train route. The generation of control tables for small railway stations can be performed manually relatively quickly, but the complexity of the work grows exponentially with the topology of the corresponding railway station, making it more susceptible to possible errors.

To reduce or even eliminate the possible errors in generating control tables, various studies and articles on automatic generation and verification have been presented in the literature, using different formal tools like EURIS, Ladder logic, Petri Nets (PNs), RailML, Controlled Natural Language (CNL), Maple, B-method, Gröbner Bases (GBs), Abstract State Machines (ASMs), Finite State Machines (FSMs), etc. All the examined papers assumed that the topological layout of a specific railway station had to be prepared manually using dedicated input tools. However, substantial progress was achieved only when the topology of the specific railway station was generated in the corresponding graphical editor before generating the control table itself, which brings a specific level of automation to the whole process.

This paper will present a methodology for the generation of station control tables using the MATHEMATICA package directly from the AutoCAD station signaling layout. This is usually prepared as the first step in the design of a railway signaling system for specific railway stations.



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sciforum-101764: Autonomous radio frequency spectrum tracker robot

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Frequency-follower robots are devices designed to detect, identify, locate, or follow radiofrequency signals. These robots are equipped with antennas and receivers calibrated to receive specific frequency ranges. Many of these robots are designed for specific purposes, such as identifying interference frequencies or analyzing the coverage of a transmitter. In this context, to provide a versatile solution for tracing frequency signals in the field or remote areas, this work presents the development of a small, easily implemented robotic vehicle that facilitates the identification of specific, pre-calibrated radio frequencies. The robot is designed with a four-wheeled configuration similar to a standard line-follower robot, allowing for stable and precise movement. It is equipped with a controlled receiver and a microcontroller that processes incoming signals and directs the robot's movements accordingly. This setup enables the robot to autonomously navigate and trace frequency signals, even in challenging environments. To ensure the robot's effectiveness, a thorough characterization process was conducted. This involved calibrating the detection frequencies and fine-tuning the robot's trajectory-tracing capabilities. The robot was tested in various field conditions, including areas with difficult access, to evaluate its performance. The characterization process confirmed the robot's ability to detect frequencies in the ranges of 10 to 100 MHz, 10-50 MHz, and 200-500 MHz. Additionally, the robot demonstrated its capability to track frequency coverage in peripheral and high-mountain areas for its versatility and adaptability.



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sciforum-104407: Classification and Fault Detection in Induction Motors Using DDACMD for Electrical Signal Analysis

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The article examines the application of the DDACMD technique for analyzing electrical current signals from induction motors to classify their operational conditions. Specifically, the study focuses on categorizing the motor into three distinct states: healthy motor, motor with one broken bar, and motor with two broken bars. To achieve this, the research involves collecting electrical current signals from the motor under various operating conditions. These signals are then processed using DDACMD, a technique designed to extract and analyze distinctive features related to each condition. The processed data are evaluated using classification algorithms that interpret these features to accurately determine the motor's condition. The results of the analysis demonstrate that DDACMD is highly effective in distinguishing between the different motor conditions with a high level of accuracy. This effectiveness highlights the technique's potential for supporting predictive maintenance strategies, allowing for early detection of faults and thereby reducing costs associated with unexpected motor downtimes. The study concludes that DDACMD provides a reliable and precise means of diagnosing faults in induction motors. Its ability to accurately classify motor conditions makes it a valuable tool for enhancing maintenance practices. The article also suggests that further research should explore the broader applications of DDACMD in various fault detection scenarios and different types of machinery to fully leverage its diagnostic capabilities. This could significantly improve preventive maintenance efforts and operational efficiency across diverse industrial settings.



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sciforum-103379: Comparing the control performance of Direct Current and Permanent Magnet Synchronous Motors based on the Stochastic Fractal Search Algorithm

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In modern electric drive systems, both Direct Current (DC) motors and Permanent Magnet Synchronous Motors (PMSMs) are widely used due to their distinct advantages and applications. DC motors are known for their simplicity and ease of control, making them suitable for various applications requiring precise speed regulation. On the other hand, PMSMs offer higher efficiency, better power density, and improved performance, which are crucial for advanced and demanding applications. This paper attempts to apply the Stochastic Fractal Search (SFS) algorithm to optimize the parameters of the PI controller for both DC motor and PMSM engine speed control and then compare their performance in order to determine which motor functions better in terms of this technique. The SFS technique uses the diffusion feature found in random fractals to find the optimal PI values by minimizing the Integral of Time-weighted Absolute Error (ITAE) to improve the performance of both engines. Our study demonstrates significant improvements in speed control stability, overshoot reduction, faster rise times, lower steady-state errors, and quicker settling times, with the overall performance of the PMSM control system being superior to that of the DC motor. These results show the superiority of the SFS algorithm for PMSM compared to DC motor applications.



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sciforum-100892: Comparative Analysis of Multicarrier Waveforms for Terahertz-Band Communications

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The terahertz (THz) band, ranging from 0.1 to 10 THz, offers substantial bandwidths that are essential for meeting the ever-increasing demands for high data rates in future wireless communication systems. This paper presents a comprehensive comparative analysis of various multicarrier waveforms suitable for THz-band communications. We explore the performance, advantages, and limitations of several waveforms, including Orthogonal Frequency Division Multiplexing (OFDM), Filter Bank Multicarrier (FBMC), Universal Filtered Multicarrier (UFMC), and Generalized Frequency Division Multiplexing (GFDM).

The analysis covers key parameters such as spectral efficiency, peak-to-average power ratio (PAPR), robustness to phase noise, and computational complexity. Simulation results demonstrate that while OFDM offers simplicity and robustness to multipath fading, it suffers from high PAPR and phase noise sensitivity. FBMC and UFMC, with their enhanced spectral efficiency and reduced out-of-band emissions, show promise for THz-band applications but come at the cost of increased computational complexity. GFDM presents a flexible framework with a trade-off between complexity and performance, making it a potential candidate for diverse THz communication scenarios.

Our study concludes that no single waveform universally outperforms the others across all metrics. Therefore, the choice of multicarrier waveform for THz communications should be tailored to the specific requirements of the application, balancing performance criteria and implementation feasibility. Future research directions include the development of hybrid waveforms and adaptive techniques to dynamically optimize performance in varying THz communication environments.



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sciforum-104226: Comparative Analysis of Rectangular and Circular Piezoelectric Sensor for Pressure-Based Energy Generation

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Piezoelectric sensors are widely used due to their high sensitivity, fast response and ability to convert mechanical energy to electrical signals for diverse applications in pressure sensing, wearable devices and energy harvesting. This study investigates the design and performance analysis of two piezoelectric pressure sensors with rectangular and circular patches using COMSOL Multiphysics. Each sensor consists of a Polydimethylsiloxane (PDMS) substrate, a Polyvinylidene Fluoride (PVDF) piezoelectric layer, and aluminium electrodes on the top and bottom. Fixed boundary conditions are applied to secure the sensor's four edges, while a pressure range of 0–60 kPa is applied to its top surface using the boundary load feature in the solid mechanics interface. The electric potential interface within the electrostatic interface connects the sensor patches in series, grounding one patch's bottom electrode while terminating the other to the electric circuit interface to measure the output voltage across a 1 k Ω load. The rectangular patch sensor yields a maximum output voltage of 26 mV, while the circular patch sensor produces a higher output of 30 mV. Additionally, to enhance sensor output, the piezoelectric element is replaced with Zinc Oxide (ZnO). The sensor employing ZnO material generates a higher output voltage of 40 mV and 47 mV for the rectangular and circular patches, respectively compared to the material PVDF. The comparative study reveals that the circular patch sensor outperforms the conventional rectangular one, offering enhanced output voltage and optimized geometry for superior performance, making it a better choice for pressure sensing applications.



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sciforum-106238: comparative study between the experimental implementation of an open loop observer and EKF observer with DTC of induction motor

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Estimation technique is a very important tool in the control of electrical machines, especially in the control of induction motors. The technique is based on the concept of "observing" unobservable states of the system by a mathematical model. There are two kinds of observer techniques available in the literature: the open loop type and the close loop type (observer).

In our study we use Direct Torque Control (DTC) which is a control strategy that allows direct control of the motor's torque and flux. This technique uses estimators or observers to calculate motor parameters, including rotor speed, torque, and stator flux.

A comparative study between the experimental implementation of an **open loop observer** and an **Extended Kalman Filter (EKF) observer** with **Direct Torque Control (DTC)** of an induction motor can be framed around several performance criteria. These criteria include accuracy, dynamic response, robustness, computational cost, noise sensitivity, and ease of implementation. The Open Loop Observer is a simpler observer, based on the mathematical model of the induction motor. It assumes perfect knowledge of the system and does not correct for measurement or model inaccuracies. Where Extended Kalman Filter (EKF) Observer is the more advanced observer that uses a stochastic approach, incorporating statistical models of noise. It estimates motor parameters by recursively updating based on measurement and system dynamics, correcting for errors and noise.



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sciforum-107826: Control of DC Microgrid with Photovoltaic and Battery Storage System

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This research paper investigates the feasibility of integrating photovoltaic batteries storage systems into a direct current (DC) microgrid for reliable electricity supply. The proposed system consists of a photovoltaic array, DC/DC boost converter, battery bank energy storage, bidirectional DC/DC converter and DC loads. First the elements of our system are modeled then the control of this elements is given. A fuzzy logic-based control algorithm is used as a maximum power point tracking to optimize power extraction from the photovoltaic panels. The energy management system (EMS) operator regulates the power output of the photovoltaic array/battery bank by transmitting reference power signals to the input side regulation unit. These units, in turn, control the DC link voltage and the state of charge of the battery energy storage system. Depending on the energy management system proposed, our system works as an islanded microgrid and as a connected to an alternating current (AC) Grid. The contribution of this paper is the use of fuzzy logic based MPPT this technique give better performance than the classical perturb and observe in terms of robustness, efficiency and response time. The system is simulated using Matlab software; variable sunshine and temperature are taken to test the effectiveness of our system. The results simulation demonstrates the high performance of the fuzzy logic maximum power point tracking controller used and the effectiveness of the energy management system (EMS) proposed.



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sciforum-107547: Design and development of smart obstacle detector using deep learning methods for vehicles to reduce the injury/death rate of human lives

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The recent surveys by WHO depicts that 50 million people are injured due to traffic accidents across the globe. This is primarily due to inattentive driving, unclear lane markings, poor visibility, and aggressive driving. The mentioned issues can be addressed by developing a smart device with advance technology that avoid traffic accidents and secure the divers/passengers. This novel design utilizes ultra high radio frequency identification that is fitted with road reflector studs, which function in a two-way system. The smart device is made with an RFID reader (ultra high frequency), Arduino controller (ATmega328p), LED's, cameras (OV7670), and speed limiter, which create a safety network for the driver. Here the RFID fitted in the reflector sends a signal to the nearby vehicle if the vehicle gets near the deadline of the road, and the RFID scanner in the vehicle receives the signal that alerts the driver using an Arduino controller, which decodes the signal and initiates the alert system so the driver can get back into the lane. Also the camera included in the smart device on a vehicle identifies the barriers such as walking people, wildlife and other harmful things in an effective manner by image classification with a deep learning method. This verifies whether the captured image is harmful to the vehicle or not, if the detected image is harmful then it activates the speed controller present in the vehicle; thereby, vehicle speed will be controlled automatically. The proposed system is modelled and verified with better results.



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sciforum-102849: Design and FEM analysis of Zeonex-Based Porous-Core Holey Fiber over telecom bands

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This paper provides a comprehensive analysis of the optical properties of a Zeonex-based porous-core holey fiber (PCHF) operating at 1550 nm. The study looks at critical parameters like dispersion, confinement loss, effective area, nonlinear coefficient, V-number, and bend loss to assess the fiber's performance in optical communication and sensing applications. The aforementioned optical properties are determined using the finite element method, which involves Comsol Multiphysics modeling and simulations. The results indicate that the Zeonex-based PCHF exhibits a significant negative dispersion of $-785.7 \text{ ps}/(\text{nm}\cdot\text{km})$, a confinement loss of $7.098 \times 10^{-2} \text{ dB/cm}$, and an effective area of $1.319 \text{ }\mu\text{m}^2$. The fiber's nonlinear coefficient is measured at $61.46 \text{ W}^{-1} \text{ km}^{-1}$, with a V-number of 2.21 and a bend loss of $4.939 \times 10^{-3} \text{ dB/cm}$. These findings demonstrate the potential of the Zeonex-based PCHF to improve the performance of optical communication systems and sensing technologies. The negative dispersion and low confinement loss indicate that it is suitable for controlling chromatic dispersion and reducing signal attenuation. Furthermore, the effective area and nonlinear coefficient values promote high-power light transmission and efficient nonlinear interactions, whereas the V-number and bend loss parameters demonstrate the fiber's structural robustness and flexibility. Finally, this study emphasizes the promising properties of a Zeonex-based PCHF, arguing for further research and development in advanced photonic applications.



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sciforum-107710: Design and implementation of novel DVR configuration for electric vehicles charging application

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In today's world, conventional vehicles are replaced by electric vehicles due to their eco-friendly operation and reduced maintenance. Though the EVs are better than the conventional vehicles, the charging stations for EVs are very few, and there are many power quality issues that have been arising in these charging stations. This is due to voltage, current, or frequencies are abnormal which leads to sudden voltage drops, voltage swells, long interruptions, and short interruptions that occur in the charging stations. Conventional FACTS devices are attached closer to the load end to overcome problems caused by client-side anomalies. One such dependable custom power gadget for dealing with voltage sag is the developed in this article and it is called enhanced dynamic voltage restorer (DVR). The proposed device continuously monitor the load voltage waveform and inject (or absorb) the balance (or surplus) voltage into (or away from) the load voltage whenever a sag occurs. A reference voltage waveform is developed to achieve the aforementioned capabilities. In this paper, the methods of compensation for these problems in charging stations are discussed. Further the power quality problems are compensated by the proposed system using a SVPWM controller. Simulation and real time implementation is carried out and the results discussed are here.



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sciforum-104326: Design and Optimisation of an Inverted U-Shaped Patch Antenna for Ultra-wideband Ground Penetrating Radar Applications

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Ground Penetrating Radar (GPR) systems with Ultra-wideband (UWB) antennas introduce the benefits of both high and low frequencies. Higher frequencies offer finer spatial resolution, enabling the detection of small-scale features and details, while lower frequencies improve depth penetration by minimising signal attenuation, allowing the system to explore deeper subsurface layers. This combination optimises the performance of GPR systems by balancing the need for detailed imaging with the requirement for deeper penetration. This work presents the design of a wideband inverted U-shaped patch antenna with a wide rectangular slot centred at a frequency of 1.5 GHz. The antenna is fed through a microstrip feed line and employs a partial ground plane. Through simulation, the antenna is optimised by varying the patch dimensions and slot size. Further modifications to the partial ground plane improve UWB and gain characteristics of the antenna. The optimised antenna is fabricated using a double-sided copper clad FR4 substrate with a thickness of 1.6 mm and characterised using a Vector Network Analyser (VNA), with a final dimensions of 200 mm x 300 mm. Experimental results demonstrate a return loss below -10 dB across the operational band from 1.068 GHz to 4 GHz and achieve a maximum gain of 7.29 dB at 4 GHz. In addition to other bands, the antenna exhibits a return loss consistently below -20 dB in the frequency range of 1.367 GHz to 1.675 GHz. These results confirm the antenna's UWB performance and its suitability for GPR applications in utility mapping, landmine and artefact detection, and identifying architectural defects.



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sciforum-104300: Design Optimal Analysis of Brushless Direct Current Motor by Fuzzy Logic

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Design investigations of Brushless DC (BLDC) motors are increasing year by year, and most motor design researchers have investigated the superior efficiency of the BLDC motor. This research presents the high performance and efficiency of the outer rotor BLDC motor by using the electric fan under optimization and an analysis of fuzzy logic to find out whether this motor shows higher efficiency and saves more energy than another traditional motor. Firstly, this research identifies a suitable design for the reference of the outer rotor BLDC motor used in electric fans. The electric fan motor is manually tested using the motor specification parameters and testing machine. To optimize the reference motor analyzed, the "one factor at a time" method involves changing one design parameter at a time while keeping all other parameters constant to observe the effect of the reference model. The simulation of the design investigation results is studied using the JMAG software. This software can produce the optimization result for the analysis of the Finite Element Method. The final proposed model achieved an efficiency of 15 % higher than the reference model, and the output power is 8 W higher than this reference model. The maximum torque of the proposed model is 0.032 Nm higher than the reference model. Moreover, the design evaluation results of the proposed model are considered, and the four methods of design optimizations are shown in the characteristics of the motor design improvements in this research.



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sciforum-104565: Development of autonomous unmanned aerial vehicle for environmental protection using YOLO V3

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Unmanned aerial vehicle also termed as unarmed aerial vehicles are used for various purposes in and around the environment, such as delivering things, spying the opponents, identification of the aerial images, extinguishing of fire, spraying the agricultural fields etc. As there are multi-functions in a single UAV model, it can be used for various purposes as per the user requirement. The UAV's are used for because of faster communication of information identified, entry through the critical atmospheres and no harm to humans before entering a collapsed path. In concern with the above discussion an UAV system is designed to classify and transmit information about the atmospheric conditions of the environment to a central controller. The UAV is equipped with advanced sensors that are capable in detecting air pollutants such as: carbon monoxide (CO), carbon dioxide (CO₂), methane (CH₄), ammonia (NH₃), hydrogen sulphide (H₂S), etc.,. These sensors present in the UAV model monitor the quality of air time to time, as the UAV navigates through different areas and transmits real-time data regarding the air quality to a central unit; this data includes detailed information on the concentrations of different pollutants. The central unit analyzes the data that are captured by the sensor and checks whether the quality of air meets the atmospheric standards. If the sensed levels of pollutants exceed the thresholds, then the system present in the UAV triggers a warning alert, this alert is communicated to local authorities and the public to take necessary precautions. The developed UAV is furnished with cameras which are used to capture real-time images of the environment and it is processed using the YOLO V3 algorithm. Here YOLO V3 algorithm is defined to identify the context and source of pollution, such as identifying industrial activities, traffic congestion, or natural sources like wildfires.



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sciforum-104012: Development of jaw controlled wireless navigation governing system for wheelchair to empower person with impaired upper limb

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The central focus of this work is to implement an effective and cost-friendly wheelchair motion control system for individuals with impaired upper body movements by utilizing the mandibular movement of an individual. The initial part of the system is the signal-gathering system that is built of two functional blocks, the magnet and sensing block. A magnet is affixed to the inferior region of the user's mandible, and the sensing block, which incorporates two static HMCL 5883L sensors, quantifies the magnetic field intensity modulated by the magnet's displacement. The processing unit deciphers these sensor signals to ascertain the wheelchair's trajectory, while the mechanical unit effects the movement directives. The methodology is embedding the HMCL 5883L sensor into the microcontroller to detect the required motion for the wheelchair. The HMCL 5883L sensors are incorporated to identify each change in the orientation of the magnet. HMCL 5883L is a sophisticated and budget technology. In order to trace the magnet in the user's jaw region, the sensor partitions the magnet's strength's path into three hypothetical axes. The magnet's configuration in the mandibular region won't create any unease, and a user jaw action isn't something new that requires a certain level. This development empowers the mobility of patients with Quadriplegia and because of the device's smaller footprint and feasible modules, it infuse sustainable development and availability.



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sciforum-107388: Dynamics and Phase Noise of Time-Delayed Laser Diode with Non-Radiative Recombination Rate

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In our study, we investigated how the strength of optical feedback and the non-radiative recombination rate impact a laser diode's dynamics and phase noise. To analyze laser dynamics, we solved numerically improved time-delay rate equations across a wide range of optical feedback strength and non-radiative recombination rates. The laser's dynamics will be categorized based on the bifurcation diagrams of the photon number. Our findings show that the non-radiative recombination rate has a significant effect on the intensity, states, and dynamic behavior of the laser diode's phase noise. A decrease in the non-radiative recombination rate results in the laser transitioning faster from a continuous wave to periodic oscillation under strong optical feedback. In the chaotic region, the non-radiative recombination rate causes a slight shift in the phase fluctuations compared to the laser operating without optical feedback. Lower non-radiative recombination rates stabilize the laser output and enable continuous wave or periodic oscillation at higher current levels. In the strong optical feedback region, a reduction in the non-radiative recombination rates shifts the chaotic operation to stable modes such as a continuous wave or periodic oscillation, and the phase noise approaches the quantum noise level. Our study emphasizes the key roles of the non-radiative rate and optical feedback in manipulating the dynamics and phase noise of a laser diode. We have shown that losses due to non-radiative rates could be practically useful for engineering laser behaviors. The strength of optical feedback can be adjusted to achieve the optimal goals of stabilizing laser operation. Our work is driven by the ongoing interest in finding effective ways to control and optimize the output of a laser diode. We believe that our findings may have potential applications in future experimental design and optimization, which will be of general interest to the community studying solid-state semiconductor laser diodes.



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sciforum-103971: Efficient PV Grid Integration Using a Three-Level NPC Converter and Advanced Control with Phase Disposition PWM

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This paper presents an innovative approach to photovoltaic (PV) grid integration using a single three-level neutral-point clamped (3L-NPC) converter with an advanced control employing a nonlinear control technique and Phase Disposition Pulse Width Modulation (PD PWM). Unlike conventional systems that utilize separate DC-DC and DC-AC converters, this study proposes a unified control strategy to regulate DC voltage and ensure unitary power factor correction (PFC) at the grid side. The DC voltage reference is generated by a Perturb and Observe (P&O) Maximum Power Point Tracking (MPPT) algorithm, optimizing the extraction of maximum power from the PV array.

The methodology includes detailed modeling of the PV system, the 3L-NPC converter, and the proposed control algorithms. The PD PWM technique is implemented to improve the harmonic performance and voltage balancing of the converter. Simulation results, conducted in MATLAB/Simulink, demonstrate the effectiveness of the proposed control strategy in maintaining stable DC voltage and achieving unitary PFC under varying solar irradiance. The results show significant efficiency improvements and reduced total harmonic distortion (THD) compared to traditional methods. In conclusion, the integration of MPPT and PFC in a single 3L-NPC converter presents a cost-effective and efficient solution for PV grid integration. The proposed system enhances overall performance and reliability, paving the way for more streamlined and sustainable renewable energy systems.



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sciforum-107742: Empowering Women's Safety with Leveraging Advanced IoT Technology for Comprehensive Protection and Security

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Globally, women entail physical assault and harassment, which emphasizes the critical requirement for proactive and efficient safety measures. However, a lot of present technologies are inadequate and often lack comprehensive information protection, integration, and real-time responsiveness, which reduces user confidence and reliability. A complete integrated platform in the form of GUARDHER and GUARDIANSTEP has been designed to provide a safety system that serves women with precautionary measures. GUARDHER is a companion app, where the user has to register and create a secure wallet that contains their personal photo and other key information within a passkey protection. This application will be linked to GUARDIANSTEP, which consist of pair of shoes with the innovative feature of force sensor connected to a high-performance Microcontroller unit. Once the threshold pressure is applied by the user to the force sensor, it eventually results in transmission of the current location with their personal profile in the wallet to the control panel using Internet of Things (IoT) for immediate remedies. Within a delay time, the user has to deactivate/turn-off the emergency button via the application after entering the passkey of their respective wallet to prevent false alerts. The difference it holds from the current-day safety apps or devices, that it is a combination of personal profile protection, transfer of personal details along with their photo, real-time location tracking, and an advanced force sensor in footwear. It is a unique combo that offers user authentication, alerts in case of emergencies, delay time to turn it off and proactive safety measures that will build user confidence and responsive ability in extreme conditions. The “GUARDHER & GUARDIANSTEP” product offers a holistic solution by providing a secure platform and also ensures the integrating safety features in mobility, fostering a society where women can move freely with confidence and empowerment.



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sciforum-102967: Energy-Efficient and Coverage-Optimized Wireless Sensor Networks using a Multi-Objective Jellyfish Search Algorithm

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This paper investigates the application of a multi-objective metaheuristic algorithm, the Multi-Objectives Jellyfish Search (MOJS), to enhance the performance and reliability of Wireless Sensor Networks (WSNs). WSNs, a recent technological advancement, facilitate the strategic deployment of numerous miniature, battery-powered sensors to monitor and gather data from diverse environmental settings. However, the implementation of WSNs faces significant challenges due to limited energy resources. We propose a novel approach, termed WSN-MOJS, which aims to optimize WSN implementation by maximizing coverage and minimizing energy consumption. Simulations were conducted using MATLAB software to design a network consisting of multiple sensor nodes to monitor a designated zone. The process begins by randomly initializing candidate node placements, which are then evaluated using two objective functions as follows: total coverage, and energy expended by the sensor nodes. The MOJS updating process is iteratively applied over multiple iterations. To test the performance of our WSN-MOJS approach, we conducted several simulations by varying the number of nodes, candidate solutions, and iterations. The results indicate that the proposed WSN-MOJS algorithm ensures maximum coverage with an average number of nodes and minimizes energy consumption within a minimal computation complexity due to its exploration and exploitation capabilities. Increasing the number of candidate solutions and iterations significantly improves the Pareto front. Consequently, the non-dominated solutions become well-distributed, and the fitness values are enhanced.



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sciforum-103798: Enhancing a Modified East–West Interface for Modern Networks

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Traditional software-defined network (SDN) systems focus primarily based on a north–south data flow to enable centralized control of network devices. However, the growing complexity and scale of modern networks, driven by emerging internet applications and services, require a more advanced approach to handle the east–west data flow, which involves communication between devices within the network. This necessitates a distributed SDN architecture with multiple controllers to simplify network management and achieve control. This paper evaluates a modified east–west interface with network policies for Distributed Control Plane Networks, designed to meet the needs of SDN in multi-domain networks such as wide area networks (WANs) while ensuring network availability. The modified east–west interface is developed by implementing network policies on a Modified Communication Interface for Distributed Control Plane (mCIDC), which is integrated with the Floodlight controller. Experimental results demonstrate that the mCIDC outperforms the Communication Interface for Distributed Control Plane (CIDC) by reducing captured transmission control protocol (TCP) packets by 15.51%, TCP errors by 29.85%, and inter-controller communication overload by 22.98%. This indicates that the mCIDC can make better decisions in line with network policies compared to the CIDC when deployed in a real-time wide-area network. This shows that SDN architectures can support network policies for management, security, and interoperability network devices.



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sciforum-108680: Enhancing the Algerian Power System for Long-Distance Transmission: A Comprehensive Study on the Implementation of HVDC Technology

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The integration of High Voltage Direct Current (HVDC) technology into power systems has emerged as a pivotal solution for enhancing the efficiency and reliability of long-distance energy transmission. This study investigates the implementation of HVDC technology within the Algerian power system, utilizing the Power System Analysis Toolbox (PSAT) to simulate its impact on power flow and voltage profiles. The Algerian power system, characterized by its extensive geographical spread and varying energy demand across regions, presents unique challenges for energy transmission, especially from renewable sources located in remote areas. By incorporating HVDC links into the system, we aimed to address these challenges, focusing on improvements in the active power distribution and voltage stability across the network. The simulation results indicate a significant enhancement in the voltage profiles of various bus bars, which previously fell below acceptable limits. The implementation of HVDC not only brought these within the 10% voltage stability margin but also optimized the active power distribution throughout the system. These findings underscore the potential of HVDC technology in bolstering the Algerian power system's capacity for efficient, reliable energy transmission over long distances, providing a valuable framework for future infra-structure development and policy formulation aimed at sustainable energy growth.



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sciforum-107150: Estimating Relativistic Errors in Satellite-Based Geolocation Algorithms with Passive Sensors

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This study focuses on improving geolocation accuracy in satellite systems using passive sensors through relativistic error estimation. Geolocation, the determination of a target's position using signals from electromagnetic emitters, becomes increasingly challenging when relativistic effects are considered, especially in space-based systems. The system under study involves a passive receiver mounted on a satellite and an emitter located on Earth's surface. The primary goal is to integrate relativistic corrections—such as time dilation, changes in potential energy, and satellite orbit eccentricity—into traditional geolocation algorithms, which primarily rely on signal time delay.

To achieve this, a theoretical model is developed, which examines the relativistic contributions to position errors arising from the finite speed of light and the effects of the satellite relative motion. Using an analytical approach, the study evaluates how these relativistic factors influence geolocation accuracy. A comparison between a Newtonian model for time delay and a modified algorithm incorporating relativistic corrections is presented. The relativistic correction algorithm, implemented through adjustments in the software layer, does not require system-level changes, making it feasible for current satellite operations.

Simulation in worst case scenarios results demonstrate that while relativistic effects are often considered negligible in many applications, they can introduce significant errors, particularly in high-precision tracking scenarios or in systems with highly eccentric orbits. In conclusion, incorporating relativistic corrections in satellite-based geolocation algorithms can enhance the precision of passive sensors, offering valuable improvements in both Earth and deep-space missions.



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sciforum-103701: Fuzzy Logic-Based Adaptive Droop Control Designed with Feasible Range of Droop Coefficients for Enhanced Power Delivery in Microgrids

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Power electronic converter-based microgrids generally suffer from poor power delivery/handling capability during sudden load changes, especially during islanded operations. This is due to a lack of transient energy support to compensate for sudden load changes. The literature has suggested the use of adaptive droop control to provide compensation during transient conditions, thereby improving their power delivery capability. In this context, fuzzy logic-based adaptive droop control is a state-of-the-art technique that was developed based on empirical knowledge of the system. However, this way of selecting the droop coefficient values without considering mathematical knowledge about the system leads to instability during transient conditions. This problem is further worsened when dominant inductive load changes occur in the system. To address this limitation, this paper proposes an improved fuzzy logic-based adaptive droop control method. In the proposed methodology, the values of droop coefficients that are assigned for different membership functions are selected based on a stability analysis of the microgrid. In this analysis, the feasible range of active power-frequency droop values that could avoid instability during large inductive load changes is identified. Accordingly, infeasible values are avoided in the design of the fuzzy controller. The performances of the proposed and conventional fuzzy logic methods are verified through simulations in MATLAB/Simulink. From the results, it is identified that the proposed method improved the power delivery capability of the microgrid by 14% compared to the conventional method.



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sciforum-107623: Implementation Of Prototype-Based Parkinson's Disease Detection System With Risc-V Processor

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In the wide range of human diseases, Parkinson's Disease has a high incidence according to the recent survey of WHO (World Health Organization). According to WHO records, this chronic disease has affected approximately 10 million people worldwide. Patients who do not receive an early diagnosis may develop an incurable neurological disorder. Parkinson's disease (PD) is a degenerative disorder of the brain characterized by the impairment of the nigrostriatal system. This disorder is accompanied by a wide range of motor and non-motor impairments symptoms. By using new technology, the PD is detected through speech signals of the PD victims by using the reduced instruction set computing 5th version (RISC-V) processor. The RISC-V MCU was designed for the voice-controlled human-machine Interface (HMI). With the help of signal processing and feature extraction methods, digital signal processing (DSP) algorithms can be used to extract speech signals. These speech signals can be classified through classifier modules. A wide range of classifier modules are used to classify the speech signals into normal or abnormal to identify PD. To analyze data, develop algorithms and create modules, we use Matrix Laboratory. We used MATLAB for algorithm development, the RISC-V processor for embedded implementation, and machine learning techniques to extract features such as pitch, tremor, and Mel-frequency cepstral coefficients (MFCCs)



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sciforum-104430: Influence of Die Backside Metallization on the Interfacial Intermetallic Compounds in Lead-Free Solder

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Semiconductors are integral to wide array of daily activities like mobile phones and modern automobiles. With rapid advancements in the electronics industry, electronic devices are evolving towards miniaturization. This evolution drives to downsizing the existing semiconductor packages and imposes higher requirements on the quality and reliability of solder joints.

This study focuses on assessing the interfacial reactions between Sn-based solder and die-backside metallizations (BSM), Ti/Ni/Ag and Ti/Al/NiP. The dice with Ti/Al/NiP BSM underwent two processes: increased backside surface roughness and increased backside Aluminum content. They were assembled onto two distinct AMB substrates: Cu-exposed and Ni-plated.

Various intermetallic compounds (IMC) were identified near the die/solder interface. They were characterized using SAM, supplemented by mechanical cross-sectioning technique, SEM, and EDX.

The results show that the Ti/Ni/Ag BSM leads to the formation of fully fragmented IMC. The Ni-plated AMB substrate results in thinner IMCs compared to the Cu-exposed AMB. Increased die-backside roughness leads to a discontinuous IMC layer, while higher Al content promotes a thin IMC with scalloped and needle-like extensions. The SnAg₅ solder results in IMCs with distinct appearance compared to SAC305 due to its initial content of Cu. Finally, thermal cycling induces heterogeneous coarsening of IMCs, and formation of cracks and delamination at the interface and within the solder.

In conclusion, the study reveals that Ti/Al/NiP BSM provided a more reliable IMC. The increased BS roughness does not represent an optimal approach, this contrasts with the increase in Al content which results in a more favorable structure. The Ti/NiV/Ag BSM leads to highly fragmented IMC detached from the interface with the dispersion of plate-like Ag₃Sn IMCs which represent a site for strain localization. Finally, the initial Cu content in SAC305 solder governs the IMC crystal growth.



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sciforum-106154: Influence of Optical Feedback Strength on the Intensity Noise and Photon Number Probability Distributions of InGaAsP/InP Laser

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Long wavelength semiconductor lasers, such as InGaAsP/InP lasers emitting at 1.3 and 1.55 μm , are widely used as light sources in optical communication systems. The dynamical behavior of semiconductor lasers is significantly influenced by optical feedback from an external reflector. To achieve the highest static and dynamic performance in semiconductor lasers, it is essential to thoroughly grasp how the strength of optical feedback affects their stability. This knowledge is fundamental for creating innovative designs that meet advanced performance standards. In this work, the instability of semiconductor lasers with external cavities in terms of noise and photon number probability distributions is investigated for the first time over a wide range of optical feedback. We successfully numerically solved improved time-delay rate equations across various optical feedback strengths [1,2]. Our analysis will classify the laser's dynamics based on detailed bifurcation diagrams of the photon number, providing valuable insights into its behavior. The study analyzes the temporal trajectory of photon numbers and intensity noise and statistically examines variations in output photon number fluctuations, probability distributions, and corresponding intensity noise at different optical feedback strengths. The simulations indicate that optical feedback strength significantly affects the intensity noise and photon number probability distributions. Intensity noise is reduced at relatively weak and strong optical feedback regimes. The shape of the photon number probability distributions is strongly influenced by optical feedback strength, transitioning from symmetric to asymmetric at weak to strong optical feedback, respectively. In the moderate optical feedback range (chaotic region), the photon number probability distributions exhibit a peak at low intensity and tail off at several times the average photon number. The authors suggest that operating semiconductor lasers under weak or strong optical feedback regimes may reduce their instability.



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sciforum-102963: MantaNet: A Novel MRFO-Based Routing Protocol for MANETs

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In this paper, we investigate the application of the Manta Ray Foraging Optimization (MRFO) metaheuristic algorithm for optimizing routing protocols within Mobile Ad Hoc Networks (MANETs). MANETs are decentralized wireless networks consisting of mobile nodes that establish temporary connections independently of any pre-existing infrastructure. Routing protocols, a critical component of MANETs, consist of rules and algorithms that manage the forwarding of data packets across the network. We propose an improved routing protocol based on MRFO, named MantaNet, to identify optimal routes for data transmission. Simulations were conducted using MATLAB software to design a dynamic network comprising nodes moving within a defined zone. The optimization problem focuses on minimizing the distance traversed by data from the sender to receiver, thereby reducing energy consumption, overload, and congestion. The MantaNet algorithm begins with a random initialization of candidate routes, which are then evaluated using a fitness function. The MRFO updating processes are applied to refine the search through multiple iterations. To assess the performance of the MantaNet approach, we conducted several simulations, varying the distance between the sender and receiver, the number of nodes, the candidate solutions, and the iterations. The results demonstrate that the proposed MantaNet algorithm consistently identifies optimal routes across various network sizes and scales. The algorithm maintains strong performance even with a small number of candidate solutions and iterations, thereby reducing computational time. Overall, the MantaNet routing method offers a promising solution for efficient data transmission in MANETs.



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sciforum-104362: Multiple Linear Regression-Based Correlation Analysis of Various Critical Weather Factors and Solar Energy Generation in Smart Homes

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The smart home culture is widely spread across the world by transforming traditional homes into smart homes with technological advancements. In addition, the consumers are becoming prosumers by adding renewable energy namely solar, wind, etc., to their homes along with traditional energy sources. However, intermittent weather conditions impact the power generation of renewable sources. Hence, there is a need to understand the correlation between several weather parameters and power generation. Traditional statistical methods such as Pearson and Spearman's, Kendall's Tau, and Phi correlation coefficients are available but are limited to only two variables. Instead, multiple linear regression (MLR) offers multivariate analysis. Thus, this paper employs MLR to analyze the correlation between weather conditions such as temperature, apparent temperature, visibility, humidity, pressure, wind speed, dew point, and precipitation, and the power generation in kW. All the weather conditions are independent variables, and the generated power is a dependent variable. The key objective is to investigate the significant predictors and their impact on power generation. To implement this, a recent smart home dataset titled "Smart Home Dataset with Weather Information" that gives the required information is downloaded from Kaggle. This dataset contains 32 columns and 503,910 observations. The whole dataset is considered for implementing the proposed correlation analysis. A regression model is developed to find the correlation between the above-mentioned parameters in the dataset, and the multicollinearity between the independent variables is presented using the variance inflation factor (VIF). If the VIF value is greater than 10, it represents high multicollinearity. The results showcase that the variables such as temperature, humidity, apparent temperature, and dew point have VIF values of 298.96, 37.54, 126.86, and 152.95, respectively, and are thereby considered critical weather parameters that significantly influence solar energy generation. This aids in better planning of generation and load management in smart homes.



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sciforum-102193: Optimal Sizing of a photovoltaic system: A Case Study of a poultry plant in Ecuador

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The poultry sector in Ecuador relies heavily on non-renewable energy sources, particularly conventional electricity from the public grid. A typical poultry plant consumes an average of 57.313 MWh per year, resulting in an annual cost of \$7100. The sheds constitute the largest portion of energy consumption, accounting for 36% of the total. The objective of this study is to model an optimal photovoltaic system that can contribute to the energy supply of the area with the highest consumption. The aim is to reduce operating costs and facilitate a transition in the energy matrix. To achieve this, historical and exploratory data were collected, including solar radiation levels, estimation of geographical resources, and energy consumption patterns in the business. Based on the analysis, an isolated photovoltaic system was designed. The system comprises 4 solar panels, 8 batteries, 1 charge regulator, 1 current inverter, 5 types of conductors, and 3 types of electrical protections. The photovoltaic system was sized to meet the energy requirements of the Type A shed, which consumes 5.89 kWh, and the Type B shed, which consumes 6.59 kWh. The design considered the lower annual solar radiation values of 4.58 kWh/m², ensuring that the system could function effectively even with reduced solar input. This approach not only addresses the immediate energy needs of the poultry sector but also contributes to a broader goal of reducing dependency on non-renewable energy sources. By transitioning to photovoltaic systems, poultry plants can significantly lower their operating costs and reduce their environmental impact.



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sciforum-106762: Optimization of Artificial Potential Fields Using Genetic Algorithm for Autonomous Mobile Robot Navigation

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Autonomous navigation in partially known or unknown environments, such as agricultural fields, poses significant challenges for mobile robots. The effective guidance of these robots is crucial for their successful operation in dynamic settings. Artificial Potential Fields (APFs) are widely employed for this purpose; however, they often lead to issues such as oscillations and local minima, which can hinder the performance. This study proposes an innovative optimization of the parameters of Artificial Potential Fields using a genetic algorithm (GA) to address these limitations. The GA fine-tunes the attractive and repulsive constants of the potential fields, significantly enhancing the navigation performance. Comprehensive simulations were conducted in a dynamic environment, incorporating various static and mobile obstacles to rigorously test the proposed method. The results demonstrate a significant improvement in the robot performance, highlighted by smoother trajectories, reduced collisions, and improved handling of dynamic obstacles. Specifically, the APF-GA method decreased the time to reach the goal from 18.8 to 16.1 seconds and the distance traveled from 7.61 to 6.43 meters. This integration of the genetic algorithm into the APF method not only enhances the smoothness of the trajectory but also increases the navigation safety in complex environments. These promising results have important implications for real-world applications, particularly in agriculture and logistics, paving the way for more efficient robotic systems.



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sciforum-107395: Optimized Backstepping control for inverted pendulum: Achieving superior robustness, speed and precision.

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The inverted pendulum is a classical benchmark in control theory, known for its inherent instability and nonlinearity, making it a challenging problem for control engineers. In this paper, we propose a novel optimized backstepping control approach to address the challenges of stabilizing the inverted pendulum while ensuring robust performance, fast response, and high precision. Backstepping, a recursive design methodology for nonlinear systems, is employed due to its ability to systematically handle the pendulum's nonlinear dynamics. To further enhance the performance of the controller, an optimization technique is applied to fine-tune the backstepping parameters, focusing on achieving a balance between robustness, speed, and precision in the pendulum's stabilization. The optimization process is designed to minimize the control error while maintaining stability under various disturbances and model uncertainties. Simulation results validate the effectiveness of the proposed approach. The optimized backstepping controller demonstrates superior performance compared to traditional control methods, particularly in terms of robustness to external disturbances and parameter variations, fast convergence to the desired state, and precise tracking of the pendulum's upright position. Additionally, the system exhibits low overshoot and minimal steady-state error, making it well-suited for applications requiring high control accuracy. The results highlight the potential of this optimized backstepping methodology for controlling complex nonlinear systems, providing a robust, fast, and precise solution for stabilizing the inverted pendulum, even in the presence of disturbances.



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sciforum-106674: Optimizing High-Bit-Rate Optical Transmission with Advanced Techniques

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This research investigates the effectiveness of various chromatic dispersion compensation (CDC) techniques, particularly numerical methods, in a Dual Polarization-Return to Zero-Quadrature Phase Shift Keying (DP-RZ-QPSK) optical transmission system. The primary goal is to evaluate how these techniques can mitigate distance penalties and improve the bit error rate (BER), a critical metric for the reliability of optical communication systems.

The study compares optical and electronic compensation scenarios, analyzing parameters such as launch power, Q factor, and bit error rates. Results indicate that electronic compensation offers superior quality and transmission distance performance. However, it requires a higher launch power (4 dBm) than optical compensation. This trade-off between power consumption and performance must be carefully considered in practical applications.

As symbol rates increase, the study finds that tolerance to chromatic dispersion decreases, leading to a reduction in the quality factor and maximum range. This highlights the importance of developing more advanced CDC techniques to address the challenges posed by higher-speed transmission. Despite these limitations, electronic compensation remains a promising solution for high-speed optical transmission due to its flexibility and adaptability.

The study concludes that the maximum reach achievable with electronic compensation is 4000 km at a 12 dB Q factor. This result demonstrates the potential of electronic CDC to enable long-haul optical communication systems with high data rates. However, further research is needed to explore the limitations of electronic compensation and develop more efficient and power-efficient algorithms.



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sciforum-107366: Photometric Visual Servoing Through Sobel-Based Image Gradient Utilization

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This paper deals with the development of a new 6-degree-of-freedom (DOF) visual servoing control law. The traditional visual servoing (VS) methods depend on geometric features to design the control law, which limits their versatility due to reliance on visual tracking algorithms. To address these limitations, direct visual servoing (DVS) approaches have been introduced, showing that the design of photometric visual servoing (PVS) can bypass geometric feature extraction by directly considering the luminance of all image pixels to control the robot. However, these methods are sensitive to illumination changes and partial occlusions, which make the control task non-robust. To overcome this, we develop a new direct visual servoing control approach based on a Sobel filter to enhance the precision of image information under changing lighting conditions by extracting image gradients. These gradients are then used to design the interaction matrix that allows real-time updates to the motion of the robot for adaptability and precision. Also, the proposed control scheme has been tested on the VISP platform and was compared to the classical photometric visual servoing in order to evaluate its efficiency in nominal and unfavorable conditions. Experimental results validate that the approach provides more performance and reliability under variable illumination conditions.



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sciforum-101715: Practical Transceptor System for Detection of Vibration in Buildings

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Vibrations are a physical effect to which buildings in cities are continuously subjected, and depending on the vibration frequency, they can be associated with a level of risk. In high-seismic-risk areas, buildings endure continuous vibrations that can produce small fractures in the building's structure and increase material damage from periodic and random seismic events. The early detection of structural damage allows for preventive decisions to minimize the risk of a potential collapse.

To provide a tool that helps detect the vibrations a building is subjected to and assess the associated risk from large vibrations, this work presents the development of a simple and practical system that remotely detects vibrations in a building. The system's development involves using vibration sensors and a signal capture system. Data processing and a simple prognosis are performed to evaluate the risk of possible fractures in the building's structure.

The preliminary results allow us to identify that most of the vibrations a building's structure endures are due to vehicular traffic around it, coupled with vibrations from surrounding constructions. The critical vibrations that increase the risk of fracture are due to natural earthquakes exceeding 3 degrees on the Gutenberg–Richter scale, detected by sensors with frequency and amplitude magnitude components. The implemented system offers a quick and effective alternative for detecting and quantifying vibrations in buildings and serves as an alert system for potential fracture risks in a building's structure.



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sciforum-103688: Quadrotor trajectory tracking under wind disturbance using backstepping control based on different optimization techniques

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Enhancing the control techniques of quadrotors to improve their precision and robustness against wind is crucial for expanding their practical applications and reliability. Quadrotors are increasingly utilized in fields such as aerial surveying, delivery services, disaster response and military operations, where stability and accuracy are paramount. Wind disturbances pose a significant challenge, often compromising the performance and safety of these drones.

This research explores the efficacy of various optimization techniques in enhancing the performance of quadrotor control under wind disturbances. After mathematical modeling of a quadrotor, a backstepping controller is developed for this system and then is optimized by different metaheuristic methods: Grey Wolf Optimization (GWO), Particle Swarm Optimization (PSO), and Flower Pollination Algorithm (FPA). Each optimization technique is applied to fine-tune the backstepping controller parameters, with the objective of improving the quadrotor's precision, speed, stability, and robustness. Extensive simulations of quadrotor trajectory tracking are conducted to evaluate and compare the performance of these optimized controllers in the presence of wind disturbances.

The results highlight the relative advantages and limitations of each optimization method in terms of response time, overshoot and the deviation rate from the desired trajectory under wind disturbance, providing critical insights into their suitability for enhancing quadrotor control in dynamic and challenging environments.



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sciforum-101758: Real-time Predictive Monitoring and Analysis of Power Quality in Hybrid Microgrid using Data-Driven Technique

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Power quality (PQ) measures system reliability, equipment security, and power availability in electrical power systems. Common PQ problems include voltage sags, swells, overvoltages, undervoltages, harmonics, transients, and grounding issues, with harmonics and sags having the most significant impact. PQ events are variations in voltage magnitudes and waveform distortions affecting low-frequency to high-frequency spectral content deviations and other phenomena. Power quality is a growing concern due to the restructuring of the electric utility industry and the proliferation of small- and medium-scale distribution generations. This study investigates the predictive monitoring and analysis of power quality (PQ) events in a three-phase microgrid using digital signal processing (DSP) and machine learning (ML) approaches. The results show that harmonics and voltage sags are prevalent issues in AC microgrids, affecting system stability and equipment performance. This study also compares the microgrid's performance with the utility grid, showing that converter-interfaced systems are more susceptible to harmonics combined with RMS voltage variations. The microgrid showed lower Total Harmonic Distortion (THD) but increased sensitivity to voltage sags, highlighting the need for careful consideration when operating high-power devices. This research emphasizes the importance of PQ monitoring in power systems and the significance of both long-term and short-term monitoring for effective power system operation and equipment safety.



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sciforum-104115: Robustness Analysis of LQR-PID Controller Based on Particle Swarm Optimization and Grey Wolf Optimization for Quadcopter Attitude Stabilization

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The robust control of quadcopters is crucial for maintaining stability and performance in dynamic and unpredictable environments. This paper investigates the effectiveness of two optimization techniques, Particle Swarm Optimization (PSO) and Grey Wolf Optimization (GWO), for tuning LQR-PID controllers specifically designed for a constrained quadcopter limited to rotational degrees of freedom. The objective is to enhance attitude stabilization and perform a comparative robustness analysis of these optimized controllers under various disturbance conditions.

LQR-PID controllers are designed for the quadcopter model using PSO and GWO to optimize the Q and R matrices of the LQR controller. Both algorithms aim to minimize a cost function based on the quadcopter's attitude error and control effort. The optimized controllers are tested in a Simulink environment where disturbances such as wind, initial condition perturbations, and sudden impulse disturbances are introduced. Wind disturbances represent varying external forces, initial condition perturbations simulate small deviations from the expected starting state, and sudden impulse disturbances model unexpected sharp forces. These disturbance types were selected to reflect real-world operational challenges faced by quadcopters and are introduced by perturbing the feedback vector of the quadcopter's control system.

The comparative analysis shows that while both PSO- and GWO-optimized controllers achieve effective attitude stabilization, they display different robustness characteristics. The PSO-optimized LQR-PID controller demonstrates better performance in terms of faster convergence and higher sensitivity to disturbances, whereas the GWO-optimized controller excels under extreme parameter variations.

This study contributes to the current state of the art by providing a detailed comparison of PSO and GWO for LQR-PID tuning in quadcopter attitude control. The results offer valuable insights for selecting the most suitable optimization method based on specific performance and robustness criteria, ultimately aiding in the development of more resilient and reliable quadcopter control systems.



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sciforum-107386: Single-Layer Parity Generator and Checker Design Using XOR Gate in Quantum dot Cellular Automata (QCA)

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Quantum-Dot Cellular Automata (QCA) emerges as a promising nanotechnology, offering a viable alternative to traditional technologies for high-performance, low-power computing at high operating speeds in a compact area. It is well known that parity generators and checkers are crucial components in processors and communication circuits. In line with recent trends in nanocircuits in electronics, this work designs a parity generator and checker using QCA, an emerging nanotechnology that is gaining popularity for nanocomputing tasks. This paper presents a dual-tasking QCA-based 3-bit parity generator and checker, implemented using an optimized modified majority voter (MMV)-based XOR gate in QCA circuitry. It is a dual-tasking circuit, as the single circuit can both generate and check parity. The efficient XOR gate design significantly enhances the reliability and importance of parity checker circuits in QCA, which is vital for error detection in communication systems. A full input-output-accessible, single-layer and scalable layout was designed and simulated using QCADesigner 2.0.3 without incorporating crossovers to minimize fabrication complexity. Detailed power dissipation analysis, conducted using two tools, QCADesigner-E and QCAPro, shows that the circuit consumes 23.86 meV, demonstrating 86% energy efficiency as well as 59% area efficiency compared to the latest reported QCA-based parity checkers. The proposed circuit exemplifies a significant advancement in nanocomputing, providing a scalable, energy-efficient solution for next-generation computing systems, further establishing QCA as a key technology for future low-power, high-density applications.



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sciforum-104638: Smart handbag with enhanced women's safety using cutting-edge technology

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A recent survey shows that 30% of women in developed countries fear going out because of violence happening to them. To ensure their safety in public places, a smart handbag is designed, which provides enhanced security for them. The handbag is developed in such a way that it operates in wireless mode so that it can be controlled remotely without any human need. Also, the smart bag includes GSM and GPS technology for tracking the needy one. This technology provides a sense of security for women in public spaces, ensuring their safety and well-being. But the tools that use only these technologies for their operation are insecure and inefficient. The proposed handbag has an alternate approach for wireless control of a device by incorporating a fingerprint identification module, which increases the authenticity of the device and enables multiple users to control the device with the integration of hardware that makes a system that endlessly communicates their location using GPS to their known men's nearby and police station via GSM network. This system is incorporated with a camera module that captures images; further, the images are classified to check whether the threat is due to humans, animals, vehicles, etc., using a learning algorithm. For enhanced security, the smart bag is equipped with an electric shock generator and siren that give instant defensive response to potential attackers and provide a space for the women to escape. All these modules are integrated in the arduino UNO controller, which triggers the entire functionalities; therefore, with all these advancements, the smart handbag provides safety to women by instant alert, location sharing, etc.



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sciforum-103799: Software Defined East-West interface East-West Interface for managing Fog-IoT architecture: An Evaluation

Abdulfatai Dare Adekale *, Risikat Folashade Adebisi, Ore-ofe Ajayi, Bashir Olaniyi Sadiq, Habeeb Bello-Salau and Emmanuel Adewale Adedokun

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Cloud computing plays a vital role in managing and processing the diverse data generated by Internet of Things (IoT) devices, creating the cloud-IoT (CloT) architecture. However, CloT is insufficient for applications that are latency-sensitive and require significant network bandwidth. To address these challenges, fog computing complements CloT, forming a distributed architecture called the Fog-IoT architecture. The diverse nature of Fog resources complicates the management of interoperability and scalability within the Fog-IoT architecture. Software Defined Network has been proposed as a solution in managing interoperability and heterogeneous resources in distributed architectures. This paper evaluates two software-defined network (SDN) east-west interfaces - the Modified Communication Interface for Distributed Control Plane (mCIDC) and the Distributed SDN Framework (DSF), in addressing the challenges of manageability and interoperability in Fog-IoT architecture. Experiments conducted using the SDN Floodlight controller indicated that mCIDC required more packets for inter-controller communication compared to DSF, with average captured TCP packets of 26,330.7 and 17,473.1, respectively. The DSF exhibited lower inter-controller communication overload (ICO) with an average ICO of 222.6, compared to 301.2 for mCIDC. Additionally, the DSF generated fewer errors than mCIDC, with average TCP errors of 2,713.4 and 3,935.8, respectively. The results show that DSF uses fewer packets and generates fewer errors during inter-controller communication, making it more reliable than mCIDC for Fog-IoT architecture.



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sciforum-105980: Speed Regulation in DC Motor-Driven Electric Vehicles Under Real-time Disturbances Using Artificial Neural Network-Based Proportional–Integral–Derivative Control Strategies

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DC machine usage in Electric Vehicles (EVs) has been gaining a notable amount of focus. The speed of DC motor-driven wheels in an EV changes as it encounters disturbances like a reduction in tire air volume, or a corrugated and rugged surface on which it is driven. This continuous disturbance and variation in speed could result in the exertion of EV circuits, which can be fatal for passengers. Hence, a control method that could respond to the disturbance and give a signal to the motors of the wheels for automatic speed control is required. Thus, this paper proposes artificial neural network (ANN)-based control strategies for enhanced speed regulation in DC motor-driven electric vehicles. This paper highlights the focus on ANN control strategies in the context of DC motors of EVs. Different ANN architectures such as radial bias network (RBNN), probabilistic neural network (PNN), feed-forward network (FFNN), Elman network, NARX network, NAR network, and recurrent neural network (RNN) are implemented to design the gains of the PID (Proportional–Integral–Derivative) control loop of the DC motor. A thorough analysis concerning different activation functions, mean squared error, mean absolute error, and weight-bias functions is provided. The efficacy of all these methods is tested when the EV system is subjected to key disturbances, namely, step, ramp, sinusoidal, and chirp. System responses under all these test conditions for all the ANN architectures are drawn. A better ANN architecture to tune the PID controller is recommended based on these transient characteristics and disturbance rejection ability. From the results, it is observed that the performance of FFNN is superior to that of other ANNs due to its shorter rise time, less peak overshoot, lower delay time, and lower steady-state error. Thus the proposed work leverages the usefulness of ANNs to achieve more precise speed control, enhancing the overall performance of EVs.



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sciforum-107853: Stability conditions of TS systems based on quadratic and non-quadratic Lyapunov functions

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This paper introduces a method for reducing the conservatism in Takagi–Sugeno (TS) fuzzy systems through the use of a non-quadratic Lyapunov function (NQLF), also known as the line integral Lyapunov fuzzy function. By leveraging this function in combination with an efficient methodological approach, the stability analysis of TS systems is significantly improved. The stability conditions for these systems are initially formulated as Bilinear Matrix Inequalities (BMIs), which present a challenge due to their nonlinear nature and computational complexity. To address this difficulty, we propose an iterative algorithm designed to transform the BMI problem into a more tractable form by converting it into a set of Linear Matrix Inequalities (LMIs). LMIs are easier to solve using established optimization techniques, thereby simplifying the stability analysis process without sacrificing its accuracy. This transformation allows for more efficient computation and reduces the conservatism typically associated with BMI-based methods. To validate the effectiveness of our approach, a numerical example is provided, demonstrating how the proposed method outperforms traditional approaches by offering an enhanced stability analysis. The example illustrates the reduction in conservatism, thereby highlighting the practicality and robustness of the approach. Overall, this method offers a promising solution for improving the stability analysis of TS fuzzy systems by reducing the complexity and providing more reliable results. This contribution underscores the potential of using non-quadratic Lyapunov functions to address challenges in system stability with increased computational efficiency.



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sciforum-105808: Systematic Control Design of an EV Charger with Bidirectional Power Transfer Capability

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A systematic control design for an electric vehicle (EV) charger with bidirectional power transfer capability is presented in this paper. The control method centers on a state feedback control system based on linear matrix inequality (LMI) with integral action. This approach guarantees stability, resilience, and efficiency in the regulation of bidirectional power flows between the grid and the vehicle. This approach effectively regulates both grid-to-vehicle (G2V) and vehicle-to-grid (V2G) operations, which are essential for incorporating EVs into intelligent power networks and enabling grid services such as V2G. The control design incorporates integral action to achieve zero steady-state error, even in the presence of disturbances such as grid voltage fluctuations. The LMI framework provides a rigorous foundation for deriving control gains that guarantee closed-loop stability while minimizing the impact of transient disturbances. The simulation results, obtained using PSIM, Visual Studio, and MATLAB with a high-resolution sampling time of 0.1 ms, demonstrate the high performance of the proposed design. The results highlight the charger's rapid transient response, precise reference tracking, and effective power management, maintaining a unity power factor in G2V mode and a 180-degree phase shift in V2G mode. The results confirm the capacity of the proposed control approach to improve the efficiency and dependability of electric vehicle chargers in smart grid systems, contributing to the progress in sustainable energy solutions.



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sciforum-104599: Techniques for Reducing Eddy Current Losses in Permanent Magnet

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This paper focuses on investigating the most effective methods for reducing magnet eddy current loss. These techniques were utilised on permanent magnets in a surface-mounted permanent magnet synchronous machine with a distributed winding. Magnet segmentation and optimization of the segmented magnet shape comprise the initial methodology. On the other hand, the second method involves placing a conductive cylinder, known as a shielding cylinder, around the magnets to provide protection. The electromagnetic field analysis and computation of eddy current losses in the studied machine were performed using a two-dimensional finite element method.

The objective of this paper is to examine various methods for reducing eddy current losses in a surface-mounted Permanent Magnet Synchronous Machine (PMSM). The initial phase focuses on reducing the loss of eddy currents in the magnet through magnet segmentation. This technique is frequently employed to enhance the efficiency of Permanent Magnet Synchronous Motors (PMSMs). In this study, the objective is to improve the efficiency of this technique through the appropriate selection of segmentation parameters, specifically focusing on the shape of the segmented magnet. To achieve this, a constrained optimization process based on a genetic algorithm method is employed. Next, the goal is to analyse the eddy current loss, which can be reduced by adding a shielding conductive cylinder around the magnets.

The finite element method was used to analyse the eddy current loss in the machine under consideration.



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sciforum-103835: Utilization of Printed Circuit Board (PCB) in an Axial Flux Machines: A Systematic Review

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Due to the fast progression of technology, the dependence on electronic and electrical devices like axial flux permanent magnet machines (AFPMMs) has increased greatly, making printed circuit boards (PCBs) crucial components of modern designs. PCBs, made up of numerous ICs connected by copper traces, are essential to the current lightweight AFPMMs. This study systematically reviews the role of PCBs in the core design of AFPMMs for both low- and high-power applications, synthesizing research published between 2019 and 2024. Utilizing the PRISMA methodology, 38 articles indexed in IEEE Xplore and Web of Science were analyzed. The review explores advancements in PCB manufacturing, defect mitigation strategies, winding topologies, software tools, optimization algorithms, and the associated losses from varying winding configurations. A structured Boolean search strategy ("Printed Circuit Board" OR "PCB" AND "axial flux permanent magnet machine" OR "AFPM") guided the literature retrieval process. Articles were meticulously screened using Rayyan software for titles, abstracts, and content, with duplicate removal performed via Mendeley software V2.120.0. The findings demonstrate substantial progress in the design of lightweight AFPMMs that incorporate PCB components, resulting in enhanced power quality and improved electromagnetic performance. Research activity over the 6 years showed inconsistent growth, with concentrated trapezoidal winding emerging as the dominant configuration, followed by distributed winding designs. These configurations were particularly applied in single-stator double-rotor (SSDR) coreless AFPM machines, characterized by minimal defects, associated losses, and optimized single-layer winding designs utilizing tools such as ANSYS and COMSOL. Additionally, there has been growing interest in double stator single rotor (DSSR) and multi-disk configurations, reflecting the potential for alternative designs. These insights underscore the evolving role of PCBs in AFPMM development, highlighting opportunities for integrating advanced optimization methods and innovative configurations to address future technological demands.



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sciforum-107567: Video surveillance and augmented reality in maritime safety

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Augmented reality (AR) is used more often in many maritime applications. In this paper, AR model is considered for improvement traffic monitoring in ports. It is useful for port authorities.

The model's input is camera installed in the port. It provides a video stream over IP connection to the facility where the processing computer is placed. Ship's detection is performed by YOLO (You only look once) artificial neural network. Developed YOLO detector detects small and large vessels. Hence, ships with automatic identification system (AIS) and non-AIS maritime traffic is detected. This creates realistic real world scenario for Mediterranean port traffic portfolio, which includes passengers' ships, fishing ships, touristic ships, yachts, and other small-type of sailing objects.

Trajectories are estimated based on the central point of the detected vessel on the video stream from the surveillance camera. The intersection of the diagonals of the boundary box gives the central point of the vessel, the position of the central point remains remembered for each frame in the last 5 seconds. Position also depends on external influences. Hence, a linear regression is performed to get the direction of the vessel's movement between the memorized positions.

The collision risk assessment is made based on the distance between the vessels and the direction and speed of the vessel's movement. If the continued movement of the vessel according to the estimated trajectories and speeds will result in the intersection of the motion vector, it is suggested to change the course or speed of the vessel in order to eliminate the potential danger of collision.

In order to be useful for port authorities, the goal is to visualize collision risks in AR environment. AR is installed on smart phone and employee of port authority can check for possible problems easily without need for powerful computers and desk.



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sciforum-104417: Immersive scenarios for practicing sports in gyms - functional design and protocols

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Many fitness devices lack the immersive features and interactions necessary to enhance user engagement and optimize athletic performance. To address this gap, we propose an innovative, open, and interoperable architectural solution that transforms sports equipment into immersive training platforms. The solution integrates videos of real-world routes with contextual data, such as speed and altitude variations, to recreate outdoor sports experiences indoors. The system dynamically synchronizes videos with fitness equipment, adjusting parameters such as resistance, incline, and inertia to simulate real-world conditions. The architecture is based on a dual-subsystem design. The first subsystem facilitates the creation and sharing of enriched videos in the cloud, fostering a collaborative community of users. The second subsystem focuses on delivering an immersive experience through advanced technologies, including cloud computing, wearables, SIG BLE standards for fitness equipment, and edge computing, all coordinated via a mobile application. These elements ensure seamless integration between videos, equipment dynamics, and user behavior, enabling personalized training based on historical and real-time data. Initial validation was conducted through prototypes and tests with real equipment, utilizing contextual data and basic device adjustments. While further advancements, such as AI-driven personalization, are still required, preliminary results demonstrate the architecture's feasibility and transformative potential. This scalable and flexible system fosters a collaborative ecosystem and drives innovation in the fitness industry.



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sciforum-104599: Techniques for Reducing Eddy Current Losses in Permanent Magnet

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This paper focuses on investigating the most effective methods for reducing magnet eddy current loss. These techniques were utilised on permanent magnets in a surface-mounted permanent magnet synchronous machine with a distributed winding. Magnet segmentation and optimization of the segmented magnet shape comprise the initial methodology. On the other hand, the second method involves placing a conductive cylinder, known as a shielding cylinder, around the magnets to provide protection. The electromagnetic field analysis and computation of eddy current losses in the studied machine were performed using a two-dimensional finite element method.

The objective of this paper is to examine various methods for reducing eddy current losses in a surface-mounted Permanent Magnet Synchronous Machine (PMSM). The initial phase focuses on reducing the loss of eddy currents in the magnet through magnet segmentation. This technique is frequently employed to enhance the efficiency of Permanent Magnet Synchronous Motors (PMSMs). In this study, the objective is to improve the efficiency of this technique through the appropriate selection of segmentation parameters, specifically focusing on the shape of the segmented magnet. To achieve this, a constrained optimization process based on a genetic algorithm method is employed. Next, the goal is to analyse the eddy current loss, which can be reduced by adding a shielding conductive cylinder around the magnets.

The finite element method was used to analyse the eddy current loss in the machine under consideration.



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sciforum-107547: The design and development of a smart obstacle detector using deep learning methods for vehicles to reduce human injury/death rates

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Recent surveys by the WHO show that 50 million people are injured due to traffic accidents across the globe. This is primarily due to inattentive driving, unclear lane markings, poor visibility, and aggressive driving. These issues mentioned can be addressed by developing a smart device with advanced technology that avoids traffic accidents and secures drivers/passengers. This novel design utilizes ultra-high radio frequency identification that is fitted into road reflector studs, which function in a two-way system. The smart device consists of an RFID reader (ultra-high-frequency), an Arduino controller (ATmega328p), LEDs, cameras (OV7670), and a speed limiter, which create a safety network for the driver. Here, the RFID fitted into the reflector sends a signal to the nearby vehicle if the vehicle approaches the edge of the road, and the RFID scanner in the vehicle receives this signal, which alerts the driver using the Arduino controller, which decodes the signal and initiates the alert system so that the driver can get back into their lane. Also, the camera included in the smart device on the vehicle identifies barriers such as walking people, wildlife, and other harmful things in an effective manner through image classification with a deep learning method. This verifies whether the captured image is harmful to the vehicle or not. If the detected image is harmful, then it activates the speed controller present in the vehicle; thereby, the vehicle's speed will be controlled automatically. The proposed system is modeled and verified to have better results.



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Session 5. Mechanical and Aerospace Engineering

sciforum-104347: An Overview of Innovative Space Propulsion Systems: Current Directions and New Technologies

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The space propulsion market has experienced steady growth in recent years, driven by increasing demand for solutions that enhance satellite autonomy, versatility, economy, payload capacity, and readiness to fly. Key trends, initiated 25 years ago with CubeSats, include system miniaturization and modularization. These trends highlight the need for simple, small, high-performing solutions characterized by streamlined procedures and rapid maneuvers, which are required to optimize mission costs and lead times. Traditional chemical and electric space propulsion technologies, such as those based on hydrazine and its derivatives or Hall-Effect Thrusters, are being surpassed by cheaper, more powerful, and leaner systems that emphasize sustainable and safer green propellants, according to the current and future global policy initiatives.

This paper presents an extensive and critical overview of innovative propulsion system solutions, already existing or currently under development, which meet these criteria. It analyzes commonalities and differences among space propulsion technologies in terms of mission goals, satellite size, architectures, and performance parameters, as well as key points of departure from traditional systems. It investigates solutions utilizing green propellants, focusing on those based on water, especially water electrolysis propulsion technology.

This overview aims to provide a comprehensive definition of stakeholder expectations in the current space propulsion scenario, serving as input to the design process of an innovative water electrolysis propulsion system.



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sciforum-107371: Analyze the performance of horns with complex working surfaces used in ultrasonic welding of car turn signals

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For ultrasonic plastic welding, the horn design has a great influence on the quality of the weld. The design requirements are more careful, especially when the welding profile is complex. There have been many results presented on the optimization of the profile for wide-like horns. However, there have not been many studies published on block-like horn, especially block-like horn with complex working surface profile. In this paper, an optimal design for a block-like horn with complex working surface profile used for welding turn signal lights on cars will be presented. The objectives are to achieve maximum vibration uniformity in the working surface. In addition, the vibration amplitude amplification and some other factors are also considered in the process of optimizing the horn design. The integration of three methods: finite element method, response surface methodology, and genetic algorithm is used as an optimization tool for the optimal design. The results show that all the selected design variables have the greatest influence on the amplitude uniformity, while the vibration amplitude amplification is most affected by the slot location. The amplitude uniformity achieved for the optimum block-like horn is 95%, while the amplitude amplification is 2.7. In addition, the frequency separation between the longitudinal frequency and the before and after frequencies are 1340 Hz and 1245 Hz, respectively. The optimal design process presented in this study can be considered as a guidance for block-like horn designs in industry with complex profiles in the working surface.



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sciforum-107753: Effects of Infill Density, Heat Treatment and Geometry on the Tensile Strength of 3D Printed ABS Specimens

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Additive Manufacturing is a relatively new technology that allows to produce intricate parts with geometries that cannot be achieved through conventional manufacturing methods. One of the most widespread methods of 3D printing is Fused Filament Fabrication (FFF). In this study different 3D-printed, bone-shaped specimens made out of ABS (acrylonitrile-butadiene-styrene) are tested, complying with norms for mechanical testing of polymeric materials, with variations on its printing parameters (percentage of infill density), shape (thickness of specimen), and an annealing heat treatment. The resistance to tension is measured, and compared. The stress-strain curves were gathered from the universal tension tester from each of the specimens. Finally a statistical method is used in order to correlate the obtained behavior with a function that predicts the tensile strength of the part based on the parameter that can be varied, whether or not the heat treatment has a meaningful effect on the part that is to be produced, and if a lesser ratio of cross-sectional area to volume has a negative effect on the tensile properties. The resulting models showed a more pronounced decrease of tensile strength as the infill density is reduced, as well as a measurable and positive impact of the heat treatment on the ultimate tensile strength of the specimens. Finally the change in ratio of area to volume doesn't conclusively show a difference in tensile strength.



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sciforum-107859: Impact of Fly Ash from Different Sources on The Mechanical Properties of Geopolymer Concrete

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The increasing levels of carbon dioxide emissions have caused a global reconsideration of approaches to addressing global warming. One of the main contributors of these emissions is cement production, which generates high temperatures during its combustion processes. A recent development in construction industry has shown promise during formation of fly-ash based geopolymer composite, offering a potential alternative to traditional Portland cement concrete that could reduce or even eliminate its use, this research focuses on the mechanical performance of fly ash incorporated composites, especially its strength related parameters. The data for this study was obtained from tests conducted on geopolymer concrete specimen created from two different sources of fly ash, each subjected to varying concentrations of sodium hydroxide solution. The compressive strength of geopolymer concrete ranged from values typical of normal-strength concrete to those associated with high strength. The primary emphasis of this paper is on the correlation between different mechanical parameters of geopolymer concrete. Geopolymer concrete requires a combination of cement ingredients and fly ash as replacement. This research is especially relevant to developing countries as it will explore the locally produced fly ash as a raw material for production of geopolymer composite. Development of suitable geopolymer composite can be an alternate construction material for the industry and reduce reliance on conventional concrete. This will also lead to reduction in production of cement and help combat the climate change. The goal of this study is to help the achieve sustainable development goals by developing eco-friendly composite material for construction of sustainable cities.



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sciforum-104243: Modeling of Stress Concentration Factors in CFRP Reinforced Circular Hollow Section KT-Joints Under Axial Loads

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Tubular structures play a crucial role in renewable energy and the oil and gas industry, particularly in offshore applications. Over time, these structures face significant load, emphasizing the importance of addressing the degradation of tubular joints for sustained operation. Carbon fibre-reinforced polymers (CFRP) offer promising solutions for rehabilitation, yet existing literature primarily focuses on SCF at the crown/saddle points, which is sufficient only for determining fatigue life under uniplanar loads, leaving a gap in SCF along the weld toe. This study aims to bridge this gap by investigating the fatigue design of CFRP-reinforced tubular KT-joints subjected to axial loads at 24 positions along the weld toe. Our research highlights the remarkable potential of CFRP in reducing stress concentration factors (SCFs) in KT-joints, with the degree of reduction correlating with reinforcement layers and elastic modulus. We also uncover the critical role of fibre orientation in optimising stress distribution, particularly when wrapping CFRP around the brace axis with fibres perpendicular to the weld toe. Through 1679 simulations encompassing various geometric and reinforcement configurations, we analyse stress fields at the chord-brace interface under axial compression. Leveraging this data, we employ artificial neural networks to develop empirical models, enabling rapid estimation of CFRP's impact on fatigue life. These models provide precise approximations of hot-spot stress (HSS) in CFRP-reinforced KT-joints under axial load, with less than a 10% difference from simulation results, facilitating accurate fatigue life predictions akin to established methodologies for unreinforced tubular joints.



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sciforum-094733: On the Electrical Resistivity Measurement Methods and Properties of Conductive 3D-Printing PLA Filaments

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The field of additive manufacturing continues to revolutionize production methods, and 3Dprinting technologies have been at the forefront of this evolution. Among their myriad of applications, conductive 3D-printing filaments hold immense promise in the development of electronics, sensors, and flexible wearable devices. However, the precise characterization of the electrical resistance within structures fabricated using these filaments can be complex, especially when measuring subtle resistance variations. This study embarks on a comparative analysis of the two-probe and four-probe methodologies used for electrical resistance measurement while further investigating the impact of different electrical contact types on experimental specimens. Specimens will be fabricated utilizing a conductive PLA filament and 3D printing technology. The effectiveness of each measurement approach, along with the influence of electrode choice, will be evaluated. Moreover, the flexibility inherent in the four-probe method will be explored further. This research has the potential to significantly refine the measurement of electrical resistance in conductive 3D-printed constructs. In doing so, it could drive further innovation in fields where intricate circuitry, advanced sensors, and seamlessly integrated wearable technology are paramount. Furthermore, by optimizing these measurement techniques, we can gain a deeper understanding of the conductivity behavior of these novel materials, leading to an expansion of their potential applications.



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sciforum-089043: Optimizing Absorption Coefficients: A Study on Acoustic Characteristics of Saturated Fluid in Porous Media

Mustapha Sadouki

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This study introduces an experimental approach for quantifying audible acoustic frequency parameters within a rigid porous medium using an impedance tube. Employing the equivalent fluid model, a derivative of Biot's theory, we explore wave propagation intricacies within porous materials, emphasizing the pivotal roles of the effective density and dynamic compressibility of the saturated fluid. Our primary focus is on resolving the inverse problem, seeking to minimize both experimental and theoretical absorption coefficient expressions across the audible frequency range. Simultaneously, we identify and determine four critical parameters: viscous and thermal permeability, the inertia factor introduced by Norris, and the thermal tortuosity introduced by Lafarge. The research results encompass a thorough comparative analysis involving experimental and simulated absorption coefficients. This examination utilizes optimized parameters and spans across four diverse polyurethane foam samples. Through this comprehensive investigation, we elucidate the nuanced interplay between experimental observations and theoretical predictions. The findings not only advance our understanding of the intricate acoustic characteristics of rigid porous media but also contribute valuable insights into optimizing absorption coefficients and the broader field of wave propagation within such materials. This work stands at the intersection of experimental acoustics, porous media physics, and inverse problem-solving, providing a nuanced exploration of audible frequency phenomena.



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sciforum-104233: Parametric Investigation of Composite Reinforcement for Repairing Fatigue-Cracked Tubular T-Joints

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For offshore jacket constructions, circular hollow sections (CHS) have been widely used due to their exceptional performance in compression and high torsional resistance. Specifically, CHS have direction-independent stiffness and drag characteristics, which provide the structure with added stability under various marine environments. Hence, CHS are commonly chosen and welded to form tubular joints. Due to the complex geometry of the joints, the environmental loads, and the corrosion and aging of the structure, the joints are prone to fatigue cracks which can lead to crack propagation. The fatigue cracks and crack propagation can be investigated by analyzing the stress intensity factor (SIF) of the crack. If the SIF exceeds the fracture toughness of the joint, the crack will propagate. To alleviate this issue and prevent crack propagation, the application of composite reinforcement has been receiving traction in the industry due to its ability to provide in-service maintenance windows, besides its renowned capability to enhance the structural integrity of affected offshore structures. However, the effect of composite reinforcement on the SIF of fatigue-cracked tubular T-joints has been insufficiently explored. Therefore, this study aims to conduct a numerical parametric study on a semi-elliptical cracked tubular T-joint to investigate the effect of crack size, crack location, and composite reinforcement on the SIF under various basic loadings.



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sciforum-094718: Wire Arc Additive Manufacturing for Industrial Part Fabrication: A Short Review

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Fabrication processes using additive manufacturing (AM) have the potential to create a variety of new products. For this reason, research and development is actively being conducted within this area. Parts with large and complex shapes are suitable for wire arc additive manufacturing (WAAM), an AM technique based on arc welding, which is classified as directed energy deposition. Studies on WAAM are being conducted within various fields, including studies examining their mechanical properties, heat input conditions, material microstructures, post-processing, artificial intelligence techniques, repairs, and the development of hybrid systems with machining. However, many of these studies are evaluations that use simple shapes such as walls. The evaluations using simple shapes are important for fundamental engineering. However, as a fabrication technology, WAAM requires various evaluations using actual part shapes that are used in industry as test pieces in order to develop industrial applications. The purpose of this review is to further clarify the industrial application value of WAAM. First, a literature review on the results of studies on WAAM for industrial parts was conducted to summarize the current literature. Then, based on the study results obtained through the literature review, the main current issues are summarized. In addition, a discussion is conducted on how WAAM can be used to improve the development of various industries. The conclusion is that WAAM has the potential to develop further into a technology that will be one of the key factors to achieve industrial innovation.



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sciforum-102825: A Solution for Predicting the Timespan needed for Grinding Roller Bearing Rings

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The optimal management of manufacturing processes can be achieved through a set of optimal decisions, which must be made to choose the best method to follow every time the process planner is in a point at which several potential manufacturing paths branch off. A dedicated method, namely the Holistic Optimization Method (HOM), has already been developed for this purpose and was validated in several studies based on artificial and real instances databases. The HOM consists of two algorithms: i) the causal identification of a manufacturing process and ii) the comparative assessment with already performed, similar manufacturing cases, recorded in an instances database. The two algorithms can be used to estimate the values of the different performance indicators of the manufacturing processes. Their application for processing cost estimation in the case of manufacturing processes of bearing components has already shown good results. In this paper, it is presented as a solution to predict the timespan needed for grinding roller bearings rings, applying the specific algorithms of the HOM, grounded on the use of a database with data collected from the industrial environment. The cause variables selected to describe the grinding process of roller bearing rings are the inner and outer diameter of the ring, its width and weight, the machined surface roughness, the grinding stone rotation speed, the feedrate and the cutting depth, while the effect variable to be used by the process planner as decision criterion is the timespan.



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sciforum-094649: An analytical model for the prediction of the stiffness behavior of thin-walled beams

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The purpose of this work is to develop and validate an analytical model that provides accurate predictions of the mechanical properties of hollow box beams, in comparison to traditional methods. The study focuses on numerical results obtained for a hollow box beam with a rectangular cross-section. To achieve this objective, a novel analytical model was created. A finite element model (FEM) of the box beam was built in the commercial FEM software ANSYS Mechanical ADPL, and the results were compared using classical theory, the new equation, and numerical techniques. Linear static analysis was performed to analyze the results, and a mathematical method was employed to compare the outcomes. Validation of the newly developed equation was performed by comparing it with both the numerical model and the classical equation, and this approach proved successful. It was shown that the new equation outperforms the classical equation in accurately predicting the mechanical behavior of the studied geometries. This superiority was demonstrated through error analysis, which revealed that the new equation resulted in lower errors than the classical equation. It was found that the maximum error between the analytical equation and the numerical method decreased from approximately 2.5% for the classical equation to around 0.24% using the derived equation.



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sciforum-093943: An Open-Source Finite Element Simulation for Enhanced Compression Analysis of Corrugated Boards

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In the packaging industry, corrugated boards are highly valued due to their biodegradability, superior strength-to-weight ratio, and ease of manufacturing. In order to make the design optimization of such corrugated boards possible, a reliable simulation, which everyone can use, is expected to make this task possible. This study presents a finite element analysis (FEA) of corrugated boards under flat compression tests using the open-source software Salome-Meca, with Code-Aster as the solver. The corrugated board, composed of a flute sandwiched between top and bottom liners, is modeled, and a Python script was developed to iteratively explore variations in flute geometry. This study aims to simulate real-life conditions, with boundary and loading conditions carefully selected to mimic laboratory flat crush tests. The load is carried with a prescribed displacement, large deformations are accounted for, and orthotropy is considered for the corrugated board structure. The key results include the identification of local stress and strains, which are usually very challenging to collect from simple analytical approaches and lab experiments. The analysis revealed areas of high-stress concentration, including the contact zones and their respective neighborhoods. Additionally, load–deformation curves were generated, demonstrating a clear relationship between flute geometry and the board's mechanical response. This simulation is then highly useful and unique compared to the literature, not only due to being open-source but also due to its capability of simulating contact, displacement prescription, and other phenomena occurring in the lab.



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sciforum-104393: Analysis of Composite Skins for Naval Sandwich Structures: Mechanical Characterization and Performance Evaluation

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This study focuses on the analysis of composite skins made from carbon fiber, glass fiber, and aramid, materials commonly used in sandwich structures for marine applications. These composites are employed in both recreational boats and competitive racing vessels. The primary objective of the research was to evaluate the mechanical performance of these composites through tensile testing. The composite skins were modeled in a dog-bone shape, a geometry chosen to optimize stress distribution during experimental testing. Tensile tests were conducted to determine mechanical properties such as tensile strength, modulus of elasticity, and fracture strain. The data collected from these experimental tests were crucial for the subsequent modeling phase. Using the experimental results, a FEM (Finite Element Method) model for the composite skins was developed and validated. This numerical model allowed for the simulation of the mechanical behavior of the materials under various loading conditions, providing a deeper understanding of their structural performance. The validation of the FEM model was essential to ensure the accuracy of the simulations and to predict the behavior of the composites in real-world applications. The findings from this study offer significant contributions to the marine industry, suggesting possible improvements in the design and production of boats. The use of validated FEM models can lead to greater efficiency in the design phase, reducing costs while enhancing the safety and durability of the vessels. In conclusion, the research demonstrated the effectiveness of carbon fiber, glass fiber, and aramid composite skins for marine applications, highlighting how the combination of experimental testing and FEM modeling can significantly improve the understanding and optimization of composite structures.



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sciforum-107090: Beetle Elytron-Inspired Structures for Enhanced Impact Resistance in Aircraft and Automotive Shell Components

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In aerospace and automotive engineering, improving impact resistance while maintaining lightweight structures is critical, particularly for shell components. Bio-inspired beetle elytron plates (BEPs) offer promising solutions due to their natural design, providing enhanced mechanical performance under impact conditions [1][2].

This study focuses on end-trabecular beetle elytron plates (EBEPs) and grid beetle elytron plates (GBEPs) fabricated through additive manufacturing with eco-friendly materials. These plates were compared to conventional honeycomb (HPs) and grid plates (GPs) under 10 J impact energy. Dynamic impact tests using a drop hammer system measured peak force and other key indicators.

The results show that EBEP and GBEP significantly outperformed conventional plates, with energy absorption increasing by 7% to 10% and with deformation reduced by over 5%. These designs provided up to 15% more stable impact resistance and around 12% higher mean force retention, demonstrating greater structural integrity under repeated impacts.

The findings highlight the potential of bio-inspired plates for enhancing impact resistance in aerospace and automotive shell components. Our research group has already developed methods to design and fabricate curved beetle elytron plates [3][4], and future studies will focus on low-velocity impact tests to further address the demands of lightweight, high-strength structures.

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sciforum-100853: Computational Analysis and Simulation of Polylactic Acid Extrusion in 3D Printing

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This research focuses on the computational analysis of polylactic acid (PLA), a biodegradable polymer widely used in 3D printing. A commercial CFD software, Ansys-Fluent, was employed to simulate the extrusion process of PLA and to understand the behavior of the deposited flow under various printing conditions, including printing height, flow rate, and travel speed. An explicit Volume of Fluid formulation was employed. The PLA was characterized based on its density, specific heat, and heat conductivity, all of which were determined to vary with temperature, as reported in the literature. Also, a comparison between Newtonian and non-Newtonian models was carried out to understand their impact on the extrusion process.

The results show that the viscosity model influences the shape of the deposited filament. Also, both travel and extrusion speeds significantly affect the quality and geometric shape of the extruded filament. Specifically, excessive speed leads to a filament width reduction and creates instability, while insufficient extrusion speed affects stability and produces less heat accumulation. Additionally, excessive printing height negatively impacts the stability of the flow and increases solidification time.

In conclusion, the present work shows a promising approach to simulate filament deposition in 3D printing. Future research will focus on validating these results through experimental studies and optimizing printing parameters to achieve high-quality printing with less material waste.



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sciforum-101994: Design and Evaluation of Aerodynamic Appendages for a Racing Motorcycle Prototype

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The study of aerodynamics in racing motorcycle prototypes has become an essential phase, significantly enhancing performance during all riding phases. In the present study, three rear fairing winglet proposals for a racing motorcycle prototype were designed and evaluated. The three designs, realized in Siemens NX, were imported into a validated Simcenter STAR-CCM+ CFD (Computational Fluid Dynamics) model. From the analysis of the results, it was observed that the designs had varying impacts on the overall drag and lift values. The design and simulation campaigns conducted allowed for a comprehensive evaluation and appreciation of the aerodynamic functions crucial for vehicle dynamics, such as closing the wake to reduce drag and preventing advantages for following riders. By analysing the aerodynamic performance of each design, this study aimed to identify the configuration that best meets the required dynamic conditions. Furthermore, this study emphasized the importance of having a rear fairing that not only optimizes aerodynamic efficiency but also contributes to the overall stability and control of the motorcycle. Through iterative design and simulation processes, one of the three analysed designs emerged as the most effective solution, providing a balanced combination of reduced drag and improved downforce characteristics essential for competitive racing. Future developments could involve implementing optimization algorithms to further enhance the performance of the best rear winglet design.



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sciforum-106328: Determining Paper Material Properties through Compression of Corrugated Boards

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Determining the material properties of paper accurately is crucial in order to ensure good performance of the material in demanding packaging applications. To this end, this work intends to adopt an optimization strategy in order to find the material stiffness properties of paper. The novelty presented is that the most likely material stiffness values are determined by considering a common paper structure - corrugated boards - subjected to the Edge Crush Test (ECT) and the Flat Crush Test (FCT). Different from the common approach, where material properties are assumed in order to compare more complex structures with the experiments, here the inverse problem is solved: material properties of paper are determined based on the experimental results themselves. The numerical simulation is based on the plate theory and a buckling analysis for in-plane and out-of-plane compression. By conducting experiments, it is then possible to minimize the difference between the results from the numerical simulation and those experiments. The machine direction stiffness (E_{MD}) and the cross-direction stiffness (E_{CD}) are primarily assigned using the ECT. Conversely, the FCT is used not only to make both assignments above more precise but also to provide an estimate of the out-of-plane stiffness (E_z). The results suggest that E_{MD} is around 3 GPa, more than twice the value of E_{CD} , being consistent with a well-known property of paper related to anisotropy. Another relevant finding suggests that the thickness of the paper had a very minimal influence on the overall mechanical characterization of the structure. These results are highly relevant to achieve reliable simulations and optimal designs of corrugated boards.



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sciforum-105271: Effect of X-ray Computed Tomography Scan Noise on Observation of Internal Defects in a Blade Part Fabricated by Wire Arc Additive Manufacturing

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The application of additive manufacturing to the fabrication process of metal parts has the potential to solve some of the problems that have existed in the industry for a long time. On the other hand, it is necessary to guarantee sufficient quality of the fabricated parts. One of the causes of functional degradation of parts fabricated by additive manufacturing is the presence of internal defects such as blowholes. In the case of turbomachinery blade parts, damage to the parts caused by internal defects may result in a noticeable loss of machine performance; therefore, it is necessary to accumulate a great deal of knowledge and make appropriate judgments. For this reason, there is an active discussion on the integrity of parts. A suitable method of additive manufacturing for large parts is wire arc additive manufacturing (WAAM). In addition, X-ray Computed Tomography (CT) scans are often used for the observation of internal defects in metal additively fabricated parts. The purpose of this study is to clarify the effect of artifacts, which are noise from X-ray CT scans, for the proper evaluation of internal defects in parts fabricated by WAAM. An axial-flow impeller made of general-purpose stainless steel, fabricated by WAAM and machining, was used as a test model. The blades of this impeller were observed for internal defects by X-ray CT scanning. Suitable imaging results and imaging results affected by artifacts were obtained by changing the imaging conditions. These results were used to consider the effects of artifacts on the imaging results. In conclusion, it was shown that artifacts may cause a misidentification of internal defects in parts fabricated by WAAM.



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sciforum-106553: Enhanced Analysis of Corrugated Board Geometries Using Computational Image Processing Techniques

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Image acquisition and processing of corrugated boards is highly complex, especially in situations where deformation is intended to be observed during compression tests. This is not only due to the very low thickness of the corrugated boards as well as due to the great influence of shadows and regions where illumination impacts the real investigation of the board liner and flute thicknesses. This work aims to develop an image analysis algorithm in order to measure the corrugated board geometry with higher accuracy, thereby improving quality control. It primarily focuses on identifying key geometric properties in corrugated board structures, such as the flute thickness, the liner thickness, wavelength, and height. Several methods are used: pre-analysis involves the experimentation of mean filtering, bilateral filtering, morphological operations (dilation and erosion), binarization, and contour detection; further analysis involves masks, sinusoidal function, RANSAC, and Segmented Fourier. Furthermore, illumination effects are studied and explored. Results suggest a significant disparity between liner thicknesses due to the illumination effect, which is then corrected when observing the dynamic compression of the specimen. Moreover, the overall decrease rate of the height along frames is also consistent with the compression speed, and the frequency peak is also maintained constant. This research advances the technological capabilities of industrial image processing, ensuring that corrugated boards are produced with the desired geometry and within the standard requirements.



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sciforum-107765: Enhancing Vortex Tube Performance through Geometric Modifications

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Vortex tubes are an intriguing application of energy separation, featuring one inlet and two outlets on either side. A high-pressure fluid is introduced into the tube via a vortex generator, where energy separation occurs, resulting in hot fluid being released from one outlet and cold fluid from the other. Despite the interest in vortex tubes over the past few decades, the exact phenomena occurring within them remain largely unknown. This research aims to analyze the effect of varying geometries on the performance of a typical vortex tube using Ansys Fluent. Specifically, the study focuses on the hot and cold outlets to determine the most efficient design. The fluid's temperature, pressure, and mass flow rate are analyzed using Computational Fluid Dynamics (CFD). Three different geometries were designed and analyzed by varying the radius of the hot and cold exits. The results indicate that the temperature difference between the hot and cold exits is maximized in the pointed cone geometry model compared to the truncated cone geometry. These findings demonstrate a clear correlation between geometry and vortex tube performance, suggesting that shape modifications can be used to control or vary the temperature for different applications, such as refrigeration and air conditioning systems.



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sciforum-104497: Evaluating the Environmental Impact of 3D Printing: A Comparative LCA of Electron Beam Melting and Material Extrusion with Metal-Filled Filament

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This study presents a comparative Life Cycle Assessment (LCA) of two 3D printing technologies: Electron Beam Melting (EBM) and Material Extrusion (MEX) using metal-filled filaments, followed by debinding and sintering processes. The primary goal is to assess the environmental impact of both technologies.

The LCA methodology employed adheres to ISO 14040/44 guidelines. Data were collected from primary and secondary sources, including direct measurements, database information, and scientific literature.

Results indicate that EBM technology, despite its high energy consumption during metal melting, produces higher quality parts with less post-processing required. However, the significant energy impact raises concerns about energy efficiency, particularly in large-scale production contexts.

Conversely, the MEX technology with metal-filled filaments, followed by debinding and sintering, exhibits lower energy consumption during the printing phase and benefits from low operational costs due to the use of conventional 3D printers that are widely accessible and maintainable. Nevertheless, this technology requires additional processing steps that can introduce complexity and variability in the final results. Furthermore, parts produced via MEX generally exhibit lower quality compared to those produced by EBM, necessitating further machining to meet desired standards.

In conclusion, the LCA analysis highlights that the choice of 3D printing technology should be carefully evaluated based on specific project requirements and available resources. EBM technology is more suitable for applications demanding high quality and precision, while MEX with metal-filled filaments offers a more energy-efficient solution, albeit with challenges related to quality and process complexity.

These findings provide a foundation for future research and optimization of 3D printing technologies, contributing to informed decisions for sustainable manufacturing in advanced production sectors.



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sciforum-100789: Fatigue Design of Mechanical Systems such as Refrigerator based on a quantum-transported life-stress model and sample size formulation

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To increase the life of mechanical product such as refrigerator and automobile, new structured reliability method – parametric Accelerated Life Testing (ALT) was provided with reliability quantitative (RQ) statements. It included: (1) ALT scheme established on system BX lifetime that will be X percent of the accumulated failure, (2) load examination, (3) tailored parametric ALTs with the design modification, and (4) judgement if product design(s) achieves the targeted BX life. A quantum/transported life-stress model and sample size formulation were proposed. This new parametric ALT enables engineer to identify the design defects and modify them in the product development. As the problematic designs are recognized and altered by utilizing this parametric ALT, companies can get away from recalls due to the product failures in the marketplace. As case studies, two products were suggested: 1) troublesome refrigerator compressor failed from the field and 2) the action of redesigning the hinge kit system (HKS) in a household refrigerator. After several parametric ALTs with modifications, the mechanical products – compressor and HKS were expected to reach the lifetime – B1 life of ten year.



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sciforum-107637: Finite element analysis for block-like horn performance of ultrasonic plastic welding systems

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Ultrasonic plastic welding technology has been widely applied in practice. Welding horn design is one of the important tasks. Many studies have presented this problem. However, most of these studies are only interested in face profiles that are flat or have symmetrical profiles. Meanwhile, ultrasonic welding horns with complex working surfaces receive little attention. This research presented the design of an ultrasonic horn with a complex working surface. Moreover, the influence of the slot width in the horn, an important design parameter, on the performance of the designed horn was considered. The finite element method was used for modal and harmonic analysis. The performance of the design was assessed through criteria that are the uniformity of amplitude, the distribution of the greatest stress at points on the working surface, and close to the target frequency. A new parameter, namely Displacement unevenness (a), was proposed to evaluate the unevenness amplitude in the working surface of the horn. Effects of three alternative slot structures width corresponding values of 12 mm, 17 mm and 20 mm, denoted by B12, B17, and B20 respectively were carried out. The results showed that the B12 and B17 designs have natural frequencies close to the target frequency of the welding machine, while the natural frequency of the B20 design is far from the target one. The B12 and B17 designs also produce an unevenness amplitude smaller than those of the B20 design. The model showing the relationship between design parameters and the required criteria must be further developed. Additionally, this result can be said for the design guidelines not fully available in the literature.



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sciforum-097574: Formulation of a torsion displacement equation for the compatibility with bending in rectangular section thin-walled hollow-box beams

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Thin-walled structures are widely used for engineering applications where lightweight structures with high stiffness and high resistance are especially advantageous or even required. In this work, a novel analytical equation is developed to accurately predict the mechanical behavior of thin-walled beams. The Finite Element Method (FEM) was used to build the model and obtain the results. The newly developed equation is designed for calculating the displacement of a simply supported beam subjected to torsional loads, which are distributed at midspan using two triangular load functions applied in opposite directions in the FEM models. The Eureka software was utilized to uncover hidden analytical models, which were subsequently validated. The goal is to provide a formula that allows for the comparison of analytical calculations with numerical results for combined bending and torsion loads. A FEM model of a hollow-box beam with a rectangular cross-section, subjected to torsion, was constructed, and analytical calculations were performed. The analytical results were compared with the numerical results to assess their accuracy, and good agreement was found. In the future, other models, such as internally reinforced beams, could be tested using this methodology. Additionally, different conditions could be applied to the model studied in this work to evaluate the limitations and validity of the developed analytical model



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sciforum-106326: Image-to-Graph Representation of Corrugated Boards under Compression: A Novel Approach

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Graphs are commonly used to reduce the data dimensionality of images without reducing the efficiency of the applications. Computational time is then reduced compared to using the original image data. Graphs can also provide deeper data insights than the original images. This work proposes a novel approach of using graphs to represent the geometry of the corrugated board profile in order to benefit from the aforementioned advantages of graphs. The objective is to develop a framework where images are converted into graphs. Common problems with such image processing are related to image noise, detection of delamination of the board as part of the structure of the corrugated board, and illumination. An algorithm is then employed in order to tackle such issues, and it is based on the properties of graphs related to the degree of nodes. In a simplified model, the maximum node degree is 3, where two members of the liner are connected and visually divided by the contact with the flute structure. The main results are as follows: several nodes at degrees 1 and 2 were observed as either noise or delamination and were removed from the processed graph structure; the graph structure is consistent with the experimental visualization along compression tests, where the cumulative length of the flute not in contact with the liners is reduced. Comparative analysis of the different data variables suggests a significant difference in sizes between storing the original image and the output graph. In conclusion, the graph representation is simpler and easier to consider in future research to simulate and optimize corrugated boards.



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sciforum-107639: Mechanical Characterization of TPMS Structures Fabricated via SLA 3D Printing using Tough Resin: Influence of Geometry on Performance

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This study investigates the mechanical behavior of six triply periodic minimal surface (TPMS) structures—gyroid, primitive, diamond, lidinoid, neovious, and splitP—fabricated using stereolithography (SLA) 3D printing with a tough engineering resin. Each structure measures 70x70x70 mm³ and maintains 75% porosity, designed to enhance properties like lightweighting and energy absorption. The resin's excellent mechanical properties make it suitable for engineering prototypes, mechanical aids, fixtures and medical devices.

Compression tests were conducted at a deformation rate of 2 mm/min to compare the mechanical response of the TPMS structures. Results indicate that, within the same strain range, stress ascends in the elastic zone in the following order: lidinoid, primitive, neovious, splitP, diamond, and gyroid. This sequence highlights the varying mechanical responses under identical testing conditions. While porosity and dimensions remained constant, most structures followed a clear trend where thicker walls resulted in higher stress in the elastic zone. However, neovious, despite having the thinnest walls (0.31 mm), performed unexpectedly well, ranking fourth in stress, surpassing some thicker structures. The wall thickness for other structures ranged from lidinoid (1.17 mm), splitP (1.33 mm), diamond (1.94 mm), primitive (1.31 mm), to gyroid (2.32 mm). The splitP and diamond structures displayed very similar stress-strain behavior, as reflected in their close curves on the stress-strain diagram.

These findings emphasize that while thicker walls generally correlate with increased stress, the geometry of the TPMS structures plays a significant role in mechanical behavior. The unique performance of neovious further underscores that wall thickness alone cannot predict mechanical outcomes. By leveraging advanced TPMS designs and tough resin, this study demonstrates the potential for creating lightweight, robust components for various engineering and medical applications, enhancing stress distribution, energy absorption, and overall mechanical performance.



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sciforum-104180: Multistep Layup Optimization of UAV Wing for Minimum Weight

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Laminated composite structures are widely used for structural applications, owing to their tailorable mechanical response. These structures are made of tens or hundreds of plies of various materials, each having a unique orientation, called the layup. The layup is a primary parameter in the design of composite structures. The numerous design variables involved in defining the layup of laminated structures are decided based on expert intuition, often resulting in overweight designs, as analysing all possible combinations may be time-consuming and sometimes impossible. Many researchers have worked on optimising the fibre orientations; however, these were limited to the problems whose analytical equations were available. Analytical models representing the behaviour of complex problems are often unavailable, such as the wing of a typical unmanned aerial vehicle. Such structures can be efficiently modelled using numerical methods such as finite element (FE) modelling, and these FE models can be further used for optimisation. The Design Optimisation module of general-purpose ANSYS has the capability of optimising such problems. However, this module is designed for the optimisation of systems made from isotropic material. This paper presents a two-step strategy for the weight optimisation of an aircraft wing fully made of composite materials. A code was developed which can cater for the range of wing span, number of ribs, spar width, and location of spars. The optimisation design variables considered were the number of composite layers, layer orientation, and their stacking sequence. The number of layers in each structural component was optimised, followed by the optimisation of layer sequence and orientation of each lamina. The weight of the specific wing was reduced by 45%, and the maximum stress values also lowered from 421 MPa to 330 MPa, meeting the material strength limits. The method presented is easily implementable for a wide range of problems, materials, and loading conditions.



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sciforum-097577: Non-linear structural behaviour of internally reinforced beams subjected to simple bending loadings

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Thin-walled structures are interesting for applications in which lightweight structures with high stiffness and high resistance are especially advantageous or even required. The mechanical behaviour of thin-walled structures is, therefore, of high importance. Thin-walled structures which are internally stiffened are of particular importance, as internal reinforcements can be designed to maximize the inertia moment, leading to higher stiffness and strength. The present study investigates the mechanical behavior of sandwich beams using the Finite Element Method (FEM) software ANSYS Mechanical APDL. This study is in the field of solid mechanics, with a specific focus on analyzing structures' non-linear mechanical response. Structural analysis was conducted on internally reinforced hollow-box beams, and a non-linear static analysis was conducted under bending loads. The material considered was structural steel. The models were solved using the iterative Newton–Raphson method. A material curve, obtained from real tensile tests, was input into ANSYS Mechanical APDL software for the FEM simulations considering the plasticity of the material. A load–displacement curve was generated to characterize the non-linear behavior of the models. To ensure high precision in the results, a mesh convergence analysis was carried out. Additionally, a comparison was made between the stiffness characteristics of the different beams and those of conventional hollow-box beams.



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sciforum-104043: Numerical Analysis of Load-Bearing Capacity in Offset Stacked Corrugated Board Packaging

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The stability of palletized corrugated board packaging is crucial for safe transportation and storage. Offset stacking, where packages are slightly shifted relative to those in lower rows, is a common technique to enhance pallet stability. However, this method can compromise the load-bearing capacity of the packaging. This study investigates the impact of offset stacking on the load-bearing capacity of cardboard packaging during palletization. While offsetting packages on a pallet can enhance stability, it adversely affects the load-bearing capacity of the packages. This is particularly critical as the load from upper packages is primarily transferred through the walls, and their misalignment can significantly reduce their structural integrity. Our research indicates that such reductions in load-bearing capacity can reach up to several percent.

Advanced numerical modeling using the Finite Element Method (FEM) was employed to estimate the decrease in load-bearing capacity due to offset stacking. This method allows for a detailed analysis of how misaligned walls affect structural performance under a load. The FEM analysis revealed that offset stacking leads to a notable reduction in the load-bearing capacity of the packaging. The structural integrity of the corrugated board is compromised, with load-bearing capacity reductions reaching up to 25% in some configurations.

This study highlights the trade-off between stability and load-bearing capacity in offset stacked cardboard packaging. The findings underscore the need for careful consideration in packaging design and palletization strategies to balance these competing factors. Future work will focus on optimizing stacking patterns and developing guidelines to mitigate the adverse effects on load-bearing capacity. This research provides valuable insights for the packaging industry, promoting safer and more efficient palletization practices while maintaining structural integrity.



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sciforum-104023: Numerical Homogenization of Bubble Deck Concrete Slabs Using General Nonlinear Constitutive Law

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Bubble Deck slabs are an innovative construction technology designed to optimize material usage and reduce slab weight through strategically placed elliptical voids. Traditional analysis methods struggle to accurately model these complex geometries and their nonlinear behavior under load. This study explores the numerical homogenization of bubble deck slabs, which incorporate elliptical voids to reduce weight and material usage while maintaining structural integrity. These slabs, characterized by lower and upper mesh reinforcement, present a complex cross-sectional geometry that benefits from advanced numerical methods for accurate modeling.

This study employs numerical homogenization techniques based on the finite element method to transform the complex geometry of bubble deck slabs into an equivalent homogeneous layer. To account for the nonlinear (plastic) behavior of the material, the General Nonlinear Constitutive Law (GNCL) is integrated into the homogenization process. The combination of these methods enables a detailed representation of the slabs' structural response. The homogenization process successfully reduced the complex bubble deck geometry to a simplified model that retains the critical nonlinear characteristics. The results indicate that this approach can accurately predict the structural behavior under various loading conditions, including those leading to nonlinear deformation (due to cracking, etc.).

This research demonstrates that combining numerical homogenization with the GNCL provides a robust framework for analyzing bubble deck slabs. The methodology allows for accurate and efficient structural analysis, promoting material efficiency and structural performance. Future research will focus on extending this approach to other complex slab geometries and incorporating additional loading scenarios. This study underscores the potential for advanced numerical methods to enhance the design and analysis of innovative structural elements, contributing to more sustainable and economical construction practices.



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sciforum-104051: Numerical Homogenization of Multilayer Laminated and Sandwich Plates Considering Delamination

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Laminated and sandwich plates are widely used in engineering applications due to their high strength-to-weight ratio. However, the presence of delamination can significantly affect their structural performance, particularly under bending loads. This study addresses the numerical homogenization of multilayer laminated and sandwich plates, incorporating the effects of compliance and a lack of integrity between layers, in particular, delamination. Previous research has described the homogenization process, but this study focuses on the impact of delamination on bending stiffness without affecting tensile stiffness.

We employed numerical homogenization techniques, incorporating interplay delamination or partial delamination to model these effects. The Finite Element Method (FEM) was utilized to simulate the behavior of delaminated plates, ensuring accurate boundary conditions through using periodic boundary conditions to capture the correct stiffness reductions. The analysis revealed that delamination leads to significant reductions in bending stiffness, while tensile stiffness remains largely unaffected. The correct implementation of periodic boundary conditions was crucial in accurately estimating stiffness reductions in delaminated plates.

This research highlights the importance of accurate boundary condition assumptions in numerical models for predicting the structural performance of partially delaminated multilayered and sandwich plates. The findings provide a basis for more reliable design and analysis of such structures, promoting better understanding and mitigation of the effects of delamination. This study underscores the potential of advanced numerical methods to enhance the analysis and design of complex laminated and sandwich structures, contributing to more resilient and efficient engineering solutions.



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sciforum-099931: Numerical Study on Film Pressure in a Helical Grooved Plain Bearing of a Canned Motor Pump

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A canned motor pump is a type of turbopump that features a non-leakage structure that integrates the pump and the motor. It differs from a typical turbopump in that the pumping liquid also serves as the cooling liquid for the motor and the lubricating liquid for the sliding surfaces. Grooved plain bearings are generally used in canned motor pumps to supply sufficient cooling liquid to the motor. However, there is no external lubricant supply system for canned motor pumps, which means that the design guidelines for standard grooved plain bearings cannot be applied without modification. The purpose of this study is to obtain knowledge to develop design guidelines for helical grooved plain bearings for canned motor pumps. Therefore, the film pressure, which is one of the important indices in bearing design, was analyzed by Computational Fluid Dynamics (CFD). CFD simulation was performed using the steady-state single-phase flow solver implemented in OpenFOAM for analyzing fundamental trends. First, a comparison with the theoretical solution was performed for a plain bearing without grooves to investigate the film pressure. Furthermore, analysis was conducted on a helical grooved plain bearing. This analysis clarified the trend of film pressure generated in the helical grooved plain bearing. The conclusion is that the peak values of positive and negative film pressure tend to be higher in the helical grooved plain bearing than in the plain bearing without grooves, so the effects of material strength and cavitation should be handled appropriately when the bearing is used in industry.



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sciforum-103996: Optimization of Concrete Rectangular Water Tank Sections Using Evolutionary Algorithms

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This study focuses on optimizing the cross-sections of free-standing concrete rectangular water tanks. The primary goal is to minimize material usage while maintaining structural integrity. Traditional design methods often lead to conservative estimates of material requirements. By employing evolutionary and global gradient-free algorithms, this research aims to find more efficient design parameters. Water tanks are essential structures in civil engineering, and their design requires careful consideration to ensure safety and cost-effectiveness. The design challenge increases with the aspect ratio of the tank, as walls behave more like cantilevers with higher width-to-height ratios.

We employed evolutionary algorithms, specifically genetic algorithms, to optimize the thickness of the tank walls and the placement of vertical ribs. These algorithms are well suited for this application due to their ability to handle complex non-linear optimization problems without the need for gradient information. The optimization variables included wall thickness, which varies with height, and rib placement, considering different tank dimensions. For the modeling of wall behavior, the finite difference method was utilized, incorporating an orthotropic description of the material to accurately represent the directional properties of reinforcing ribs. The optimization process demonstrated that evolutionary algorithms could effectively identify optimal cross-sectional parameters.

The results indicated a potential material saving of 10-15% compared to traditional design methods. The optimized designs maintained structural integrity while using less concrete, making them more economical and sustainable. This research validates the effectiveness of evolutionary algorithms in optimizing the design of reinforced concrete water tanks. The findings suggest significant material savings, contributing to more cost-effective and environmentally friendly construction practices. Future work will extend these methods to other structural elements and consider additional constraints such as seismic loads. This study provides a robust framework for engineers to adopt advanced optimization techniques, enhancing the efficiency and sustainability of civil engineering projects.



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sciforum-107477: Optimizing Laser Processing Parameters for Enhancing Wear Resistance of R6M5 Steel Gears in Industrial Applications

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The wear resistance of gears plays a crucial role in ensuring the longevity and efficiency of machinery, particularly in industries like textile manufacturing, where gears are subjected to continuous operation under high loads and long-term motion. R6M5 steel, commonly used for high-performance gears, possesses excellent hardness and durability but still faces wear challenges under extreme conditions. Laser processing has emerged as an effective technique to enhance the wear resistance of such materials through precise surface modification. This study investigates laser processing parameters for a miniature-sized (10 mm diameter) R6M5 steel gear to achieve the desired melting depth and improved surface properties. The objective is to enhance wear resistance while maintaining the structural integrity of the gear. Experiments were conducted using laser powers ranging from 1.5 to 2.4 kW and scanning speeds from 15 to 25 mm/s. The results were analyzed to identify the best-performing combination of parameters within this range.

The study found that using a 2.4 kW power and 25 mm/s speed achieved a melting depth of 0.30 mm, enhancing the surface hardness without causing excessive thermal distortion. This combination significantly improved the gear's wear resistance, making it more suitable for high-demand applications in textile manufacturing. However, as these were the maximum tested values, further studies are needed to determine whether increasing power or speed beyond this range would lead to additional improvements or adverse effects. In conclusion, laser processing with these parameters offers a reliable method for improving the durability and wear resistance of mini R6M5 steel gears, providing a foundation for further optimization and application in high-demand industries.



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sciforum-104196: Parametric Analysis of Transduction Mechanisms (Piezoelectric, Electro-Capacitive, and Electromagnetic) in a MEMS Accelerometer

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Accelerometers are extensively utilized in various applications to measure vibrations (in the form of acceleration) across different vibrational structures. Researchers have already been exploring different mechanisms to interpret acceleration values. In this regard, over the past decades, Microelectromechanical Systems (MEMS) accelerometers have been prominently describing the interconnectivity between the generated electrical signal and the accelerated motion. However, there has been a major gap in the comparative assessments of the different transduction mechanisms. Therefore, in this research work, a classical dynamics approach is utilized to mathematically model the MEMS accelerometer by incorporating three different designing mechanisms: Piezoelectric, Electro-Capacitive, and Electromagnetic transductions. The transfer functions of all three designs of the MEMS accelerometer are developed by incorporating different structural parameters, material properties, and external input conditions. The piezoelectric accelerometer relies on the inherent compliance of the piezoelectric material, the electric field generated, and the material's dimensions. The electro-capacitive model's key parameters include the number of rows of capacitive plates in a comb-like structure, the area of each plate, and the voltage produced by these capacitive elements. On the other hand, the electromagnetic accelerometer depends mainly on the change in flux produced by the magnet in the coil, the coil length, and the magnetic field strength. MATLAB has been utilized to investigate the electrical response of the designed MEMS accelerometers by considering several controllable factors of each modeled system. The tangible findings highlight that under the same environmental as well as external input conditions, the Piezoelectric accelerometer produces the highest output voltage as compared to the electro-capacitive and electromagnetic MEMS accelerometers. Therefore, this article provides a well-established theoretical, mathematical, and semi-numerical interpretation of the MEMS accelerometers for multipurpose engineering applications.



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sciforum-107872: Performance Evaluation of 3D Printed Mortar Composite developed using Waste Materials

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This research addresses the need for a sustainable alternative by focusing on the performance evaluation of 3D printed mortar using recycled materials. The overarching problem lies in the environmental impact of conventional construction methods and the lack of comprehensive studies on the viability and sustainability of 3D printed mortar. This project aims to investigate the mechanical and environmental performance of 3D printed mortar while considering its potential to contribute to a circular economy. By conducting a detailed analysis, the study aims to provide insights into the feasibility of implementing 3D printed mortar as a sustainable solution in construction practices, thereby addressing the broader challenges of resource conservation and environmental sustainability in the construction industry. The purpose of studying 3D printing is to develop a technology-based alternative for construction. The methodology of study is to compare the strength of conventional mortars of cubes to 3D printed Mortars by strength performance analysis. In this study brick dust powder was used as partial replacement of cement. The compressive strength achieved for control sample was (24.3MPa) and it increased up to (27.6 MPa) by partial replacement of cement with 10% brick dust powder. The benefits of study of mechanical properties of 3D printed mortar utilizing waste materials are anticipated to result in a range of favourable composite materials. Together, these effects collectively promote construction practices that are both environmentally conscious and economically feasible. After successful testing of developed mortar, this technology can be recommended for housing construction at large scale.



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sciforum-104404: Phase-Field Modeling of Crack Propagation for brittle materials by finite elements method (FEM)

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Phase-field models are used to represent the geometry of defects in a diffuse manner, without introducing sharp discontinuities. Due to this feature, these models demonstrate a high level of efficiency in simulating crack propagation compared to numerical techniques that rely on a discrete crack model. This particular advantage becomes exceptionally evident when confronted with complex crack models, highlighting the superior capabilities of phase-field models to accurately represent the complex behaviors exhibited by cracks, and the phase field method can essentially be treated as a multi-field problem, even for a purely mechanical problem. The current study focuses on the area of crack modeling in brittle materials, using the phase-field methodology specifically adapted to these materials. In the field of computational mechanics, many research efforts have focused on the complex task of fracture modeling through the use of phase fields. Among this body of academic work, the present study stands out for its use of a phase-field model to describe crack initiation and propagation in brittle two-dimensional materials using the finite element method (FEM). Numerical simulations are meticulously presented and carefully studied to vividly illustrate the remarkable efficiency and robust capability of the phase field method to address and handle this particular type of modeling.



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sciforum-106329: Predicting Deformed Corrugated Boards Using a Logistic Regression Classifier

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Ensuring the durability and performance under compression of packaging materials, especially corrugated boards, is essential to quality control, as protection of the contents in packages is expected and required. Therefore, predicting deformations in such structures becomes demanding. In this work, the authors present a Machine Learning model to predict the deformation of corrugated boards. The considered hypothesis is that frequency-domain features can predict deformation accurately, as corrugated boards have wavy patterns whose prediction models can take advantage of. The methodology consists of filtering and removing the regions depicting the liners of the corrugated boards before retrieving relevant features from the processed images. The data structure consists of several candidate frequency-domain values as features, while the deformation status (deformed or not deformed) is labeled as the output. A logistic regression classifier was trained using these features, expecting to yield a highly accurate model for predicting the deformation of corrugated boards. The results suggest the model performed with high accuracy - over 80%. The results underscore how well frequency-domain features can be used for machine-learning models to serve in corrugated board quality control. They also set the stage for future advancements in packaging technologies, such as optimizing the design and manufacturing of corrugated boards that make use of predictive algorithms.



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sciforum-107465: Relationship between Fabrication by Wire Arc Additive Manufacturing and Pump Performance in Low-Solidity Axial-Flow Impellers with Different Numbers of Blades

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The fabrication of parts by metal additive manufacturing may reduce environmental impact, cost, lead time, and other factors compared to traditional fabrication processes. In particular, several studies have shown that the fabrication of impellers, one of the key elements of turbomachinery, by wire arc additive manufacturing (WAAM) can improve the fabrication process compared to traditional fabrication methods. However, there are problems that have not been discussed in the analyses conducted in these studies with regard to the relationship with the hydraulic performance of the impeller. As the mechanical design in industrial turbomachinery requires appropriate evaluation and determination of impeller hydraulic performance and fabrication methods, it is important to clarify these relationships for industrial applications of WAAM.

In this study, an analysis was conducted for low-solidity axial-flow impellers with a focus on the number of blades. Two aspects were analyzed for axial flow impellers with different numbers of blades. First, an evaluation of the fabrication method by WAAM in the fabrication of impellers was conducted. Second, the pump performance was measured for a centrifugal pump with axial-flow impellers installed as an inducer to evaluate the hydraulic performance. In addition, these results were analyzed comprehensively. The conclusion is that there is a trade-off between the fabrication process advantage of WAAM and pump suction performance.



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sciforum-104057: Renovation of Water and Sewer Manholes Using a Three-Layer Polyurea and Closed-Cell Rigid Foam Coating

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Water and sewer manholes are prone to chemical degradation, resulting in concrete erosion and structural weakening. Traditional repair methods often fail to restore the original load-bearing capacity adequately. This study investigates an innovative method for renovating water and sewer manholes using a three-layer coating of polyurea and closed-cell rigid foam. The chemical degradation of manholes leads to significant concrete loss, necessitating robust repair methods. Finite Element Method (FEM) analyses were conducted on axisymmetric manhole structures subjected to soil pressure and tanks with internal water pressure, considering existing concrete damage.

This study employed FEM to simulate the structural behavior of damaged manholes under various loading conditions. A three-layer repair coating comprising polyurea and closed-cell rigid foam was applied to address these damages. Numerical homogenization was used to reduce the complex cross-section of the repaired manhole to a single equivalent layer, facilitating simplified yet accurate structural analysis. The homogenization process enabled the transformation of the geometrically complex cross-section into an effective single layer with equivalent properties. This approach allowed for the re-evaluation of the manhole's load-bearing capacity, demonstrating significant improvements due to the innovative repair method.

This research underscores the efficacy of using a three-layer polyurea and closed-cell rigid foam coating for manhole renovation. The combination of FEM and homogenization techniques provided a reliable framework for assessing and enhancing the structural integrity of repaired manholes. This study's findings support the adoption of this innovative repair method, promising improved durability and performance of water and sewer infrastructure. This work contributes to the field of civil engineering by presenting a practical and effective solution for extending the lifespan of critical infrastructure elements.



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sciforum-107219: Robust Backstepping Sliding Mode Control for a Morphing Quadcopter UAV

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Morphing quadcopters have recently gained unprecedented popularity due to their flight flexibility, geometric reformation, and self-controlled arm management and the diversity of their applications. It has been established that in morphing quadcopter control, morphing formations in flight introduce time-varying parameters into the dynamic models, thereby increasing the complexity of the control problems, in addition to the non-linearity, coupling dynamics, and external disturbances present in the model. Thus, to address these challenges, this research therefore developed a robust backstepping sliding mode controller for morphing quadcopter position and orientation control. In the first stage, a mathematical model of an active morphing quadcopter (a foldable drone) was presented considering five morphing formations (X, H, T, O, and Y). Following the development of the system model, the proposed control method was designed in two stages: a high-performance sliding mode controller (HSMC) for attitude control to ensure chattering-free and fast convergence of the angles of orientation and a backstepping controller applied to position control were developed. Then, Lyapunov stability was used for an analysis of the stability of the closed-loop system. Finally, the robustness and effectiveness of the controller were investigated and benchmarked against a backstepping control approach using the mean square error and the sum of tracking errors as the performance metrics. The simulation results obtained show the effectiveness of the developed controller for the backstepping approach in the presence of parameter variations and external disturbances.



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sciforum-094650: Sensitivity analysis of conformal CCs for injection molds: 2D Transient Heat Transfer Analysis

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The fabrication of conformal cooling channels (CCCs) has become increasingly efficient and cost-effective throughout the past few years. Conformal cooling channels, also known as CCCs, are superior to straight-drilled channels in terms of efficiency in injection molding engineering applications owing to their ability to provide superior cooling. The ability of CCC to conform to the curves of molded geometry is the reason for this. The implementation of CCCs results in a significant reduction in the amount of time required for cooling, total injection time, thermal stresses, and warpage. When compared to the construction of a regular channel, the construction of a CCC channel is usually more complex. To maximize the development of designs that are both economically viable and highly efficient, computer-aided engineering (CAE) simulations are necessary. The purpose of this study is to conduct a sensitivity analysis of a full injection mold, with eight cooling channels, by means of a thermal analysis done in 2D. The objective is to achieve the best possible placement of CCCs to diminish the amount of time required for ejection and to enhance the uniformity of temperature distribution. The results show that all the variables have significant sensitivity to the maximum and Average temperature on the injected part and, therefore, are suitable for design optimization procedures.



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sciforum-094651: Sensitivity analysis of conformal CCs for injection molds: 3D Transient Heat Transfer Analysis

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Recent developments in additive manufacturing have resulted in a reduction in the costs and the level of complexity connected with the manufacturing of conformal cooling channels (CCCs). Conformal cooling channels, also known as CCCs, offer a higher level of cooling efficiency in the injection molding process when compared to the more traditional straight-drilled channels. The fundamental reason for this is that traditional machining processes do not have the potential to properly follow the contours of the molded form. However, CCCs are able to offer this capability. Using CCCs makes it possible to improve cycle times, achieve a more uniform temperature distribution, and reduce thermal strains and warpage. When it comes to developing a design that is both productive and cost-effective, computer-aided engineering (CAE) simulations are an absolute necessity nowadays. The primary purpose is to determine the optimum placements of CCCs, to improve temperature uniformity and reduce the amount of time that ejections take place (ejection duration). For the sake of future optimization techniques, it is possible to infer the practicability and potential usefulness of the design variables and parametrization that were accomplished in ANSYS Parametric Design Language (APDL). In fact, all the considered geometric/design variables present significant sensitivity in the studied CAE model.



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sciforum-104061: Shape Optimization of Trapezoidal Sheet Metal for Maximum Bending Stiffness and Coverage Area

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Trapezoidal sheet metal is widely used in construction due to its high strength-to-weight ratio. However, optimizing its shape for both bending stiffness and coverage area poses a significant challenge. This study focuses on optimizing the shape of trapezoidal sheet metal to achieve maximum bending stiffness and coverage area, with the constraint of fixed working length. Using Pareto front analysis, we identified the optimal shape incorporating stiffeners on the flanges and web. The dual objectives of maximizing stiffness and coverage area often conflict, making the optimization problem complex. The proper formulation and selection of optimization algorithms are crucial. We employed both global and local minimization algorithms with multistart methods to effectively explore the design space.

We utilized Pareto front analysis to balance the conflicting objectives of maximizing bending stiffness and coverage area. The shape of the sheet metal, including stiffeners on the flanges and web, was optimized using both global and local minimization algorithms. Multistart methods were applied to ensure comprehensive exploration of the design space. The optimization revealed that achieving an optimal shape for trapezoidal sheet metal requires careful consideration of the trade-offs between bending stiffness and coverage area. The Pareto front provided a range of optimal solutions, highlighting the importance of selecting appropriate algorithms for different aspects of the optimization problem.

This research demonstrates that the shape optimization of trapezoidal sheet metal is a complex yet feasible task when using advanced optimization techniques. The findings emphasize the critical role of problem formulation and algorithm selection in achieving effective results. Future work will explore further refinements in the optimization process and application to other structural components. This study provides a robust framework for engineers to optimize the design of trapezoidal sheet metal, enhancing its performance and efficiency in construction applications.



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sciforum-107372: Simulation of ultrasonic transducer for plastic welding system using finite element method

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Ultrasonic transducers combine coupling elements such as bolt, piezoelectric disk, back mass, and front mass. The quality and performance of the transducer greatly influence the quality of the ultrasonic weld. The design of a transducer requires good coordination with the design of other components such as bolt, piezoelectric disk, back mass, front mass, and sometimes booster, and horn. There have been many studies presenting how to build models for transducer design. However, there are not many articles presenting the design and simulation of transducers using finite element models. This paper will present a finite element model to simulate the coordination of all the above components. The influence of the interaction creation methods of the elements as well as the influence of the choice of bolt load on the predicted axial resonance frequency. In addition, the model also considers whether the simplification of some factors on the elements in the simulation affects the simulation results. The dynamic properties of the transducer obtained from the simulation model will be verified by experiment. The results show that the choice of host surface and slave surface in the interaction affects the simulation results. Meanwhile, the simplification of some parts also has a significant effect on the simulation results. The results of the calculation of longitudinal resonance frequency from the simulation are compared with the results obtained from the experiment and are very consistent with each other.



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sciforum-088947: Structural Analysis of Euler–Bernoulli Beams using Radial Point Collocation Meshless Technologies

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Beams, as flat slender structures primarily subjected to bending and transverse shear stresses and likely used in every engineering structure, are among the most important topics in mechanical and structural engineering training and practice today. Despite the long history of man's understanding of structural behavior and the various shear deformation theories for beams proposed, the Euler–Bernoulli beam theory (or classical beam theory) is still the most widely used engineering approach today. Although the finite element method (FEM) is now the standard engineering method for analyzing all types of beam problems, meshfree methods have also been used to analyze beams in recent years. The assumption that any function can be written as an expansion of a set of continuously differentiable basis functions is a simple, easy to implement, and very popular non-symmetric meshless method for solving partial differential equations (PDEs) nowadays which, provided the basis coefficients are properly determined by a collocation method, can, in general, be used as an approximation scheme for the solution of PDEs. This article addresses radial point collocation numerical technologies for the static analysis of Euler–Bernoulli beams involving fourth-order spatial derivatives, including how to apply the method to uniform and isotropic beams with arbitrary boundary conditions and loadings, as well as a performance comparison of the meshless approach to traditional analytical and FEM solutions, demonstrating its appeal and competitiveness for a broader engineering application.



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sciforum-107817: Structural integrity evaluation of polymers used in additive manufacturing under UV light and humidity exposure

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The mechanical properties of polymers change over time when they are exposed to UV light and moisture. This work presents the results of continuously exposing a nylon-based composite used in additive manufacturing (AM) to UV light and humidity for 24-, 48-, 96-, 168-, 336- and 504-hour periods. Sample coupons were printed in a Markforged Two ® composite printer using Onyx ®, which is a nylon matrix composite reinforced with short carbon fibers. For UV exposure, the samples were exposed to commercial 253 nm UV lamps, whereas for humidity, an ACE UV-260 humidity chamber was used at 50% relative humidity and 22°C with bi-distilled water. The effects of said variables were measured using the Charpy impact energy (per ASTM D6110), water absorption, and Shore hardness D (per ASTM D2240). It was found that nylon indeed presents 1.03% $\pm$ 0.28 water absorption over as little as 24 hr of exposure and about 5.6% $\pm$ 0.48 water absorption for 504 hrs. Regarding the Charpy impact energy, the absorbed energy decreases from 450 kJ/m² $\pm$ 15.96 at 24 hr to 254 kJ/m² $\pm$ 33.9 at 504 hr of humidity exposure. The Shore hardness D varies from 59.1 $\pm$ 0.82 for zero exposure to 59.7 $\pm$ 1.5 at 24 hr and 66.8 $\pm$ 2.5 after 504 hr of UV exposure. We can conclude that water absorption makes nylon a more fragile material, whereas UV exposure hardens the material. Future results could include using tensile axial tests and infrared spectroscopy to assess water absorption.



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sciforum-094648: Structural Strength Behavior and Optimization of Internally Reinforced Beams Subjected to Three-point Bending Load

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Thin-walled structures are particularly advantageous for applications that require lightweight designs with high stiffness and strength. Therefore, understanding their mechanical behavior is essential. Internally stiffened thin-walled structures are of particular interest, as internal reinforcements can be designed to optimize the moment of inertia, leading to increased stiffness and strength. This investigation applies structural finite element analysis (FEA) to assess the strength behavior of internally reinforced hollow-box beams. A total of twelve different beams were subjected to static three-point bending stresses, with loads applied to beams that had previously undergone stiffness optimization for enhanced performance. These beams were carefully modified to achieve the highest possible stiffness while minimizing mass. The strength was evaluated using von Mises equivalent stress values, and various metrics were provided to analyze the behavior of the optimized models. The optimized beams were compared with both the initial models and a reference model of an unstiffened beam to assess the impact of stiffness-based optimization on strength results. The findings indicate that the optimization technique, originally developed to increase stiffness while reducing mass, also improves specific strength while maintaining mass reduction. The primary benefit of reducing material in certain parts is not only the decrease in material costs but also the enhanced motion capability of mobile components, which allows for faster movement. The technological complexity of producing such structures was high until recent years, when additive manufacturing emerged as an affordable and high-quality solution for fabricating complex parts like those studied here. Future research could focus on exploring the long-term stability and safety of these structures.



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sciforum-097543: The aerodynamic and flight characteristics of the UEFA EURO 2024 football

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Recent international tournaments have seen various changes in the design of official footballs. Especially since the 2006 Germany World Cup, the balls used in World Cups and Euro Championships have continuously evolved in terms of surface roughness and other characteristics. This study compares the flight characteristics of the footballs used in Euro 2024 and the 2022 Qatar World Cup footballs.

A wind tunnel experiment was conducted comparing the drag force characteristics of the footballs used in the 2022 Qatar World Cup (Al Rihla) and Euro 2024 (Fussballliebe). Drag force was measured using a sting-type balance detector, which is capable of detecting drag force accurately.

Comparing the subcritical drag coefficients ($C_{D,sub}$) of each football, the 2022 World Cup ball exhibited approximately 0.17 (at $Re=2.2 \times 10^5$), while the Euro 2024 ball showed about 0.19 (at $Re=1.9 \times 10^5$). Based on these findings, simulations were conducted to calculate the respective distances when kicked at an initial velocity of 30 m/s and an angle of 25 degrees. The results showed that the 2022 World Cup ball traveled approximately 46.5 meters, whereas the Euro 2024 ball traveled a shorter distance of 45.1 meters. Additionally, when each ball was kicked from 25 meters away with an initial velocity of 30 m/s and an angle of 12 degrees, the landing point in front of a goalpost was lower for the Euro 2024 ball (0.82 meters) compared to the 2022 Qatar World Cup ball (0.91 meters).

Consequently, in football tournaments where balls vary between competitions, it has become crucial for players to quickly adapt to the specific characteristics of each ball. This adaptability directly impacts performance, highlighting the significant importance of understanding and adjusting to the unique properties of tournament-specific footballs.



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sciforum-103934: The effect of thickness of Jacketing on the response of square RC sections

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The load resisting capacity of reinforced-concrete (RC) structures reduces due to various sources such as earthquakes, corrosion and aging effects. Even under neutral circumstances, the performance of buildings can be reduced over time due to the strength and deformation degradation of concrete and steel. Reconstruction of such structures may be an option, but it may cause significant costs, labor and time. Therefore, depending on the priority of the structure, strengthening becomes one of the alternatives and may be a sustainable solution to increase the capacity in terms of both strength and ductility.

There have been many studies on the strengthening of buildings and the different methods that have been improved and applied. Among these strengthening methods, RC jacketing is considered one of the most common methods in over the world. The advantage of this method is that it needs little labor and equipment, with low costs, and method itself can improve the strength, stiffness and, to some degree, ductility of structural elements by increasing the cross-section and lateral confinement, thus increasing the performance and service life.

Based on the above, this study examines the behavior of different cross-sections' strength with RC jacketing. Using the improved jacketing behavior models in the experimental studies, the mechanical behavior of RC jacketing was investigated using three different reinforced-concrete square sections with varying jacketing thicknesses. The axial load ratio of a column before strengthening was taken as 30%, and the longitudinal reinforcement ratio of the jacketed and as-built sections was assumed to be 1%. The compressive strength of the existing column and RC jacket was 15MPa and 40MPa, respectively. The changes in the strength and ductility of the sections were evaluated using parameters such as ratio of jacket thickness to cross-section depth (Δ/h) and ratio of cross-sectional area to area of jacketed RC section (A_1/A_2). The evaluations revealed a strong relationship between these parameters and the section responses.



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sciforum-103572: Thermal and Mechanical Performance of Cement Mortar Containing Microencapsulated Phase Change Material

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For both residential and commercial buildings, one of the largest portions of the total energy consumption and environmental impact lies within the heating and cooling of the building and the thermal inefficiencies of the building envelope. To meet the Paris Climate Agreement's goal of reducing global warming by 2 degrees Celsius, the thermal efficiency of buildings should be increased by 30%. Phase Change Materials (PCMs) have been used in gypsum wallboard with great success but have not performed as well in concrete due to the resulting decrease in the concrete's compressive strength and the survivability of the PCM during mixing and curing. Testing has shown that concrete walls containing PCMs consistently show a 3-degreesCelsius change in temperature compared to similar walls without PCM. This study aims to build upon previous work in the literature and further explore the effect of the water-cement ratio, aggregate content, and PCM content on the thermal and mechanical properties of PCM concrete. The PCM concrete used in the study was composed of Type I cement, silica fume, sand, and 24 degree Celsius microencapsulated dry PCM. The compressive strength of the concrete was measured at 7 days, and the compressive strength and thermal performance were measured at 28 days. The thermal performance was assessed using a radial heat flow method that involved recording the temperature rise in a cylindrical concrete specimen as it was heated using a cartridge heater.



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sciforum-107723: A comprehensive analysis of the impact of the properties of water and its mineralogical components, and their interactions, on the concrete qualities

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Water is an essential resource for humans and a key component in the creation of concrete. However, the availability of this vital resource is being strained by the lack of fresh water brought on by population increase, climate change, and rising pollution. The concrete industry is increasingly using unusual waters, such as treated wastewater, brackish water, and industrial water, in response to the scarcity of fresh water. Although using these waters has benefits for the ecology and economy, there are concerns about how it may affect the quality of concrete. Despite the importance of the subject, there is a lack of scientific articles synthesizing the effects of all water characteristics and their interactions on concrete properties. With this in mind, this study aims to investigate the influence of the main characteristics on the strength, consistency and durability of concrete, using a qualitative approach based on a detailed synthesis of the literature. Our analysis of various water sources reveals that several key parameters in the mixing water significantly impact concrete. These include: pH - low pH leads to reinforcement corrosion, concrete cracking, and strength loss. High pH can degrade mechanical strength and cause setting and hardening issues. Chlorides promote reinforcement corrosion, cracking, loss of adhesion, and reduced mechanical properties. Sulfates contribute to swelling, cracking, strength loss, and aesthetic deterioration. Finally, suspended matter decreases mechanical strength, increases porosity, reduces durability, and hinders workability. Beyond their individual influences, the interaction between these different parameters is of particular importance, especially between pH and other parameters, as well as between chlorides and sulfates.



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Session 6. Energy, Environmental and Earth Science

sciforum-107565: Evaluating the Ecotoxicological Impacts of Heavy Metals in Freshwater Ecosystems: A Comparative Study of Sediment Quality Guidelines

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This research investigates the evolution of sediment quality guidelines (SQGs) since the 1980s, highlighting a shift from basic comparisons of contaminant concentrations to more sophisticated assessments that account for ecological impacts. Historically, the reliance on background or reference values for sediment contamination assessments neglected the biological diversity and potential adverse effects on aquatic organisms. In response, various national and regional agencies have developed comprehensive SQGs aimed at safeguarding sediment-dwelling organisms within freshwater ecosystems. These guidelines are categorized into threshold effect concentrations (TECs) and probable effect concentrations (PECs). Utilizing statistical analyses performed with Statgraphics 19 and Microsoft Excel 2019, this study reveals notable variability in PECs, ranked as follows: chromium (Cr) at 11.00%, Nickel (Ni) at 30.04%, zinc (Zn) at 32.84%, copper (Cu) at 33.11%, lead (Pb) at 40.44%, cadmium (Cd) at 43.47%, arsenic (As) at 48.48%, and mercury (Hg) at 52%. These results indicate that chromium is the least variable contaminant, while mercury exhibits the highest variability. Additionally, the toxicity levels of various metals (loids) were investigated using box-and-whisker plots, revealing that mercury was the most toxic, whereas zinc was found to be the least toxic. For TECs, the ranking is lead (11.43%), mercury (16.67%), zinc (18.70%), nickel (20.00%), arsenic (25.79%), cadmium (29.58%), chromium (30.29%), and copper (37.14%), indicating lead as the least variable and copper as the most among the examined guidelines.



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sciforum-107740: A Systematic Review of Biomass-Derived Potassium Extraction for Potassium-Ion Batteries: Techniques, Challenges, and Sustainable Energy Solutions

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The increasing demand for food has intensified agricultural practices, leading to environmental degradation and economic loss. Simultaneously, the need for sustainable energy has spurred research into alternatives like potassium-ion (K-ion) batteries, which have emerged as a promising substitute for lithium-ion batteries. This systematic review evaluates the current methods of extracting potassium from biomass, with a focus on its application in K-ion batteries (KIB). Following PRISMA guidelines, a systematic search was conducted across major databases using broad keywords related to biomass-derived potassium extraction and its use in energy storage. Articles were reviewed for relevance, and a subset was selected based on criteria such as extraction techniques (pyrolysis, acid leaching, and alkaline hydrolysis), biomass types, and battery applications. The review highlights the potential of agricultural waste, particularly in developing sustainable energy solutions through KIBs. However, challenges remain, including the need to improve extraction methods and address scalability issues. Further research is required to refine these processes, explore alternative biomass sources, and evaluate long-term battery performance. Linking waste management with K-ion battery technology, this review outlines a pathway toward more sustainable energy solutions benefiting both the environment and economy. Continued research is vital to fully unlock the potential of biomass-derived potassium in renewable energy.



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sciforum-094634: Earth-Integrated Renewable Energy Systems: Pioneering Sustainable Solutions for a Greener Future

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Introduction:

The quest for sustainable energy solutions amidst environmental concerns has led to the emergence of innovative approaches integrating renewable energy with earth science principles. This research article explores the novel concept of Earth-Integrated Renewable Energy Systems (EIRENS), highlighting their potential to revolutionize energy production while mitigating environmental impacts.

Methods:

A comprehensive synthesis of recent advancements and cutting-edge research in renewable energy and earth science was conducted. Key methodologies, including geothermal heat extraction, underground pumped hydro storage, and enhanced geothermal systems, were explored to demonstrate the feasibility and sustainability of EIRENS.

Results

and

Discussion:

The findings underscore the transformative potential of EIRENS in addressing energy challenges while minimizing environmental footprints. By harnessing the Earth's natural resources, such as geothermal energy and subsurface storage, EIRENS offer reliable, dispatchable power generation with reduced greenhouse gas emissions and land use impacts compared to conventional renewable energy systems.

Conclusions:

EIRENS represent a paradigm shift in sustainable energy solutions, offering a holistic approach that integrates renewable energy generation with earth science principles. By leveraging the Earth's geological features and natural energy reservoirs, EIRENS can provide clean, reliable power while mitigating environmental impacts and promoting energy security. This research article emphasizes the importance of advancing EIRENS as a viable pathway towards a greener and more sustainable future.



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sciforum-095605: A Cellular Automata Markov (CAM) model for land use change prediction using GIS and Python

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Knowledge of future land use changes is crucial, as they are interlinked to various factors of human-environmental systems. Land use changes have a profound impact on urban planning, environmental sustainability, resource management, and overall quality of life. Spatial data can often be computationally heavy, so the provision of accessible and ready-to-use tools is crucial for the analysis of land use changes in any case study. In this work, a Cellular Automata Markov (CAM) model is presented and applied through a combination of Geographic Information Systems (GIS) and Python, to predict land changes and provide future land use maps. The inputs are historical land use maps at a five-year time-step from 2006 to 2021, and the outputs include future land use maps until 2051. The Cedar Creek Watershed (CCW) in Indiana, US, is used as a case study; it is an area of great natural beauty, mainly consisting of agricultural lands, forests and water bodies. Various validation techniques are explored for the predicted maps, based on the historical data, including Accuracy, Mean Absolute Error (MAE), Root Mean Square Error (RMSE), the Kappa coefficient (κ), and Confusion Matrix statistics. The results indicated a gradual increase in urban areas at the expense of agricultural land. Forested areas showed stability with minimal change, while water bodies maintained consistent coverage. Some minor shifts from barren land to both urban and forested categories were also observed. Validation results showed a high accuracy of 99.63%, a mean absolute error (MAE) of 0.0094, and a root mean square error (RMSE) of 0.1613. The Kappa coefficient indicated strong agreement at 0.9925. A step-by-step GIS guide and the Python script are provided to contribute to the reproducibility and improvement of the model. Similar analyses can find multiple applications in a variety of studies on human-environmental systems (including water, agriculture, economy).



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sciforum-106723: A Comparison Between Methanol And Carbon Nanotube Production From Co₂ Inside A Cement Industry

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Carbon dioxide (CO₂) represents more than 70% of the greenhouse gases (GHG), which are responsible for the greenhouse effect, a natural phenomenon that directly affects and allows life on the Earth. However, over the last half-century, the CO₂ atmospheric concentration has rapidly increased to about 400 ppm due to human-related emissions, causing the well-known climate change. Of these emissions, 21% are originated from industry, in which the cement production has the largest impact.

In this scenario, many solutions using either CO₂ capture storage (CCS) or CO₂ capture and utilization (CCU) in cement industries have been investigated, including the synthesis of chemicals, polymers, fuels, and nanomaterials.

In this work, one functional unit with 2 Mtons of cement/year was adopted to compare the conversion of the captured CO₂ to carbon nanotubes (CNT) and methanol. Along with emission factors and economic evaluations, the proposed analyses were employed using material and energy balances.

The results showed that, currently, methanol seems more attractive since it can increase profits per functional unit up to 322 M€/year and allows a reduction of 8% of the total CO₂ emissions inside the cement industry, while for CNTs the values are respectively 90 M€/year and 0.01%.

Nevertheless, CO₂ conversion to CNT has the potential to increase its attractiveness in the cement sector according to the CNT market expansion in the future (carbon nanotubes would replace the large markets of iron and aluminum).



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sciforum-107788: A Model Based Analysis of Direct Methanol Production from CO₂ and Renewable Hydrogen

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Methanol synthesis from CO₂ is a key strategy for carbon capture and utilization, offering a viable solution to mitigate climate change. Direct synthesis of methanol not only reduces greenhouse gases but also produces valuable chemicals for industrial applications. The aim of this study is to model and optimize the methanol synthesis process from CO₂, focusing on maximizing methanol yield while minimizing CO₂ content in the product stream. In this work, a detailed methanol synthesis process simulation was developed using the Soave-Redlich-Kwong equation of state in the Aspen Plus commercial software environment. Pure CO₂ stream which comes out of post-combustion carbon capture process and renewable hydrogen stream are used. The results are compared with open literature sources. Apart from that, a sensitivity analysis was employed to evaluate the effects of pressure, temperature, and recirculation fraction on process efficiency. The results showed that the highest methanol yield of 76,838 kg/h was obtained at 80 bar, 276°C, and a recirculation fraction of 0.9. The lowest CO₂ content in the final product (73 kg/h) occurred at 80 bar, 220°C, and a recirculation fraction of 0.6. These findings demonstrate the trade-off between maximizing methanol output and reducing unreacted CO₂. In conclusion, optimal operating conditions for both high yield and low CO₂ content were identified, providing a foundation for further process refinement. Future work will involve developing a more complex multi-reactor model and conducting economic assessments for large-scale industrial implementation.



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sciforum-103858: Ab-initio life-cycle analysis assisting the selection of ecofriendly additives in biobased coatings

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The formulation of ecofriendly coating compositions with protective properties against corrosion and/or mechanical degradation requires appropriate selection of bio-based binders and functional additives. Although the concentration of additives remains limited, they highly contribute to the enhanced lifetime and may alter processing conditions of the coating. Their influences on processing conditions also affect the selection of appropriate end-of-life options with specific technological challenges on recycling and re-processing of the coating. Therefore, the replacement of fossil-based additives into bio-based additives may deliver an important contribution improving the carbon footprint of a coating over its full lifetime. However, the role of bio-based additives in life-cycle analysis is often neglected and minorly considered, as up to present only few dedicated case-studies have been identified in literature. Reasons for this are further pointed out in this paper, including lack of data, methodological inconveniences and appropriate design of realistic scenarios. Within this work, a simplified approach is followed by ab-initio cradle-to-gate analysis of coating compositions focussing on the replacement of specific fossil additives into bio-based additives. Particular case-studies are presented in relation with replacement of carbon black, silicates, calcium carbonate into biochar, bio-based wax and recovered calcium carbonate. There is a main interest in improving coating performance by substituting cellulosic additives into nanocellulose from different sources, where environmental benefits are associated with their high performance at low concentration. The environmental impact parameters (human health, ecotoxicity, resource scarcity, carbon footprint) are calculated from ecocost analysis (Idemat 2024 v2.2 database) indicating a 15 to 30 % gain in environmental footprint for given coating formulations. The need for intermediate processing of the bio-based additives is a main parameter contributing to their environmental impact, but is abundantly compensated by their carbon storage credit and performance improvement.



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sciforum-099140: Abrasivity assessment of Triassic limestone and volcanoclastic sandstone in Mae Mon Basin, northern Thailand: comparison between RAI and CAI

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The ability of rocks to wear tools used for ground excavation, tunneling, or drilling, is referred to as rock abrasivity. There are a variety of testing methods to estimate rock abrasiveness, ranging from microscopic to pilot scales. This study tests the abrasivity of selected sedimentary rocks observed in the Mae Moh Basin, northern Thailand, using the two abrasivity testing methods, including RAI (rock abrasivity index) and CAI (CERCHAR abrasivity index). The method of RAI involves mineralogical analysis coupling with the uniaxial compressive strength tests of the rock. The mineral assemblage formed in the rock and its content are microscopically observed under a conventional microscope. Each mineral is also compared to quartz in terms of hardness. The CAI method, on the other hand, observes the wear of a steel stylus tip after direct scratching on a rock surface under a systematic setup. The diameter change of the eroded tip is subsequently used for the calculation of the CAI. The results show that the limestone exhibits an RAI of 2.12, indicating it is not abrasive, and a CAI of 1.24, which indicates it has medium abrasivity. The volcanoclastic sandstone exhibits an RAI of 30.88, indicating medium abrasivity, whereas its CAI is 2.72, which indicates high abrasivity. The calculated CAI provides a more abrasive indicator than the RAI and significantly increases with the increasing equivalent quartz content. The findings of this study support a strategy for rock abrasivity assessment and tool wear prediction, which is essential in the fields of mining and georesource engineering.



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sciforum-089070: Advancements in Spectral Remote Sensing for Aquatic Ecosystem Quality Assessment: Integrative Approaches Using Convolutional Neural Networks and Spatio-Temporal-Spectral Fusion Models

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The study meticulously explores the cutting-edge domain of spectral remote sensing technologies tailored for the nuanced monitoring of water quality across diverse aquatic ecosystems. It places a strong emphasis on the innovative integration of Convolutional Neural Networks (CNNs) and groundbreaking spatio-temporal-spectral fusion models, setting a new precedent in environmental data analytics. Through a rigorous examination, we unveil the unparalleled efficacy of spectral remote sensing in unraveling the complexities inherent in key water quality parameters, including but not limited to, the concentration of phytoplankton pigments and fluctuating salinity levels. This is achieved via the strategic deployment of sophisticated computational algorithms that dissect and interpret the intricate data derived from spectral signals. Our discourse extends to illuminate the transformative impact of satellite-based remote sensing, revolutionized by the introduction of high-resolution spectral imaging coupled with the prowess of machine learning techniques. Such advancements facilitate not only the precision but also the expansiveness of water quality assessments, encompassing vast geographical terrains with remarkable accuracy. Through a methodical comparative analysis of various inversion models, the paper delineates the subtle yet powerful capabilities of these methodologies in extracting and decoding accurate environmental data from the complex interplay of spectral signatures. Moreover, the research accentuates the critical importance of hybrid analytical models that seamlessly blend spatial, temporal, and spectral data streams. This holistic approach furnishes a more intricate and dynamic understanding of aquatic ecosystems, enabling stakeholders to navigate and manage the nuances of these environments with greater efficacy. The synthesis of avant-garde remote sensing technologies with advanced computational models encapsulated in this study not only signifies a pivotal advancement in the realm of environmental monitoring but also lays down a robust framework poised to catalyze future innovations in the sustainable stewardship of water resources.



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sciforum-104564: Detection and Mitigation of hazards using advanced sensor technology with decision making system

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Pollution makes our environment endangered; the pollutants present in the air, such as N₂O, S₂O, CO, etc., affect living things and cause climatic changes in our environment. This leads to an increase in mortality rates and economic burdens. In order to address the above challenges, a new design of an IoT-powered air pollution monitoring system is introduced. This design utilizes an advanced sensor that monitors the harmful gases present in the air continuously. Furthermore, the proposed design incorporates a Kalman filter supported by an AI architecture that enhances the data accuracy and real-time processing by refining sensor data. The AI structure triggers the automatic response once it detects hazardous conditions; further, the automated response activates the instant alert and ventilation system that are placed in the proposed design. This increases safety and provides protection to the surroundings. The IoT system supports continuous data transmission from the sensor to the cloud; this enables seamless monitoring and time-to-time decision-making. Based on the predefined index, the proposed model predicts the air quality with three conditions: good, moderate, and danger. After air quality observation, the proposed system alerts the pollution control board for further action. The preliminary result obtained from the proposed model shows a significant improvement in the data accuracy and response time compared to conventional methods.



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sciforum-099026: Earthquake Potential Zones Identification using MCDA, Machine Learning and Geospatial Techniques in Sikkim

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Sikkim, nestled in the North-Eastern Himalayas, is a region frequently disturbed by earthquakes and are triggered by a myriad of factors, including tectonic plate movements, volcanic activities, subterranean explosions, human-induced quakes, and environmental conditions. This leads to loss of human lives, destruction of human properties and deformation of earth crust plates. The study aims to refine earthquake vulnerability assessment by incorporating Machine Learning Weighted Overlay methods over traditional Analytical Hierarchy Process (AHP) techniques. Unlike AHP, where users assign weightage based on their knowledge, ML models use feature importance for objective weightage assignment. A comprehensive set of parameters—fault characteristics, peak ground acceleration, earthquake magnitude, proximity, slope, and elevation which previous studies were somewhere lacking in their study. These parameters are weighted and superimposed using the AHP method. We used Google Earth Engine (GEE) to facilitates the extraction of weighted stacked images, which are then analyzed to pinpoint earthquake-prone locations via machine learning models, namely Random Forest and SmileCart classification. The earthquake vulnerability zones are stratified into five distinct categories: Very High (4.54%), High (28.37%), Medium (27.84%), Low (23.60%), and Very Low (15.65%). The Random Forest and SmileCart models outperformed the AHP method, yielding accuracies of 0.89 and 0.78, respectively, compared to 0.57 for the AHP approach by the validation points and ROC Curve/AUC values corroborate these findings, with respective scores of 0.71, 0.75, and 0.60. The integration of advanced machine learning algorithms over conventional AHP methods significantly enhances the precision of seismic susceptibility estimations. This synergy illustrates the potential of modern analytical techniques in the realm of natural disaster risk evaluation.



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sciforum-101741: Evaluation of Internal and External Radiation Exposure Doses from Concrete Samples Using a Computer Code (RESRAD-Build)

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Building materials naturally contain radionuclides, potentially leading to internal and external radiation exposure in human dwellings. This study collected and analyzed data on natural radionuclides such as Ra-226, Th-232 and K-40 in concrete samples from 16 countries worldwide. Internal and external doses for these concrete samples were estimated using the RESRAD-BUILD computer code. The RESRAD-BUILD model facilitates the evaluation of radiation exposure over a 70-year period, providing insights into the long-term health effects. The calculated long-term effective doses showed variations in external and internal doses over the years and among countries. The variations among countries underscore the importance of considering each country's geographical location and geological characteristics when establishing norms and guidelines related to emitted radiation limits from building materials.

These findings highlight the need for continuous monitoring of commonly used building materials, especially as radiation exposure is likely to increase in the near future due to the growing use of recycled materials and materials formerly considered waste in the building industry. Environmental quality, both indoor and outdoor, is crucial for human well-being and can serve as an indicator of human development, particularly since the majority of the population spends almost 80% of their time indoors. Therefore, measuring and controlling natural radiation in buildings is of great interest for ensuring human safety.



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sciforum-104412: Hybrid Fuel Cell And Solar-Powered Charging Station For Micro-Mobility And Stem Education

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The increasing demand for sustainable energy solutions in transportation has driven significant advancements in renewable energy technologies, with applications in electric vehicle charging stations, for example. Thus, a hybrid fuel cell and solar-powered charging station for micro-mobility, where such local transportation is utilized, would be beneficial. Moreover, such a hybrid charging station can be used to promote STEM education as it showcases the integration of solar-energy panels and hydrogen fuel cell technology to provide a sustainable power solution for micro-mobility and portable devices. This project aims to address the growing demand for eco-friendly transportation options while serving as an educational tool for science and engineering students. The methodology involved assembling, testing, and evaluating a system composed of a solar panel of up to 200 W, a solar charge controller, a set of battery banks, a hydrogen generator, a fuel cell, and a power inverter. The preliminary results indicated that while the system could power various devices from a fan of 3 Watts to a laptop of about 90 Watts, the hydrogen generators underperformed a bit to run at sub-optimal pressure at a flow rate of about 1 L/min, and thus limited the fuel cell's performance to below 100 Watts. The solar charging system successfully charged batteries to power the hydrogen generator for the tested duration.



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sciforum-096147: Key players in the adsorption process: engineered adsorbent surfaces for cleaner water

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A clean water source is essential for the continuity of the vital activities of all living things in the world. However, water pollution has become a global problem that threatens all living and non-living ecosystems. In response to this problem, both proven and alternative technologies have been used recently for the treatment of wastewater. Among these technologies, the adsorption method has gained popularity as it is a simple and environmentally friendly, highly effective method. The main role of the method is the adsorbents used, especially the different designed adsorbents obtained from waste materials and their surfaces come to the fore. The main goal in designing or modifying is to increase adsorption capacity by improving properties such as specific surface area, pore distribution and modification ability. The main purpose of this research is to evaluate the surface and functional structures of materials such as tuff, olive stone, coffee waste and date waste. In many studies, these materials are modified in terms of their surface structure to ensure the removal of different pollutants. In order to investigate the surface structure and chemistry of the adsorbents selected in the study, including functional groups, analyses were performed with Fourier-Transform Infrared Spectroscopy (FTIR) and Scanning Electron Microscopy (SEM).



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sciforum-107831: Leveraging Technology To Optimise Tertiary Education Trust Fund Building Projects For Public Universities In Delta State Nigeria

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Public tertiary institutions in Nigeria have been beneficiaries of the Tertiary Education Trust Fund(TETFUND), aimed at enhancing the quality of education by providing essential structures. The TETFUND is a government agency in Nigeria, established by an Act in 2011 to provide financial support to public tertiary institutions in the country. Despite this initiative, many projects encounter setbacks such as budget overruns and suboptimal resource allocation, leading to uncompleted or abandoned building construction projects. Deployment of technologies has enhanced the concept of intelligent construction, which has impacted the processes of building construction. These stalled projects hamper the universities' ability to expand infrastructure, improve educational quality, and accommodate growing student populations. Identifying the root causes of project abandonment and exploring the potential role of technology in addressing these issues is crucial for utilizing available funds. This study examines how technology can enhance the efficiency and transparency of TETFUND construction projects in public universities in Delta State, Nigeria. The research methodology to be adopted is a descriptive approach where a review of the literature would be performed and advantages drawn from them. The focus was on TETFUND-sponsored buildings randomly selected from the research population. Technology can enhance the projects by optimizing material usage, reducing waste, and improving energy efficiency, thus contributing to more sustainable university campuses. TETFUND building construction projects involve multiple stakeholders, including Architects, Project Managers, Contractors, Academia, Universities, and TETFUND. Understanding how leveraging technology impacts these stakeholders can help improve collaboration and communication throughout the project lifecycle. Keywords: artificial intelligence



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sciforum-096341: Natural Hazards and Spatial Data Infrastructures (SDIs) for Disaster Risk Reduction

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When there is an absence of or no implementation of measures targeting disaster prevention, natural hazards can be promptly converted into disasters. An essential part of disaster risk management is the geospatial modelling of devastating hazards, where the polygon shapefiles containing the extent, time period and cause of various disastrous events are significant input datasets in the context of early-warning systems. However, equally important are Earth observation satellite data for constructing remote sensing indices, a high-resolution digital elevation model, updated land cover data, socio-economic data like demographics and spatially referenced data, such as wind characteristics, temperature and precipitation. This research work points out the usefulness of Spatial Data Infrastructures (SDIs) in disaster risk reduction through a literature review, focusing on the necessity of data unification and disposal. Initially, the principles and implementations of SDIs are presented, and subsequently, their benefits for achieving the specific targets and priorities of the Sendai Framework for Disaster Risk Reduction 2015-2030 are elaborated. Thereafter, the challenges in SDIs are investigated in order to underline the main drawbacks the stakeholders in emergency management have to come up against, namely a lack of semantic alignment, which induces a time-consuming data search, and malfunctions in the interoperability of the datasets and web services, the non-availability of the data in spite of their existence and a dearth of quality data. Thus, diachronic observations on disasters will not be found, despite these comprising a meaningful dataset in disaster mitigation. Consequently, recommendations for an efficient SDI that is geared towards natural hazards are proposed to the involved participants for the purpose of disaster preparedness. SDIs constitute an ongoing collaborative effort intending to offer valuable operational tools in decision-making under the threat of a devastating event. Notwithstanding the functionality of SDIs, data collection is an intricate task.



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sciforum-104405: P3HT:PCBM as an active layer to enhance the efficiency of organic solar cells

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Organic solar cells have gained significant attention in recent years due to their properties of having low material costs, being lightweight, and undergoing high-throughput roll-to-roll production. However, their low efficiency and stability remain major challenges. Through our study, we aimed to address these issues by optimizing the optical and structural properties of the active layers to enhance performance and stability. Here, we investigated how optical interference impacts device performance. Solar cell efficiency is influenced by various factors, including the materials used within their structures. To analyze the impact of structural geometry, we used bulk heterojunctions with P3HT as the donor layer and PCBM as the acceptor layer, forming the active layers. We examined various computed optical properties, such as the intensity of optical electric fields, the generation rate, absorption profiles inside the device, and reflection within the device. Additionally, we calculated the short-circuit current density concerning the active layers and found a high value of 11.35 mA/cm² for P3HT:PCBM active solar cells, which corresponds to the high absorption within the device structure. High performance was achieved in the case where high absorption was localized within the active-layer cells using the finite element method. The numerical simulation, conducted with COMSOL Multiphysics software, shows a strong correlation with published experimental data.



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sciforum-106943: PbO₂ Potential in Anodic Oxidation for Microplastics Removal from Bay Water in Philippines

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The increasing abundance of microplastics in the water bodies poses a huge threat to the survival of marine organisms and to the health of people. Presently, a bay is one kind of surface water that has been contaminated by microplastics. One of the recently developed treatment techniques for eliminating microplastics from water is anodic oxidation. This study examined the potential of anodic oxidation with a lead dioxide (PbO₂) anode to remove microplastics from real water samples collected from Bacoar Bay, Philippines. Microplastics are broken down into nontoxic molecules like CO₂ and H₂O by hydroxyl (•OH) radicals produced during anodic oxidation, which eliminates the need for additional chemicals that could cause pollution of another form. Two factors, reaction time and current intensity, were investigated for their effects on removal efficiency. The concentration of microplastics in Bacoar Bay was discovered to be 49.56 mg/L. The water samples contained a variety of microplastics types, the bulk of which were fragment-shaped and ranged in size from less than 1 mm to 5 mm. The study's findings demonstrated that anodic oxidation resulted in a 42.53% microplastics removal efficiency and a 55.64% turbidity removal efficiency. Considering the results of this study, anodic oxidation using PbO₂ anode is a promising treatment method for microplastics, which can help alleviate the problem regarding microplastics.



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sciforum-105115: Satellite and Geographic Information System-Incorporated Multi-Platform Monitoring of Coastal Erosion on the Northwestern Coast of Sri Lanka

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Coastal erosion is the degradation of shorelines caused by natural factors such as sea level rise, currents, and wave action, as well as human activities like construction, deforestation, and fisheries. This process leads to the loss of land and sediments. In Sri Lanka, this phenomenon has impacted 15 tourist attractions in Kalpitiya, altering coastal landforms, including beaches, cliffs, dunes, and barrier islands. Over time, a 50-meter stretch of beach has been destroyed, resulting in the loss of valuable coastal habitats and infrastructure. This study investigated shoreline changes and calculated erosional and depositional rates using Geographic Information Systems (GIS) and remote sensing techniques. The region of interest (ROI) covered the coastal area from Mannar to Puttalam on the northwest coast of Sri Lanka. To analyze shoreline changes, vector data were processed using the Digital Shoreline Analysis System (DSAS V5_0) integrated with ArcGIS 10.5. Secondary data sources included topographic maps, digitized shorelines, and satellite maps obtained from the Survey Department and the United States Geological Survey (USGS) website. Coastal slope and contour lines were created to understand coastal geomorphology and its characteristics. Moreover, the Topographic Wetness Index (TWI) and Normalized Difference Vegetation Index (NDVI) were examined for supportive analysis. Weighted linear regression rate analysis revealed that the Kalpitiya vulnerability region experienced approximately 69% erosion and 30% accretion. The Erosion Potential Rate (EPR) parameter was used to calculate erosional and depositional rates, showing a maximum erosional rate of 13.48 m/year and a maximum depositional rate of 25.36 m/year.



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sciforum-107499: Statistical Methods for Optimizing Industrial Energy Systems

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Optimizing industrial energy systems is vital for meeting sustainability targets, reducing operational costs, and enhancing overall system performance. This paper explores the integration of advanced statistical methods—including regression analysis, time-series forecasting, Monte Carlo simulations, and machine learning algorithms—to optimize energy utilization and drive efficiency gains in industrial settings. A comprehensive analysis of energy data demonstrates significant improvements in efficiency through precise demand forecasting, reductions in energy consumption, and cost-effective operational strategies. Machine learning-driven predictive maintenance models effectively forecasted equipment malfunctions, reducing downtime and maximizing energy use efficiency. This study emphasizes the power of data-driven strategies to identify inefficiencies, forecast energy requirements, and enhance resource allocation. Techniques such as regression and time-series models offered precise demand insights, while Monte Carlo simulations provided robust risk assessments amid operational uncertainties. Machine learning-based predictive maintenance reinforced system reliability by proactively addressing potential breakdowns and improving resource utilization. Key challenges, including data quality issues, system complexity, and model scalability, are examined, highlighting the necessity of enhanced data integration and improved model interpretability. These factors are critical for the widespread adoption of statistical optimization approaches in industrial energy systems. The findings underscore the transformative role of statistical techniques in energy management, yielding substantial cost reductions and advancing sustainability efforts. The integration of these approaches with emerging technologies such as IoT and AI holds significant potential to further optimize system efficiency, bolster resilience, and drive sustainable industrial practices.



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sciforum-103616: Tetrabromobisphenol A (TBBPA): Ecotoxicity Assessment and Interactions with Low-Density Polyethylene Microplastics

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Tetrabromobisphenol A (TBBPA), a widely used brominated flame retardant, is prevalent in various environmental matrices due to its extensive use and release from plastic products. TBBPA exposure is linked to endocrine disruption, reproductive toxicity, and potential carcinogenicity. Microplastics (MPs), defined as plastic particles smaller than 5 mm, have become common persistent pollutants in marine, inland, and freshwater environments, including remote regions like the polar areas. Ionic strength and dissolved organic matter (DOM) can influence the sorption behavior of MPs, which due to their small size and large areas can significantly facilitate the transfer and accumulation of hydrophobic organic contaminants (HOCs) and heavy metals (HMs). Humic acid (HA), a mainly negatively charged natural organic matter, can interact with MPs, creating new sorption sites and potentially altering contaminant dynamics.

This study investigates the toxicity of TBBPA on the seawater microalgae *Tisochrysis lutea*. Additionally, the study evaluates the toxicity of TBBPA after adsorption onto LDPE MPs, both in the presence and absence of humic acid (HA) in four water matrices (seawater, lake water, wastewater and ultra-pure water), on *Tisochrysis lutea*.

The results showed significant inhibition of microalgae growth due to TBBPA exposure. The toxicity decreased in the presence of LDPE microplastics due to the potential adsorption of TBBPA onto the LDPE. In contrast, the presence of humic acid increased the toxicity of TBBPA, possibly by altering its sorption behavior on LDPE, making it more bioavailable. The findings aim to elucidate the complex interactions between MPs, TBBPA, and environmental factors, contributing to a better understanding of the ecological impact of these co-existing contaminants.



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sciforum-106375: Model Development of Nitrification in Premise Plumbing using Artificial Neural Network

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Nitrification is the process by which reduced forms of nitrogen are oxidized to produce nitrite and nitrate. When chloramine is used in potable water systems for secondary disinfection, there is a serious potential issue. The usage of monochloramine as a secondary disinfectant is growing in place of free chlorine. Water is treated with ammonia to promote the creation or breakdown of monochloramines. Regulations may be broken as a result of nitrification's detrimental effects on water quality. A study was conducted to look into the quality of the water, the impact of pipe material on the beginning of nitrification, and the effects of nitrification on In-Premise Plumbing. Here, the impact of pipe material on nitrification in premise plumbing was investigated along with examining its effects on water quality. Empirical modeling approach using Artificial Neural Network (ANN) was taken to observe and predict these effects. Input variables of ANN modeling are copper dose concentration, pH level and number of days while output variables are nitrite and ammonia utilization. The best-fitted models are, for ammonia utilization, ANN model with Levenberg-Marquardt algorithm and 50 hidden neurons, which had a coefficient of determination of 0.738 and a mean squared error of 65.8, and, for nitrite utilization, ANN model also using Levenberg-Marquardt algorithm and 50 hidden neurons, which had a coefficient of determination of 0.601 and a mean squared error of 0.0063.



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sciforum-102879: Bioconcentration and translocation of heavy metals from landfill leachate by selected plants

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It is reported in the literature that the most common pollutants in landfill leachate, apart from ammonium nitrogen, chlorides and sulfates, include heavy metals. Municipal waste landfills are considered a potential source of heavy metal contamination of groundwater, soil and plants. In high concentrations, they may pose a threat to human health and cause toxic effects in plants. Therefore, the aim of the study was to verify the content of heavy metals in leachate from four municipal waste landfills in Poland. The bioconcentration factor of heavy metals (BCF) from landfill leachate by emerged macrophytes (*Phragmites australis*) and submerged macrophytes (*Ceratophyllum demersum*) was assessed. Heavy metal translocation factor (TF) following exposure to landfill leachate were also analyzed. The obtained results showed that the content of selected heavy metals (Cu, Ni, Pb, Cr and Cd) in leachate remained at a low level (i.e. 1 mg/l), which shows that heavy metals are not currently a serious problem in landfill leachate in Poland. The BCF values were >1 only in a few cases (e.g. for Cr, where the BCF ranged from 1.02 to 4.62). For most variants, slightly higher metal contents were recorded in the roots than in the shoots. The TF of heavy metals in *P.australis* in almost all cases it was 1.0 except for Cd, where values up to 784 were achieved in the control variant.



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sciforum-103665: Green upgrading of biodiesel derived from biomass wastes

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With the increasing demand for edible oils for food and fuel purposes, non-edible oils have become more attractive for biodiesel production. Nevertheless, biodiesel has significant drawbacks that hinder its broader utilization, necessitating its blending with conventional diesel for current applications. These drawbacks include low oxidative stability (OS) and inadequate cold flow properties. These fuel properties are influenced by the composition of fatty acid methyl esters (FAMES), with a particular emphasis on their degree of unsaturation. Compression ignition (CI) engines can effortlessly handle blends of up to 30% biodiesel mixed with diesel fuel without necessitating any modifications. However, surpassing this threshold and utilizing biodiesel to a greater extent demands engine upgrade. Partial hydrogenation in aqueous/organic biphasic catalytic systems of polyunsaturated FAMES aims for maximum selectivity towards cis-monounsaturated FAMES. This approach optimizes oxidative stability while preserving satisfactory cold flow properties to the greatest extent possible.

The method used in this work includes the characterization of biodiesel samples using EN ISO standard methods and gas chromatography–mass spectrometry (GC-MS) for qualitative and quantitative analysis. Based on the composition of biodiesel samples in polyunsaturated FAMES, partial hydrogenation in aqueous/organic biphasic catalytic systems using transition metal complexes aims at improving the properties of produced biodiesel to meet specific standards while acting as a purification step, effectively eliminating impurities.

The highlighted results are (i) the research and development of an aqueous/organic biphasic catalytic system for the partial hydrogenation of biodiesel, and (ii) the improvement of biodiesel properties that do not meet EN ISO standard specifications.

Given the ongoing research and development in this field, the catalytic upgrading of biodiesel through partial hydrogenation in aqueous/organic biphasic catalytic systems seems promising. Further exploration of innovative catalysts and techniques holds potential for advancing biodiesel production and its application.



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sciforum-103621: Optimal sizing and Energy Management/Control of RES-Based Hybrid Systems

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During the past decade and more, the conventional energy production has led to the exaggeration of Climate Change due to the continuous emissions of greenhouse gases. To this end, renewables are the means of energy transition under the installation of Photovoltaics (PVs) and Wind Turbines (WTs) either in grid-dependent or stand-alone operation mode.

Aim of this study is the development of a combined sizing and energy management/control that will simultaneously provide optimal solutions for the accurate sizes of RES-based units that are able to incorporate short-term energy shortage with accumulators. Two options will be presented with this study: a) sizing of PV/WT-grid dependent and b) PV/WT-off grid systems. In the 1st option, the net-metering strategy will be applied and the optimal problem set-up will seek solution for sizing PV/WT hybrid systems towards satisfying a variable load demand with minimum power losses. In the 2nd option, the same strategy will be applied but in this case, the optimal sizing will take into account the use of short-term energy storage (accumulators) under a flexible energy management strategy (protecting the overutilization of charging/discharging cycles). As a reference region, two areas in Greece will be selected, Kozani at the Western Macedonia and Crete at the Southern part of Greece. In all modeling and simulation results, validated mathematical models of PV/WT units will be used for highest accuracy.

Based on the above results, this study will close by presenting a novel optimal sizing and energy management/control strategy for the operation of PV/WT systems along with hydrogen production (through PEM electrolyzers and high-pressure storage) and accumulators. As will be presented, this novel strategy can lead towards a completely optimal hybrid system with minimum power losses, minimum capital and operating expenses (CAPEX+OPEX) and satisfying both hydrogen and load demands.



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sciforum-102667: Techno-Economic Analysis of Solar-Powered Hydrogen Production in Western Algeria: Optimizing PV-Electrolyser Integration for Cost-Effective Green Hydrogen

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Hydrogen production, a promising avenue for reducing greenhouse gas emissions, is advancing through renewable energy sources. This study focuses on the techno-economic analysis of hydrogen generation using solar energy in western Algeria, a significant step toward sustainable energy solutions. The research optimised the arrangement between photovoltaic panels and electrolyzers, aiming for the most cost-effective low-energy capacity system.

A multi-objective function based on artificial intelligence was employed to ensure comprehensive analysis, seeking to maximise green hydrogen production at the lowest cost. The study considered technical aspects such as the performance of PV panels under real climatic conditions, converter and electrolyser modelling, total system expenditure evaluation, and hydrogen production costs. Simulations were conducted across several provinces in western Algeria, known for their high solar potential.

Results indicate the southern provinces have significant potential for hydrogen production at a cost of 3.022-3.106 \$/kg. In contrast, the central western region shows a slightly higher cost range of 3.1973-3.2217 \$/kg, while the northwestern part has the highest range of 3.2787-3.3452 \$/kg. These findings highlight the economic viability of hydrogen production in the southern regions. However, further investigation into transportation logistics is necessary due to the remoteness of these areas.

This study underscores the feasibility and economic potential of solar-powered hydrogen production in Algeria, contributing to the global efforts in renewable energy and sustainability.



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sciforum-104515: Advanced Virtual Synchronous Generator Control Scheme for Improved Power Delivery in Renewable Energy Microgrids

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Renewable energy and voltage source inverter-driven microgrids generally lack natural inertia to provide transient energy support during sudden load demands. Thus, the virtual synchronous generator (VSG) is a state-of-the-art control technique applied for power controllers to emulate virtual inertia during sudden load changes. This allows stable power delivery from the source to the loads during sudden active power load demands. However, in the case of large inductively dominant load demands, the VSG-based power controller's power delivery capability is relatively poor. To address this limitation of VSG control, this paper proposes an advanced control scheme in which VSG is supported by appropriately designed voltage and current controllers. Conventionally, classical tuning techniques were used to design the controllers in the forward paths of the voltage and current controllers (CVA). Accordingly, the conventional control scheme is a combination of VSG and CVA. Recently, the hybrid-modified-pole-zero-cancellation technique has been discussed in the literature for the design of voltage and current controllers (HVA) to improve the vector control of the inverter. This method supports better tuning for controllers of both forward and cross-coupling paths. Thus, to improve the power delivery with VSG-based control when subjected to inductive load changes, this paper proposes an advanced control scheme that is based on the combination of VSG and HVA. The performance of both conventional and proposed control schemes is verified through simulation in MATLAB/Simulink under two different test load conditions, namely good and poor power factor loadings. Based on the results obtained during these test cases, the response and power delivery capability of the proposed control scheme is compared with that of the conventional control scheme. From the results, it is verified that the power delivery capability of the microgrid with the proposed control scheme is improved by 25% than the conventional control scheme.



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sciforum-089070: Advancements in Spectral Remote Sensing for Aquatic Ecosystem Quality Assessment: Integrative Approaches Using Convolutional Neural Networks and Spatio-Temporal-Spectral Fusion Models

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The study meticulously explores the cutting-edge domain of spectral remote sensing technologies tailored for the nuanced monitoring of water quality across diverse aquatic ecosystems. It places a strong emphasis on the innovative integration of Convolutional Neural Networks (CNNs) and groundbreaking spatio-temporal-spectral fusion models, setting a new precedent in environmental data analytics. Through a rigorous examination, we unveil the unparalleled efficacy of spectral remote sensing in unraveling the complexities inherent in key water quality parameters, including but not limited to, the concentration of phytoplankton pigments and fluctuating salinity levels. This is achieved via the strategic deployment of sophisticated computational algorithms that dissect and interpret the intricate data derived from spectral signals. Our discourse extends to illuminate the transformative impact of satellite-based remote sensing, revolutionized by the introduction of high-resolution spectral imaging coupled with the prowess of machine learning techniques. Such advancements facilitate not only the precision but also the expansiveness of water quality assessments, encompassing vast geographical terrains with remarkable accuracy. Through a methodical comparative analysis of various inversion models, the paper delineates the subtle yet powerful capabilities of these methodologies in extracting and decoding accurate environmental data from the complex interplay of spectral signatures. Moreover, the research accentuates the critical importance of hybrid analytical models that seamlessly blend spatial, temporal, and spectral data streams. This holistic approach furnishes a more intricate and dynamic understanding of aquatic ecosystems, enabling stakeholders to navigate and manage the nuances of these environments with greater efficacy. The synthesis of avant-garde remote sensing technologies with advanced computational models encapsulated in this study not only signifies a pivotal advancement in the realm of environmental monitoring but also lays down a robust framework poised to catalyze future innovations in the sustainable stewardship of water resources.



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sciforum-102010: Air Quality Health Index and Discomfort conditions in a heatwave episode on the island of Rhodes in July 2024

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Climate conditions in combination with the concentration of pollutants increase human health stress and exacerbate systemic diseases. The city of Rhodes is a desirable tourist destination that is located in a sensitive climate region of the southeastern Aegean Sea in the Mediterranean. In this work, hourly recordings from a mobile air quality monitoring system which is located in an urban area of Rhodes city were employed in order to measure the concentration of regulated pollutants (SO₂, NO₂, O₃, PM₁₀ and PM_{2.5}) and meteorological factors (pressure, temperature and relative humidity). The Air Quality Health Index (AQHI) and Discomfort Index (DI) were calculated to study the impact of air quality and meteorological conditions on human health. The analysis was conducted during a hot summer period, from 29 June to 14 July 2024. During the second half of the studied period, a heatwave episode occurred, affecting the bioclimatic conditions over the city. The results show that despite the fact that the concentration of pollutants was lower than the pollutant thresholds (according to Directive 2008/50/EC), the AQHI and DI conditions degraded significantly over the heatwave days. In particular, the AQHI suggested a reduction in outdoor activities and the DI indicated that most of the population suffered discomfort. The AQHI and DI simultaneously increased during the days of the heatwave episode, showing a possible negative synergy for the health risk. Finally, both the day maximum and night minimum temperatures were increased (about 0.8 and 0.6 °C, respectively) during the heatwave days as compared to the whole studied period.



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sciforum-106817: Analysis of natural vaporization in LPG tanks

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At standard atmospheric pressure and temperature, the main components of liquefied petroleum gas (LPG)—propane and butane—exist in gaseous form. Moderate pressurization converts LPG into liquid form, which is suitable for storage in cylinders and tanks. When gas is required for consumption, the valve at the top of the tank opens, pressure drops, and the liquid LPG vaporizes. This natural vaporization process relies on ambient heat from the surroundings, which is transferred through the walls of the LPG tank. The natural vaporization rate depends on several factors, such as the ambient temperature, the surface area of the tank in contact with the liquid (i.e., the filling percentage), the exact composition of LPG, and the design and positioning of the LPG tank. When natural vaporization rates cannot meet the gas demand, as in the case of colder climates and large commercial applications, an additional LPG vaporizer is necessary. The literature's data on natural vaporization in LPG tanks are incomplete and ambiguous, often limited to the most prevalent conditions. This leaves engineers and designers in doubt on whether an LPG vaporizer is actually required. Therefore, the aim of this study is to provide an exact calculation procedure for the natural vaporization in LPG tanks that is capable of taking into consideration different ambient conditions, propane–butane mixtures, LPG tank designs, and the system's working conditions. Aboveground and underground installations, as well as horizontally and vertically positioned LPG tanks, are also accounted for in the present study. The analysis reveals that LPG vaporizers are necessary in situations of high demand, low-temperature environments, limited tank size, and when using butane-heavy LPG mixtures.



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sciforum-102194: Assessment of the anthropogenic load levels of heavy metals: a case study on the example of the Styr River

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Introduction: The increasing levels of heavy metals in natural waters pose significant environmental and health risks. This study focuses on the Styr River, particularly in the area affected by cooling water discharge from the Rivne Nuclear Power Plant in Ukraine. The primary aim is to analyze the distribution and sources of eight heavy metals: Zn, Cd, Pb, Cu, Ni, Mn, As, and Cr.

Methods: Monthly water samples were collected from 2018 to 2022 and analyzed using an inductively coupled plasma mass spectrometer (ICAP 7400 Duo). The analytical lines used were Zn (213.857 nm), Cd (226.502 nm), Pb (220.353 nm), Cu (324.754 nm), Ni (231.604 nm), Mn (257.610 nm), As (193.696 nm), and Cr (267.716 nm). Calibration was performed with standard solutions, and results were checked against internal quality standards. Statistical analyses included Pearson correlation and cluster analysis to identify relationships and potential sources of heavy metals.

Results: The average concentrations of heavy metals in the Styr River water followed the sequence: Cu > As > Zn > Mn > Ni > Cr > Pb > Cd. Seasonal and annual variations were observed, with notable decreases in Zn, Cu, and Mn in 2021, likely due to reduced anthropogenic activities. Pearson correlation and cluster analysis revealed distinct patterns, suggesting both natural and anthropogenic sources. Heavy metals like Pb, Cr, and Ni were associated with industrial emissions and urban pollution, while Cd and As showed more isolated sources. Despite the presence of these metals, their concentrations did not exceed the allowable limits set by the Council Directive 98/83/EC for drinking water.

Conclusions: This study provides a comprehensive assessment of heavy metal pollution in the Styr River. The findings indicate that the water quality remains within safe limits for human consumption, although continuous monitoring is essential. The results highlight the complex interplay of natural and anthropogenic factors influencing heavy metal levels, emphasizing the need for sustainable environmental management practices.



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sciforum-107162: Bibliometric analysis of renewable energy resources in the context of extreme weather event: Case megadroughts

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Introduction

The global energy transition towards renewable sources is a critical challenge to mitigate the effects of climate change. With an energy system highly dependent on hydropower, Chile faces a unique challenge due to the megadrought that limits water resource availability. This situation drives the need to diversify the energy matrix with non-conventional renewable sources, such as solar and wind energy, to reduce vulnerability to extreme weather events.

Methodology

This study conducts a bibliometric analysis to identify the main research lines on using renewable energy resources in megadrought. The search was carried out in the Scopus database using critical terms related to renewable energies, drought, and the optimization of photovoltaic and wind plants. Data were analyzed using Bibliometrix and VOSviewer, generating co-authorship, keyword, and publication networks. After applying exclusion filters, 82 documents were selected, and a quantitative and qualitative analysis of the results was conducted.

Main Results

The bibliometric analysis showed an exponential increase in the scientific production of renewable energies over the last six years. The most studied areas include solar energy (26.83%), climate change (29.27%), and renewable energies in general (25.61%). The most relevant keywords were "renewable energy," "solar energy," and "wind energy," reflecting the focus on energy diversification and the search for solutions to water scarcity. China and the United States lead scientific output, with Stanford University and Nanjing University being among the top institutions.

Main Conclusions

This study highlights the importance of non-conventional renewable energies in Chile's energy matrix, especially in prolonged droughts. The integration of solar and wind technologies offers high potential to mitigate the impacts of climate change and ensure the country's energy security. Further research on optimizing these energy sources and policies that promote the energy transition and reduce dependence on vulnerable water resources is needed.



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sciforum-107243: Bland-Altman Analysis of Open-Access Online Weather Data

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Solar radiation data is essential for evaluating solar energy potential; designing, optimizing and developing predictive models for solar energy systems; and other applications. While weather stations provide reliable data, their high installation and maintenance costs lead to data gaps in many regions. Satellite-derived data presents a cost-effective alternative, offering broad coverage. However, satellite-derived data require continuous evaluation to prove them as reliable substitutes for ground measurements. This study compared satellite-derived (SD) solar irradiation data from two sources, NASA's POWER and PVGIS, against ground-measured (GM) data from the World Radiation Data Centre (WRDC). The comparison relied on data from 171 WRDC stations spanning 2005 to 2020. The Bland-Altman method was the primary statistical measure used because of its ability to determine agreement between data sources and identify systematic bias; this involved constructing Limits of Agreement (LOA), within which the most differences between the two data sources are expected to lie. Additional statistical measures, including r-correlation, root mean square error analysis, and t-value analysis, were employed to validate the BA findings and to investigate the influences of latitude, diurnal periods and annual seasons on the agreement between the SD and GM data. The results of the study showed that, when compared with the WRDC data, the POWER data exhibited limits of agreement (LOA) of 0.45 ± 4.78 MJ/m²/day, while PVGIS data had LOA of 0.47 ± 5.11 , with the range of LOA being 9.55 and 10.23, respectively. In addition, distinct relationships between the range of LOA and latitude and season were visually identified from the plots, indicating that these factors affect the agreement between the SD and GM data. The narrower LOA range of the POWER data suggested it to be the more reliable substitute for GM data.



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sciforum-104314: Circularity assessment of municipal waste management scenarios using a MFA-LCA based approach: A case study in Brazil

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One of the critical elements of the so-called circular green transition is to move from waste minimization to materials circularity, i.e. to implement a systems engineering approach in which the residues of a process are not seen as waste but as a resource to another process of an integrated circular economy network. So, this study aims to apply a circularity assessment of municipal waste management scenarios combining Life Cycle Assessment (LCA) and Material Flow Analysis (MFA) approach. Four scenarios were considered: scenario 1: the existing conditions of the system, scenario 2: based on recovery of the organic fraction by composting, scenario 3: focused on the circularity of the organic fraction by anaerobic digestion, scenario 4: using recycling and incineration. The LCIA approach used was CML 2001. The circularity of each scenario was compared in terms of materials and energy recovery and effect of circularity solutions in the impact categories. A multicriteria analysis was used to aggregate the results of circularity in all impact categories and obtain a ranking of scenarios to determine the final result. From the results it could be noted that even if the three considered scenarios correspond to a significant improvement compared to the base scenarios in terms of materials recovery, scenario 4 was ranked in first place as it results in both materials and energy recovery rates higher than the others. Moreover scenario 4 also has less impacts related to the emissions involved during the biological processing of the organic fraction, mainly eutrophication and acidification potential. So, the LCA approach was shown to be an efficient way to support circular economy assessment by providing a more holistic circularity overview than considering only MFA.



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sciforum-104340: Comparative assessment of the toxicity of bisphenol A and its alternatives: an in vitro study

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Plastic additives comprise many substances that serve numerous purposes in the plastic industry, such as assisting in the moulding of plastics and improving optimal performance. One of the bisphenols, namely, bisphenol A (BPA), is a widely used additive in the plastic industry and is now restricted by the European Union due to its proved toxicity. This additive is being replaced by analogues such as bisphenol E (BPE) and bisphenol Z (BPZ). However, there is a need to better understand their potential toxic effects to validate if they constitute safer alternatives. Thus, this study aimed at making a comparative assessment of the cytotoxicity of BPA, BPE, and BPZ to amphibian cell lines (A6 and XTC-2 - cell lines of *Xenopus laevis*), as Amphibia is the class of vertebrates with the highest proportion of species threatened with extinction. The cell lines were exposed for 24 h, 48 h, and 72 h to eight concentrations of each bisphenol and cell viability was assessed through each time point. Overall, the median lethal concentrations (LC₅₀) revealed that A6 cells are more sensitive to these chemicals than XTC-2. The obtained data support the premise that BPE and BPZ are less toxic to amphibian cell lines than BPA. Thus, based on the 72h LC₅₀, the cytotoxicity can be ranked as BPA>BPZ>BPE (45.48 mg/L, 57.1 mg/L, and 64.7 mg/L, respectively) for XTC-2 cells. A similar trend was observed for A6 cells (24.6 mg/L, 32.1 mg/L, and 41.6 mg/L for BPA, BPZ, and BPE, respectively). Thus, the data support that these BPA alternatives appear less toxic, but more studies must be performed and other endpoints assessed to fully understand their highest environmental safety.



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sciforum-104252: Comparative Life Cycle Assessment of Ultra-High Performance Concrete with Graphene Oxide

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Several studies have been conducted on Ultra-High Performance Concrete (UHPC) to enhance the mechanical properties of this construction material, but the benefits of this new material to the natural environment is still to be assessed. So, this study aims at comparing the environmental impacts of conventional concrete and UHPC with graphene oxide (GO) by applying life cycle assessment (LCA). Four scenarios were considered in the LCA: (1) conventional concrete, (2) UHPC without graphene, (3) UHPC with a low content of GO, and (4) UHPC with a high content of GO. The compression strength for these scenarios was 30 MPa, 160 MPa, 160 MPa, and 180 MPa, respectively. The LCA was carried out in four phases: goal and scope definition, Life Cycle Inventory (LCI), Life Cycle Impact Assessment (LCIA), and Result Interpretation. For impacts per m³ of concrete produced, scenarios with UHPC (scenarios 2, 3, and 4) led to a much higher environmental impact (2,5 times higher) for most of the impact categories compared to conventional concrete results (scenario 1). For impacts per MPa of compression strength, the UHPC scenarios showed a much lower environmental impact than scenario 1. Notably, the higher strength UHPC, with the higher content of GO (scenario 4), resulted in a lower environmental burden due to a higher increase in strength due to the GO addition compared to the increase in impact. Therefore, UHPC with GO has a high potential to support more environmentally friendly construction if it results in less demand for concrete.



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sciforum-104406: Designing and Testing of a Solar Charging Station for Micro-Mobility, Portable Devices and Energy Education

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The urgent need for sustainable energy solutions, particularly in addressing urban mobility challenges and promoting environmental stewardship, has underscored the critical importance of integrating renewable energy sources. This necessity is especially evident in underrepresented communities, where access to renewable energy education and resources remains limited. To address this disparity, the development and deployment of a Solar Charging Station for Micro-Mobility, Portable devices and Renewable Energy Education represents a significant stride forward. The project is a collaborative initiative between the University of Texas at Tyler and Houston Community College, aiming to serve the Greater Houston area. The project consisted of three main phases: feasibility study, design and construction, and operation and evaluation. The solar charging station uses a solar panel with maximum 300 W and maximum of 45 degree tilt, a set of batteries of up to 1000 Wh, a solar charge controller, a power inverter, and a data acquisition system to harness solar energy and convert it into electrical energy for charging various devices of up to 500 W. The system successfully addressed the functionality to be used in the educational setting and looks energy gaps in disadvantaged communities by providing clean energy alternative as well as enhance educational opportunities in the areas of science and engineering. **Community-Based Renewable Energy Innovation:** The project pioneers a localized approach to renewable energy deployment by addressing both the technical challenges of integrating solar power into everyday life and the social impact of clean energy access. Its focus on combining energy generation using a charging station in an underserved area presents a novel approach to utilizing solar energy as part of a community infrastructure, potentially contributing to new frameworks for community-based renewable energy systems.



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sciforum-104564: Detection and Mitigation of hazards using advanced sensor technology with decision making system

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Pollution makes our environment endangered; the pollutants present in the air, such as N₂O, S₂O, CO, etc., affect living things and cause climatic changes in our environment. This leads to an increase in mortality rates and economic burdens. In order to address the above challenges, a new design of an IoT-powered air pollution monitoring system is introduced. This design utilizes an advanced sensor that monitors the harmful gases present in the air continuously. Furthermore, the proposed design incorporates a Kalman filter supported by an AI architecture that enhances the data accuracy and real-time processing by refining sensor data. The AI structure triggers the automatic response once it detects hazardous conditions; further, the automated response activates the instant alert and ventilation system that are placed in the proposed design. This increases safety and provides protection to the surroundings. The IoT system supports continuous data transmission from the sensor to the cloud; this enables seamless monitoring and time-to-time decision-making. Based on the predefined index, the proposed model predicts the air quality with three conditions: good, moderate, and danger. After air quality observation, the proposed system alerts the pollution control board for further action. The preliminary result obtained from the proposed model shows a significant improvement in the data accuracy and response time compared to conventional methods.



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sciforum-106583: Deterioration of cement-based materials in wastewater treatment plant facilities- A comparison between sewage gases and sewage liquid exposure environments

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Cement-based materials are preferred in constructing various infrastructures including wastewater treatment plants (WWTPs) due to their durability, low processing cost, and watertightness. However, the increasingly reported maintenance in many cement-based WWTP facilities is raising concerns about their performance in aggressive environments such as WWTPs. Wastewater contains different chemical substances (e.g., sulfates, organic compounds, and nitrates) which have known deterioration effects on cement performance. Still, less is known about the deterioration process occurring on cement-based materials exposed above sewage line and submerged in sewage liquid.

This study aimed to understand the difference in cement deterioration between submerged and above sewage structures in WWTP facilities. This was an in-situ experiment that involved 23 specimens of ordinary Portland cement. The specimens were exposed to above sewage in the pumping station and below sewage in sand-trap structures. The specimens were exposed for different durations: 30, 75, and 24 days. After exposure, specimens were analyzed. The analysis involved material physical observation (using stereo microscopy), morphology (SEM), and mineralogical analysis (using XRD).

The results of our study show that (a) specimens exposed to sewage gases had a notable physical change compared to those submerged in sewage liquid in sandtrap locations. (b) SEM-SE images show that specimens from sewage gases had massive spongy and prismatic needle crystals, whereas, in sewage liquid, specimens showed little or no such morphologies. (c) These crystals observed in samples from sewage gases in the pumping station were confirmed by XRD to gypsum ($\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$), ettringite ($3\text{CaO} \cdot \text{Al}_2\text{O}_3 \cdot 3\text{CaSO}_4 \cdot 32\text{H}_2\text{O}$), and thaumasite ($\text{CaSiO}_3 \cdot \text{CaCO}_3 \cdot \text{CaSO}_4 \cdot 15\text{H}_2\text{O}$) minerals. These minerals are secondary minerals in cement and are characterized by high volume expansion and their presence in hydrated concrete results in volume expansion crack formation. These results suggest that cement-based concrete above sewage line are more prone to deterioration than those submerged in sewage liquid.



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sciforum-104349: Early-life stage exposure to the antidepressant paroxetine compromises later-life behavioural phenotypes and animal fitness

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Intraspecific behavioural variability (e.g., coping styles) ensures an optimal adaptive response to environmental stressors. These individual stress-coping skills are expressed along a fundamental axis of behavioural variation, the bold-shy continuum. Exposure to neuroactive compounds intended for human use, like paroxetine, may affect behavioural phenotypes, through action on evolutionarily conserved neurological pathways found in humans and other species, such as teleost fish, even at low doses. Although paroxetine is prevalent in water systems worldwide at concentrations in the ng/L range there is no available data on its influence on fish coping styles. Accordingly, this study aimed to assess if early exposure (up to 48 hours post fertilisation (hpf)) to PAR environmental levels (0.04 and 0.4 µg/L) may compromise zebrafish's (*Danio rerio*) bold and shy behavioural phenotypes at later-life stages (larval and juvenile). The obtained data show that both larval and juvenile stages are sensitive to early-life PAR exposure, as differences between bold and shy behavioural profiles were lost at 8dpf (larval stage) and 45dpf (juvenile stage) for basal swimming activity and stress response (e.g. total swimming distance, inactivity time, thigmotactic behaviour, boldness). These results highlight the need for further studies to understand the ecological implications of these behavioural phenotype modifications.



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sciforum-099026: Earthquake Potential Zones Identification using MCDA, Machine Learning and Geospatial Techniques in Sikkim

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Sikkim, nestled in the North-Eastern Himalayas, is a region frequently disturbed by earthquakes and are triggered by a myriad of factors, including tectonic plate movements, volcanic activities, subterranean explosions, human-induced quakes, and environmental conditions. This leads to loss of human lives, destruction of human properties and deformation of earth crust plates. The study aims to refine earthquake vulnerability assessment by incorporating Machine Learning Weighted Overlay methods over traditional Analytical Hierarchy Process (AHP) techniques. Unlike AHP, where users assign weightage based on their knowledge, ML models use feature importance for objective weightage assignment. A comprehensive set of parameters—fault characteristics, peak ground acceleration, earthquake magnitude, proximity, slope, and elevation which previous studies were somewhere lacking in their study. These parameters are weighted and superimposed using the AHP method. We used Google Earth Engine (GEE) to facilitates the extraction of weighted stacked images, which are then analyzed to pinpoint earthquake-prone locations via machine learning models, namely Random Forest and SmileCart classification. The earthquake vulnerability zones are stratified into five distinct categories: Very High (4.54%), High (28.37%), Medium (27.84%), Low (23.60%), and Very Low (15.65%). The Random Forest and SmileCart models outperformed the AHP method, yielding accuracies of 0.89 and 0.78, respectively, compared to 0.57 for the AHP approach by the validation points and ROC Curve/AUC values corroborate these findings, with respective scores of 0.71, 0.75, and 0.60. The integration of advanced machine learning algorithms over conventional AHP methods significantly enhances the precision of seismic susceptibility estimations. This synergy illustrates the potential of modern analytical techniques in the realm of natural disaster risk evaluation.



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sciforum-104337: Ecotoxicity of a mixture of polyhydroxybutyrate (biological-based) and polymethylmethacrylate (petroleum-based) micro(nano)plastics: implications for the physiology and behavior of *Danio rerio*

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There has been a recent trend to replace petroleum-based plastics with greener and more sustainable alternatives, such as bio-based ones. During this transition, there is a high probability that both types of polymers will be encountered and interact in environmental matrices. An integrated ecotoxicological test, that is, covering standard physiological parameters, such as mortality or growth, with behavioural characteristics, can be extremely important to understand the potential environmental and human impacts of these mixtures. This study aimed to evaluate the effects on *Danio rerio* embryonic-larval stage of exposure to micro(nano)plastics of polyhydroxybutyrate (PHB-MNPLs) and polymethylmethacrylate (PMMA-MNPLs) at concentrations of 0.1, 1, 10, 100, and 1000 µg/L on a full cross design. A control group was also included. Generally following the OECD 236 Fish Embryo Toxicity (FET) adapted for a period of 120 hours, the following endpoints were observed: mortality, malformations, heartbeats (only at 48 hours), hatching rate (starting at 48 hours), and overall length (at 120 hours). At 120h of exposure, the total time active, the total distance swum, thigmotaxis behaviour, and trajectory angles were analyzed.

The individual exposure to PHB-MNPLs and PMMA-MNPLs had no impact on mortality, malformations, or hatching rates of *D. rerio*. The PMMA-MNPLs alone induced tachycardia at 100 and 1000 µg/L and reductions in larvae length at concentrations between 0.1 and 100 µg/L. The PHB-MNPLs induced effects on fish swimming-related parameters, similar to those induced by PMMA-MNPLs (decreased total time active under light periods; decreased high amplitude movements at 0.1-10 µg PHB-MNPLs/L. These effects were also observed at 100 and 1000 µg PMMA-MNPLs/L under light periods. The mixture of both polymers induced patterns of response different than those observed for both MNPLs alone (e.g., in heartbeat rates and swimming parameters). This study highlights the need to Assess the effects of combined nanoparticles of different polymers.



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sciforum-103843: Effects of halogens and alkali metals on guanidinium/ethylammonium-doped perovskite photovoltaic devices

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Perovskite solar cells are expected to be alternative materials to silicon solar cells because of their high conversion efficiencies and easy device fabrication with various compositions. Recently, research is being conducted to develop low-cost and flexible devices. For the typical $\text{CH}_3\text{NH}_3\text{PbI}_3$ perovskite, CH_3NH_3 (MA) migration and high reactivity have a significant impact on instability and low durability in the atmosphere. To solve this problem, research has been conducted to improve crystal stability by introducing elements and molecules into perovskite crystals. Among organic molecules, guanidinium (GA), which has three different resonance structures and is stable, and ethylammonium (EA), which has a larger ionic radius than MA, will contribute to crystal stabilization by introduction into the crystal lattice. Additionally, alkali metal cations are expected to be difficult to desorb due to their inorganic nature. In this study, effects of substitution of halogen anions and addition of alkali metal cations for GA/EA-doped perovskite solar cells were investigated by fabricating devices and comparing their photovoltaic properties. The halogen compositions of the additives were found to contribute to the improvement of preferred orientations of perovskite crystals, and the order of the effectiveness was I, Cl, and Br. In addition, the addition of alkali metal cations contributed to improvement of the conversion efficiencies, and addition of a small amount of cesium at the MA site was the most effective. It was also found that the short-circuit current densities and fill factors depended on the (100) preferred crystal orientation of the perovskite compounds.



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sciforum-103299: Efficacy Of Ozonation As A Method Of Decontamination Of Hydrocarbons In Seawater

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Rising maritime traffic and activities have caused oil pollution of the marine environment to increase considerably in recent decades, with illegal dumping of bilge water from ships being one of the main sources of this type of pollution. Numerous studies have established that the main hydrocarbons found in seawater are *n*-alkanes from diesel and polycyclic aromatic hydrocarbons (PAHs). This source of pollution could be reduced through the installation, on the vessels themselves, of systems that allow the degradation of hydrocarbons. Advanced oxidation processes are of great importance as techniques for the degradation of organic pollutants, among which ozonation stands out. In this context, the aim of this work was to establish the effectiveness of ozonation to oxidise *n*-alkanes contained in diesel and PAHs declared by the EPA as priority pollutants in seawater. For this purpose, artificial seawater was prepared and contaminated with one of the two types of hydrocarbons of interest and the samples were then subjected to an ozonation process. After ozonation, the samples were extracted by SPME and then analysed by GC-MS. The results show that, under the conditions of this study, ozone was able to degrade 94.6% of the total PAHs in only 60 minutes, however, longer ozone exposure times (720 minutes) were needed to degrade 87.3% of the total *n*-alkanes present in the medium. It is noteworthy that, for both, PAHs and diesel, only 100% oxidation of the lower molecular weight compounds was achieved, therefore for the heavier compounds more aggressive oxidation conditions should be applied.



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sciforum-102136: Evaluation of Corncob Pellets: Drying Methods, Densification, and Energy Potential

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Growing concerns about environmental pollution and climate change are driving the use and research of renewable energy sources. One possible solution is the use of biofuel derived from agricultural waste. Corn is one of the primary crops grown in the agricultural sector, generating large amounts of waste after harvesting and industrial use. This study focuses on the drying of corncocks, the evaluation of their properties before densification into pellets, the densification process, and the assessment of their suitability for energy needs.

The research found no significant difference between drying with active ventilation in a dryer and drying under outdoor conditions. The optimal moisture content for the pellets is 12.39%, with a compression coefficient of 3.43 ± 0.011 , and the highest pellet density of $1012.96 \pm 3.35 \text{ kg/m}^3$. The change in pellet density at optimal moisture content is minimal at 0.78%. The compression coefficient of pellets produced using a granulator with a horizontal matrix is 9.75% higher than those made with a laboratory automatic press. The lower heating value of corncocks is $17.35 \pm 0.14 \text{ MJ/kg}$, with an ash content of $1.78 \pm 0.24\%$. The produced pellets are sufficiently durable and suitable for combustion. This study can help better understand the properties of corncocks and their potential in the energy sector. By mastering preparation techniques and optimizing raw material moisture during compaction, as well as through ongoing research, biofuel preparation technologies can be refined to enhance efficiency, reduce production costs, and minimize environmental impact.



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sciforum-103522: Evaluation of ecotoxic effects of PFOS, PFOA, and their mixture on aquatic organisms

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Per- and polyfluoroalkyl substances (PFASs) are man-made chemicals with high persistence, that are utilized in numerous consumer and industrial applications. The most well-known substances of this group are perfluorooctane sulfonic acid (PFOS) and perfluorooctanoic acid (PFOA). They are used in various products such as non-stick cookware, textiles, paint, firefighting foams, surfactants, food packaging, and personal care items. Due to their extensive usage, they are frequently detected in water sources globally, with PFOS's reported concentrations reaching 187 and PFOA's 1371 ng L⁻¹. PFOS and PFOA have also been reported in all levels of aquatic life. Indicatively, PFOS has been found in *Crassostrea virginica* in concentrations up to 1225 ng g⁻¹ (dw) and PFOA in *Sebastes mentella* at 5.3 ng g⁻¹ (dw). As PFASs are widely detected in the environment, they may induce toxic effects on a variety of aquatic organisms, and thus their investigation is crucial.

The present study aimed at investigating the potential toxic effects of PFOS and PFOA (individually), as well as those of their mixture, on a saltwater microalga and a bacterium. The tested organisms were exposed to different concentrations of the studied compounds, and the growth inhibition percentages, alongside the IC₅₀ values, were calculated. The microalga and the bacterium presented different sensitivities to the target compounds. The mixture of PFOS and PFOA presented more adverse effects in comparison to the individual compounds in the bacterium. Dissimilarly, the highest effect on the microalga was observed when the organism was exposed to PFOA.



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sciforum-101741: Evaluation of Internal and External Radiation Exposure Doses from Concrete Samples Using a Computer Code (RESRAD-Build)

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Building materials naturally contain radionuclides, potentially leading to internal and external radiation exposure in human dwellings. This study collected and analyzed data on natural radionuclides such as Ra-226, Th-232 and K-40 in concrete samples from 16 countries worldwide. Internal and external doses for these concrete samples were estimated using the RESRAD-BUILD computer code. The RESRAD-BUILD model facilitates the evaluation of radiation exposure over a 70-year period, providing insights into the long-term health effects. The calculated long-term effective doses showed variations in external and internal doses over the years and among countries. The variations among countries underscore the importance of considering each country's geographical location and geological characteristics when establishing norms and guidelines related to emitted radiation limits from building materials.

These findings highlight the need for continuous monitoring of commonly used building materials, especially as radiation exposure is likely to increase in the near future due to the growing use of recycled materials and materials formerly considered waste in the building industry. Environmental quality, both indoor and outdoor, is crucial for human well-being and can serve as an indicator of human development, particularly since the majority of the population spends almost 80% of their time indoors. Therefore, measuring and controlling natural radiation in buildings is of great interest for ensuring human safety.



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sciforum-106664: Geographical distribution of fluorine containing contaminants in the Hungarian section of the Danube River

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Per- and polyfluorinated alkyl substances (PFAS) have gained significant attention due to their persistence in the environment and potential bioaccumulative effects on ecosystems and human health. Specifically, perfluorooctanoic acid (PFOA) and perfluorooctanesulfonic acid (PFOS) have been widely detected in European rivers, leading to restrictions on their use. A 2015 study of the Danube River reported PFOA concentrations of 5–40 ng/L and PFOS concentrations of 5–30 ng/L. To evaluate the impact of these restrictions, this study measured the concentrations of PFOA and PFOS using UHPLC-QTOF systems, revealing a decreasing trend in their levels compared to earlier data.

Simultaneously, the growing demand for new organofluorine chemicals, particularly in lithium-ion battery production and the agrochemical and pharmaceutical industries, poses additional challenges. Municipal wastewater treatment plants are generally ineffective at removing these resistant fluorine-containing contaminants. To assess the fluorine content in riverine environments, the inorganic fluoride and total organofluorine concentrations in the dissolved water phase must be determined.

This study was focused on the analysis of PFAS compounds in water samples collected monthly from July to December 2023 at twelve sampling sites along the Hungarian section of the Danube River. Inorganic fluoride concentrations ranged from 28–106 µg/L, with a median of 45.3 µg/L, while total organofluorine concentrations ranged from 0.22–12.5 µg/L, with a median of 2.43 µg/L. The findings highlight the ongoing presence of fluorine-containing contaminants in the Danube River, despite regulatory efforts to reduce PFAS levels. These results underscore the need for continued monitoring and the development of more effective wastewater treatment technologies to address emerging environmental challenges.



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sciforum-106894: Glucan production by *Rhodotorula* yeasts and phenolic content reduction in olive mill wastewaters under nitro limited conditions

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Olive mill wastewaters is one of the most difficult wastewaters to treat in the agricultural industry due to its chemical composition, especially its phenolic content. In this study, *Rhodotorula* yeast strains were examined for their ability to reduce the phenolic content of the influent but also for their ability to produce glucans. *Rhodotorula diobovatum* EXF-6843, *Rhodotorula kratochvilovae* Hamam. 1988 EXF-3471, *Rhodotorula mucilaginosa* EXF-8984 and *Rhodotorula toruloides* NRRL Y-27012 were cultivated in sterile shake flask fermentations under nitro-limited conditions (C/N=120, glucose equivalents) in wastewater from olive mills with a phenol content of $\text{pH} = 3.2$ g/L including a blank fermentation in distilled water by *Rhodotorula toruloides* NRRL Y-27012. The results showed the maximum total glucan production: *Rhodotorula toruloides* NRRL Y-27012 (blank) - 1.75 g/L at after 96 hours, *Rhodotorula toruloides* NRRL Y-27012 (OMW) - 0.97 g/L (44.81% phenol reduction) after 76 hours, *Rhodotorula kratochvilovae* Hamam. 1988 EXF-3471 - 1.19 g/L (46.71% phenol reduction) after 48 hours, *Rhodotorula mucilaginosa* EXF-8984 - 0.77 (66.02% phenol reduction) after 96 hours and *Rhodotorula diobovatum* EXF-8984 - 1.15 g/L (62.93% phenol reduction) after 72 hours. In summary, the results suggested that glucan production by *Rhodotorula* yeasts, can be optimized by fermentation conditions (carbon/nitrogen source, C/N, pH, temperature, etc.), and the phenol reduction were at a very satisfactory level, making them suitable to develop potential biological recovery technologies for phenols from olive mill wastewater.



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sciforum-107270: Heatwaves and power peaks: Analyzing Croatia's record electricity consumption in July 2024

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This study investigates the unprecedented electricity consumption in Croatia, which was driven by an intense heatwave in July 2024. Daytime temperatures consistently exceeded 30 °C, and the intense tourist season caused air conditioning usage to skyrocket. The previously recorded maximum from August 2023 was surpassed on several occasions during July 2024. In the evening hours of July 17, 2024, a new record high demand of 3381 MW was recorded. More troublesome, in the hours of high demand, about 50% of the electricity had to be imported because domestic power plants could not generate the entire demand. As a consequence, electricity prices went up to 480 EUR/MWh, four times the daily average price in Croatia. In response to power peaks and increased electricity imports, Croatia has intensified efforts to expand the share of renewable energy in the electricity mix. From 44.8% in 2020, the share of renewables increased to 58.5% in 2023. This marks a significant increase, mostly driven by the expansion of the wind and solar markets. However, as of 2023, Croatia's per capita electricity generation from wind and solar PV combined was 676 kWh per person, which is only about half the EU-27 average (1410 kWh per capita). Croatia and Southern Europe alike will continue to experience hotter summers, and power systems will have to handle higher peak loads. As the energy system transitions to a larger share of renewables, power grid flexibility will become crucial. Flexible power generation could be used to fill gaps in the renewable output. Pumped hydro and batteries could store excess renewable energy and release it during demand peaks. Demand response is another option, as shifting electricity usage to periods when wind and solar generation are high could help adapt to their intermittent nature.



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sciforum-103497: Leveraging RFID for Road Safety Sign Detection to Enhance Efficiency and Notify Drivers

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With exponentially growing pollution along with unfavorable natural conditions like snow and fog, the menace of road accidents has increased because most people will not be able to clearly view the safety board signs. Furthermore, it generally gets collected in most western countries which enhances the hindrance of these essential signs. The proposed solution makes use of Radio Frequency Identification (RFID) technology with the help of IoT to forward real-time warning messages to the drivers. In this system, an RFID reader is attached inside a vehicle and passive RFID tags are mounted on road safety signboards. If a vehicle falls in the range of the tag, it permits its reader to transmit the message alert of the tag towards the reader that then shows the warning to the driver. Hence, the system reduces the risk of accidents in harsh environments. The system has multi-lingual audio alerts, which it transmits through speakers and gives visual notice through a display screen; the multilingual audio output can be exploited to break the language barrier between various regions. The use of solar panel makes the system more energy efficient. This enhances road safety significantly and uses traditional signboards on roads along with RFID technology. Use of modules such as GPS and GSM modules allows for real updating of a vehicle's location in the cloud and, therefore, enhanced warnings and prevention of accidents. Besides this improvement in road safety, this solution also ensures environmental sustainability possibly by reducing emissions because of accidents and wastage of resources. The data collected through this system has been useful in studying the pattern of traffic and thereby adding towards more efficient and environmentally benign transportation systems. Quick and accurate notification to the driver aids in developing intelligent vehicle networks to make roads safer and sustainably used.



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sciforum-107831: Leveraging Technology To Optimise Tertiary Education Trust Fund Building Projects For Public Universities In Delta State Nigeria

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Public tertiary institutions in Nigeria have been beneficiaries of the Tertiary Education Trust Fund (TETFUND), aimed at enhancing the quality of education by providing essential structures. The TETFUND is a government agency in Nigeria, established by an Act in 2011 to provide financial support to public tertiary institutions in the country. Despite this initiative, many projects encounter setbacks such as budget overruns and suboptimal resource allocation, leading to uncompleted or abandoned building construction projects. Deployment of technologies has enhanced the concept of intelligent construction, which has impacted the processes of building construction. These stalled projects hamper the universities' ability to expand infrastructure, improve educational quality, and accommodate growing student populations.

Identifying the root causes of project abandonment and exploring the potential role of technology in addressing these issues is crucial for utilizing available funds. This study examines how technology can enhance the efficiency and transparency of TETFUND construction projects in public universities in Delta State, Nigeria. The research methodology to be adopted is a descriptive approach where a review of the literature would be performed and advantages drawn from them. The focus was on TETFUND-sponsored buildings randomly selected from the research population. Technology can enhance the projects by optimizing material usage, reducing waste, and improving energy efficiency, thus contributing to more sustainable university campuses. TETFUND building construction projects involve multiple stakeholders, including Architects, Project Managers, Contractors, Academia, Universities, and TETFUND. Understanding how leveraging technology impacts these stakeholders can help improve collaboration and communication throughout the project lifecycle.

Keywords: artificial intelligence



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sciforum-097973: Methods for Processing Signal Conversion in Velocity and Acceleration Measurement Considering Transducer Characteristics

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This study presents an innovative approach to processing vibration signals in bridge structures, focusing on enhancing the accuracy of dynamic response measurements and structural health assessment. The research addresses the critical challenges in signal processing, particularly the uncertainties in determining filtering parameters for isolating dynamic components from static displacements.

A novel method for adaptive filter parameter selection is proposed, taking into account the variability of resonant frequencies and the non-linearity of quasi-static displacements due to moving loads. This approach significantly reduces errors in determining forced and natural vibration parameters, leading to more accurate assessments of the bridge's mechanical characteristics.

The study introduces an optimized algorithm for processing acceleration and velocity signals, improving the resolution in identifying natural frequencies of the structures. This method combines traditional Fast Fourier Transform (FFT) techniques with an innovative approach to spectral analysis, enabling more precise identification of resonant frequencies and damping coefficients.

A comprehensive evaluation framework is developed, integrating the analysis of vibration amplitudes, frequencies, and damping ratios. This framework provides a more robust assessment of the bridge's structural health, enhancing the ability to detect and characterize potential defects or changes in load-bearing capacity.

The practical value of this research lies in its application to real-world bridge diagnostics. Guidelines for sensor selection and configuration are provided, tailored to different bridge types and sizes. The proposed methods demonstrate significant improvements in the accuracy of dynamic coefficient determination and overall structural assessment, potentially reducing maintenance costs and enhancing safety.



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sciforum-096341: Natural Hazards and Spatial Data Infrastructures (SDIs) for Disaster Risk Reduction

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When there is an absence of or no implementation of measures targeting disaster prevention, natural hazards can be promptly converted into disasters. An essential part of disaster risk management is the geospatial modelling of devastating hazards, where the polygon shapefiles containing the extent, time period and cause of various disastrous events are significant input datasets in the context of early-warning systems. However, equally important are Earth observation satellite data for constructing remote sensing indices, a high-resolution digital elevation model, updated land cover data, socio-economic data like demographics and spatially referenced data, such as wind characteristics, temperature and precipitation. This research work points out the usefulness of Spatial Data Infrastructures (SDIs) in disaster risk reduction through a literature review, focusing on the necessity of data unification and disposal. Initially, the principles and implementations of SDIs are presented, and subsequently, their benefits for achieving the specific targets and priorities of the Sendai Framework for Disaster Risk Reduction 2015-2030 are elaborated. Thereafter, the challenges in SDIs are investigated in order to underline the main drawbacks the stakeholders in emergency management have to come up against, namely a lack of semantic alignment, which induces a time-consuming data search, and malfunctions in the interoperability of the datasets and web services, the non-availability of the data in spite of their existence and a dearth of quality data. Thus, diachronic observations on disasters will not be found, despite these comprising a meaningful dataset in disaster mitigation. Consequently, recommendations for an efficient SDI that is geared towards natural hazards are proposed to the involved participants for the purpose of disaster preparedness. SDIs constitute an ongoing collaborative effort intending to offer valuable operational tools in decision-making under the threat of a devastating event. Notwithstanding the functionality of SDIs, data collection is an intricate task.



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sciforum-107735: Optimization and Energy Efficiency in the Separation of Butadiene 1,3 from Pyrolysis Products: A Model-Based Approach

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The separation of Butadiene 1,3 from pyrolysis products is a critical step in the petrochemical industry, as Butadiene is a key raw material for producing synthetic rubber and other polymers. This study presents a detailed model-based analysis of the separation process, focusing on optimizing operational parameters to maximize butadiene recovery, enhance product purity, and reduce energy consumption. The simulation was conducted using Aspen Plus, evaluating critical variables such as the solvent-to-feed ratio, reflux ratio, number of column stages, and energy integration between distillation units. The simulation results indicated that an optimal solvent-to-feed ratio of 1.5:1 and a reflux ratio of 4.2:1 in the extractive distillation column provided the highest separation efficiency. Under these conditions, the recovery rate of Butadiene 1,3 reached 98%, with a final product purity of 99.5%. Furthermore, the study revealed that increasing the number of theoretical stages in the distillation column improved the separation process without significantly increasing energy demands. Energy integration between the primary distillation and extractive distillation columns led to a 12% reduction in total energy consumption. These findings demonstrate the importance of fine-tuning operational parameters to achieve high separation efficiency and product quality while minimizing energy use. This model-based analysis provides valuable insights into the design and optimization of industrial-scale butadiene separation processes, offering strategies to reduce operational costs and improve sustainability in production. The methodology and results can serve as a basis for further improvements in similar separation processes across the petrochemical industry.



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sciforum-107237: Outdoor Performance of a Thermoelectric Heat-Pumping Solar Air Heater

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Thermoelectric (TE) devices reliably convert electricity to heat (and vice versa) without moving parts. They can be integrated into solar energy devices to improve thermal energy conversion in various applications. This study aimed to experimentally investigate the improvement in the efficiency of a solar air heater (SAH) by incorporating TE modules. Eleven TEC1-12706 TE modules, with their cold sides affixed to the rear of the SAH absorber plate, were installed in the model SAH we assessed. Photovoltaic modules provided direct current to the TE modules to create a temperature difference across the surface of the TE modules. This propelled heat transmission to the air moving beneath the absorber plate as the TE modules extracted heat from the absorber plate through their cold to their hot sides. Under the same ambient conditions of 38.6°C maximum ambient temperature and maximum insolation of 380.6 W/m², this thermoelectric heat-pumping solar air heater (TE-SAH) demonstrated a notable gain in efficiency over the classic SAH, with an average efficiency of 23% compared to the latter's 18%. The maximum collector outlet temperatures were 61°C and 56.5°C, respectively. These indicated mean efficiency and outlet temperature gains of 31.5% and 8%, respectively. At an air mass flow rate of 0.013 kg/s, the TE-SAH achieved a peak efficiency of 74%, whereas the standard SAH recorded a peak efficiency of 57%. This work introduces a new strategy for enhancing the performance of SAH systems. It shows the significant improvement in efficiency that thermoelectric technology can produce when paired with a conventional SAH system.



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sciforum-104527: Performance Enhancement of Energy Charging Stations Through Zeta Converter Integration in Bidirectional V2G Technology

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Battery-operated electric vehicles store energy during the charging from the grid. This stored battery energy is extensively used for driving the vehicle, known as the grid-to-vehicle (G2V) technology. However, the battery storage energy is not utilized when the vehicles are parked in the parking lot. To utilize this energy, vehicle-to-grid (V2G) technology is introduced, where the stored battery energy will supply the grid when the vehicles are not in drive. This can reduce the burden on the utility grid. During the power transition from G2V and V2G, the transient and switching losses are present in the system. This can affect the grid-side parameters (namely frequency, real power, reactive power, and inverter current) and converter-side parameters (namely converter output voltage, converter switching losses, and SOC of the battery). To overcome this problem and to improve the performance of the system, this paper proposes the integration of a DC/DC zeta converter. The effectiveness of this integration is verified under various test conditions and is compared with the results of the conventional buck-boost converter. From the simulation results, it is observed that when the system is operating in G2V mode, the output voltage and frequency are settled very quickly at 0.035 sec and 0.12 sec respectively and the ripple voltage is reduced by 120 V, with the proposed converter. Similarly, in V2G mode, the output ripple voltage is reduced by 10V and the response quickly settles compared to conventional converter. In the overall operation, the converter switching losses are minimized, thereby improving the entire system's performance. From all these findings, it is recommended that the DC/DC zeta converter integration in V2G and G2V systems leads to superior and fast charging/discharging of the energy.



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sciforum-101820: Projected Changes of Wind Power Potential over a vulnerable eastern Mediterranean area using EURO-CORDEX RCMs according rcp4.5 and rcp8.5 scenarios

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Under the threat of climate crisis, renewables are an alternative that are aligned to European principles for the clean energy and green transition strategy. The revised Renewable Energy Directive of European Union set as a target for renewables a minimum of 42.5% till 2030. Past studies have shown that Eastern Mediterranean presents notable short and long term wind speed variability due to climate change. In this context, this work investigates the mean changes in Wind Energy Potential (WEP) in a typical height of offshore turbines (80m) over the climatic sensitive area of Aegean Sea during early (from 2010 to 2039), middle (from 2040 to 2069) and late (from 2070 to 2099) periods of 21st century with reference to a basis period (the historical period from 1970 to 2005). Data, available from EURO-CORDEX project under the moderate and extreme future scenarios (rcp4.5 and rcp8.5) as well as the recent past (historical) period (from 1970 to 2005), are analyzed here. In both future scenarios, the majority of model simulations indicates increase of the WEP over the Aegean area as compared to the basis (historical) period. In particular, the maximum increase of WEP is presented in extreme (rcp8.5) as compared to moderate (rcp4.5) scenario. The most significant changes are shown over the southeastern (the straights between Crete and Rhodes Island) and central-eastern Aegean area.



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sciforum-107238: Successful application of the biosorption process in wastewater treatment: insights of bacterial biomass use to assess the process environmental impacts

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Decision-makers have begun to take an increasing interest in identifying the environmental impacts through the application of Life Cycle Assessment (LCA) for the management of contaminated sites. The analysis of scientific literature shows that impact assessment studies using life cycle assessment are rare for bioremediation processes using biosorbents. More studies are therefore needed to develop sustainable bioremediation processes for the removal of pollutants such as heavy metals that can subsequently be successfully applied in large-scale facilities. We propose an impact analysis for the wastewater treatment by biosorption of 1 liter of water contaminated with Cr(VI) at a concentration of 25 mg/L. We evaluated the environmental impacts potentially generated by Cr(VI) bioremoval in batch and column conditions to demonstrate the environmental and human health impacts and benefits of this type of bioremediation process. Biomass of *Rhizobium viscosum* CECT 908, previously classified as *Arthrobacter viscosus* was used as biosorbent for Cr(VI). Environmental impacts were quantified through LCA methodology, within the Sphera Product Sustainability Solutions Software. All major factors that can lead to environmental impacts, such as transportation or electricity, have been considered. The lowest environmental impact value was quantified for the impact category human toxicity cancer (HTc) for Cr(VI) ions removed by biosorption in the batch and continuous systems. The category human toxicity cancer (HTc), is the category with a negative value, and therefore indicates no quantified environmental impact. The study has shown that energy consumption needs to be reduced in the process in order to record lower environmental impacts.



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sciforum-099994: Temporal and spatial variability of thallium in urban topsoils from Alcalá de Henares (Spain)

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Background: Although thallium (Tl) is scarce in soils, it is highly toxic and can accumulate in plants. Previously, we have observed an increment of 100% in its content in urban topsoils monitored across Alcalá de Henares (Spain) in a year in 2001. A further monitoring study was carried out in July 2017 to identify potential risks for inhabitants.

Methods: Tl was quantified in 66 urban, 24 industrial and 4 public garden topsoil samples collected in 2017 by ICP-MS. Data was compared with 97 topsoils collected in the same locations in the urban area in 2001.

Results: The presence of Tl, which was detected in all the 2017-topsoil samples (LoD=0.022 mg/kg), showed a 38.3% significant increment in the urban area when compared with the previous sampling (0.166 vs. 0.12 mg/kg), suggesting some accumulation in these topsoils. The increment of Tl detected may be attributed to its inorganic nature and the growth of the city, which may increase its anthropogenic inputs in manufacturing processes and use of cement. A significantly higher contamination in industrial (0.249) and garden (0.246) topsoils was detected versus urban soils (p -value 0.001), which would be logical due to its uses in the manufacture of electronics, detectors, optical lenses, smelting. Thus, the content of Tl was significantly higher in the suburban area that supports more industries when compared with the other subareas (0.214 vs. 0.184, 0.150, 0.127; all in mg/kg). These levels were lower than, or similar to, the background concentration level suggested in soils from south-east Spain (0.2 mg/kg), and much lower than those detected in two mine-affected catchments in the north-west Madrid Region (0.87-2.65 mg/kg), suggesting a minor contamination by Tl in Alcalá's topsoils.

Conclusions: The levels of Tl recently monitored in Alcalá's topsoils would not represent a significant risk for the population derived from the ingestion/inhalation of Tl present in the urban soils.



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Session 7. Food Science and Technology

sciforum-103785: “Cadherin Switch” Initiated By Royal Jelly Regulates Motility Of Colorectal Cancer Cells

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The basis of the negative reaction of colorectal cancer (CRC) to the application of certain treatment strategies is the acquisition of aggressive features during the process of epithelial-mesenchymal transition (EMT). It is known that the Wnt/ β -catenin signal pathway is deregulated in CRC, and some specific markers are observed to be overexpressed in this disease, such as β -catenin transcription factor. Under the regulation of Wnt/ β -catenin signaling appears the expression of the membrane proteins E-cadherin and N-cadherin, which are constitutive elements of intercellular junctions based on which the migration of cancer cells is controlled. Royal jelly (RJ) has already been recognized as a natural treatment with certain anti-cancer activities and antimetastatic potential, yet the exact molecular mechanism of these activities is still unknown.

This study aimed to assess the migratory potential of the colorectal cancer cell line SW-480 by applying the Transwell test, as well as to evaluate the expression of β -catenin, E-cadherin and N-cadherin at the gene level by using the qPCR method. Additionally, the E-cadherin and N-cadherin protein expression rates were determined by using immunofluorescence. All assays were carried out 24 h after treatment with RJ at two selected concentrations (10 and 100 μ g/mL).

The results showed significant inhibition of SW-480 cells' migratory potential and downregulation of *β -catenin* gene expression after treatment with RJ. Concurrently, an increase in E-cadherin and the inhibition of N-cadherin at the protein level were induced by RJ at both applied concentrations. The difference in the SW-480 cells' responses to the two applied RJ concentrations was obvious, and the higher concentration (100 μ g/mL) was more effective.

This study presents RJ as a promising therapeutic candidate for inhibiting the migratory potential of colorectal carcinoma cells by targeting regulatory and effector markers of EMT, thus offering potential avenues for modulating the aggressiveness of CRC.



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sciforum-103717: Applications of QMRA (Quantitative Microbial Risk Assessment) for Assessing Major Foodborne Pathogens in Fresh Vegetables

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With the increased consumption and production of fresh vegetables, the safety risks of vegetables, especially the risk of foodborne disease outbreaks, are also increasing. The food safety risks caused by pathogenic microorganisms in contaminated fresh vegetables are becoming leading threats to human health. Quantitative Microbial Risk Assessment (QMRA) is the core of preventing and controlling microbial hazard risks. This study aims to identify the main foodborne pathogens in fresh vegetables and review the applications of QMRA for assessing these major foodborne pathogens in fresh vegetables.

A comprehensive review was conducted by searching the databases including Web of Science, PubMed, Scopus and CNKI for the articles with terms related to “applications of QMRA” and “foodborne pathogens in vegetables” or “foodborne diseases caused by fresh vegetables” between 2000 and 2024. The main pathogens in fresh vegetables that cause outbreaks of foodborne diseases have been identified through analyzing the reports of foodborne disease events that have occurred internationally in recent years. The studies of Quantitative Microbial Risk Assessment applications for these main pathogens have been reviewed. The current applications and future studies of QMRA in assessing main pathogenic microorganisms in fresh vegetables and ready to eat vegetables have been summarized.

The review identified the top four pathogens associated with fresh vegetables that cause foodborne disease outbreaks are Salmonella, E. coli, Listeria monocytogenes, and Norovirus. Monte Carlo simulation approach is the most common and widely used technique for QMRA models applied to fresh and ready-to-eat vegetables, as it is easy-to-implement. The study on the applications of QMRA methods highlighted the key contamination variables and processes in the fresh produce chain as the cross-contaminations from farm to fork including soil, irrigation water, manure, human handling, storage, temperature, packaging, retail conditions, and evaluated the effectiveness of the preventive measures that have been implemented.



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sciforum-104305: Enhancing fruit and vegetable shelf-life by applying edible coatings: towards a more sustainable packaging system

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Currently, the Food Industry is confronted with significant challenges due to the detrimental impact of plastic usage and food waste on sustainability. Consumers are becoming increasingly aware of these issues and are demanding eco-friendly packaging solutions that preserve the quality of food products. This demand is particularly challenging when dealing with perishable items such as fruits and vegetables. In this context, edible coatings emerge as a viable alternative to traditional packaging. These coatings, comprising thin layers of biopolymers, are applied to the surface of food products, providing protection by inhibiting microbial growth, preventing mechanical damage and the oxidation of some nutrients such as polyunsaturated fatty acids, and reducing water loss, among other benefits. Furthermore, the biopolymers used in the formation of edible coatings can be enhanced with additional compounds such as nanoparticles, essential oils, and nanoemulsions, thereby improving the physicochemical properties of the coating and enhancing product preservation, which ultimately leads to the reduction of food waste. This review consolidates current data on edible coatings applied to both fruits and vegetables, offering a comprehensive overview of the formulation process and various methods for enhancing the coatings. Additionally, this review considers the principles of circular economy, noting that several by-products from the food industry can be utilized in the formation of edible coatings.



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sciforum-103977: Fermentation of carob syrup (*Ceratonia siliqua* L.) by SCOBY to produce a polyphenol-rich kombucha

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Introduction: Kombucha tea is a probiotic fermented acidic tea obtained from a symbiotic culture of bacteria and yeasts (SCOBY) mainly acetic acid bacteria (AAB), lactic acid bacteria (LAB) and yeasts attached to a floating biofilm of bacterial cellulose, in a medium containing sugars and tea and its consumption is linked to beneficial effects. The aim of this study was to prepare kombucha tea by using alternative plant raw materials used in the Mediterranean basin in order to increase the bioactivity of the final product. **Methods:** Two kombucha systems were fermented for 12 days, one system by using SCOBY (10g/L), sugar (10 % w/v) and a mixture (1% w/v) of equal quantities of green tea and mountain tea (*Sideritis* spp) and in the second system, sugar was replaced by carob syrup from *Ceratonia siliqua* L., a xerophytic endemic species typical of the Mediterranean climate. Physicochemical and microbiological analyses were performed and total phenolic content and antioxidant activity were measured at 0, 6 and 12 days of fermentation. The SCOBY was observed by Scanning Electron Microscopy (SEM). **Results:** Both systems fermented the available sugars and produced a slightly carbonated, aromatic and acidic (pH 3.12-3.39) probiotic beverage with a low alcohol content (0.5-0.7% ABV). Yeasts and AAB remained at high probiotic levels (>7 logCFU/mL) and LAB at 4-5 logCFU/mL. The kombucha produced with carob syrup had at the end of fermentation an increased polyphenol content, more than three times than the sugar-based kombucha (773 mgGAE/L and 233 mgGAE/L respectively) and the antioxidant activity was increased by 2.4 times. SEM revealed an extended net of bacterial cellulose with bacteria and yeasts attached. **Conclusion:** Carob syrup can be used as an alternative and sustainable fermentable substrate for the preparation of Kombucha and increases significantly its bioactivity.



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sciforum-103123: Improvement of tomato aromatic compounds through novel organic substrates from *Posidonia oceanica* residues

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Tomato (*Solanum Lycopersicum* L.) is the most popular fruit crop worldwide. However, the deterioration of the flavor quality of commercial tomatoes is one of the main causes of consumer complaints. One of the most important factors influencing the synthesis of aromatic compounds in tomato is the growing medium, though studies on the effect of the growing substrate on its volatile profile are limited. Therefore, the main objective of this work was to improve the aromatic and flavor properties of tomato through the use of novel growing media obtained from the remains of *Posidonia oceanica* (PO), favoring the revalorization of residues. A greenhouse experiment was carried out in pots with tomato seedling cv. sweet cherry with three treatment groups—control (50% peat–50% perlite), PO (50% PO washed/sieved–50% perlite), and IP (50% PO unaltered–50% perlite)—for 9 weeks under controlled temperature conditions (18°C/27°C (night/day)), 60% relative humidity, and two daily irrigations of 100 mL with tap water. To evaluate the effectiveness of the treatments, fresh weight, total soluble solids, and the concentrations of organic and volatile compounds were measured by SPME-GC/MS. The average weights of the fruits obtained were 4.97, 5.77, and 4.65 g, and they had sugar contents of 8.7, 7.4, and 10.0 °Bx for the control, PO, and IP groups, respectively. This variation was due to the high salinity of the IP sample, which resulted from not washing away the salts from the *Posidonia oceanica* debris, favoring the production of sweeter, although smaller, tomatoes. Among the volatile compounds identified by SPME-GC/MS, it stands out that the tomatoes from the IP substrate, followed by PO and the control, presented the highest concentrations of octanal and hexyl acetate, conferring citrusy, fresh, and sweet aromas. Additionally, the tomatoes from PO also had a notable concentration of nonanal and alpha-terpineol, contributing to their herbal and fresh notes.



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sciforum-104071: Influence of oil content and different thickeners on microstructure and rheological characteristics of food emulsions based on aquafaba beans

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There is a strong trend in the global food industry towards using plant-based ingredients in food technologies. The aim of this study was to develop ten o/w emulsions with a sunflower oil content of 30 and 60 % using bean aquafaba as an emulsifier. The emulsions were stabilized by increasing their viscosity. For this purpose, xanthan gum or cold-soluble corn starch were added as thickeners. The effects of oil content and different thickeners on the microstructure and rheological properties were evaluated using laser diffraction and rotational viscometry. A pre-optimised water to seed ratio of 1.5:1 resulted in a bean aquafaba with a low protein content of 0.5%. Further evaporation was used to increase the protein content to 0.8% w/w. The aquafaba-based emulsion samples were characterized by a bimodal droplet size distribution with peaks at approximately 2.8 and 10.5 μm , with the exception of corn starch systems. Increasing both the oil and xanthan gum content had little effect on the change in the mean volume diameter of the emulsion droplets in the range of 6–8 μm , while adding corn starch increased this value. All emulsions were characterized by pseudoplastic flow behavior. The flow curves were approximated using the power-law and Hershley–Barkley models. The calculated dynamic yield shear stresses consistently increased with increasing content of both oil and thickener in the range of 0.3 to 5.0 Pa. It is worth noting that in emulsions with an oil content of 30%, the addition of xanthan gum had a significant impact on this indicator, while in emulsions with an oil content of 60%, the addition of corn starch did. Thus, the higher concentration of the selected polysaccharides resulted in more viscous systems with improved stability. The developed food emulsions based on bean aquafaba are promising precursors in the technology of vegetarian products.



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sciforum-088849: Partial replacement of wheat with fava bean and black cumin Flours on nutritional properties and sensory attributes of bread

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Blending wheat with fava bean and black cumin flours can improve the nutritional content of wheat-based bread. The current study investigated the effects of flour blending ratios of wheat, germinated fava bean, and black cumin on the physicochemical and sensory attributes of bread. A total of sixteen bread formulations were produced using Design Expert software: mixtures of wheat (64–100%), fava bean (0–30%), and black cumin (0–6%). The findings showed that the mixed fraction of composite flours affected the sensory attributes and nutritional value of bread. The mineral contents [Fe, Zn, and Ca] and proximate compositions [ash, fiber, fat, and crude protein] increased with an increase in fava bean and black cumin flour content and decreased with an increase in wheat flour content. The carbohydrate content and crumb lightness (L^* value) increased with a decrease in black-cumin and germinated fava bean flour proportion. The sensory attributes were significantly affected by the blend proportion ($p < 0.05$). Sensory scores increased with an increase in the level of germinated fava bean flour and decreased with an increase in the level of black cumin. Generally, the best bread blending ratio was found to be 72.5% wheat, 25.6% germinated fava bean, and 1.9% black cumin, in terms of overall qualitative attributes. This could lead to healthier and more appealing bread options.



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sciforum-104628: Repurposing of natural compound derivatives for control of foodborne fungi and mycotoxins

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Controlling agricultural or foodborne fungal pathogens is becoming increasingly problematic since effective agents available for antifungal treatment are often very limited. The development of new antifungal agents is expensive and time-consuming; therefore, an alternative approach, termed antifungal drug or compound repurposing (ADCR), has recently been employed. ADCR is the repositioning of already marketed chemicals approved for treating other diseases or for use as food additives (flavorings, antioxidants, etc.) to control fungi. One of the merits of ADCR is that the mechanisms of action, cellular targets and safety of the chemicals have already been characterized.

We investigated the antifungal efficacy of the natural product salicylaldehyde (SA), a generally-recognized-as-safe (GRAS) compound, in corn and pistachio kernels. SA has been utilized as a food flavoring agent or an intermediate for synthesizing pharmaceuticals. Since SA emits volatiles, test crops were remotely exposed to SA (0.1 to 1.0 mM) for 1, 2 and 3 days (Petri plates, raised bed containers). This transient exposure of crops to SA would allow for minimal deposition of chemicals on crop surfaces. The results showed that SA treatment (0.5 mM or higher) for 3 days almost completely inhibited the growth of fungi (aflatoxigenic *Aspergillus flavus*, seedborne filamentous fungi). We also studied the antifungal activity of 4-isopropyl-3-methylphenol (4I3M), a derivative of the natural products thymol and carvacrol, against *A. flavus* and seedborne fungi, and determined that 4I3M possesses potent antifungal and anti-aflatoxigenic activity against *A. flavus*, while it exhibits less antifungal efficacy against seedborne filamentous fungi compared to SA.

We concluded that natural compounds that do not have any significant environmental impact are a potent source of antifungal/anti-mycotoxigenic agents, either in their nascent form or as lead structures for more effective derivatives.



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sciforum-091611: The effect of temperature on the upscaling process of medicinal compound extraction from *Zingiber officinale* using subcritical water extraction

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Subcritical water extraction (SWE) is a green technology with interesting advantages, including a cheap and selective process for various applications, including the extraction of bioactive compounds. However, knowledge and data on upscaling from studies related to this process are limited. Therefore, this study reports comparative experimental data for the upscaling process of subcritical water extraction. Two SWE processes with different scales, namely the commercially available high-pressure system ASE 200 with a capacity of 28 ml and a locally fabricated high-volume SWE process with a capacity of 1000 ml, were employed for the extraction of medicinal compounds from *Zingiber officinale*, namely 6-gingerol and 6-shogaol. The effect of temperature for both setups on the compounds' concentrations was studied from 130°C to 200°C at a constant pressure of 3.5 MPa and for a duration of 30 minutes. The quantitative analysis for each compound was performed using High-Performance Liquid Chromatography (HPLC). The optimum temperature for the extraction of 6-gingerol using the high-volume SWE was 130°C, with a concentration of 1741.54 ± 0.96 µg/g, which differs from ASE 200, in which the optimum extraction temperature for 6-gingerol was 140°C, with a concentration of 1957.22 ± 2.55 µg/g. Meanwhile, for the extraction of 6-shogaol, both pieces of equipment recorded the same optimal temperature—170°C—with concentrations of 541.78 ± 3.16 µg/g and 1135.23 ± 1.18 µg/g for high-volume SWE and ASE 200, respectively. This is possibly due to the difference in the scale of the extraction process, which was up to 35-fold, from a 28 ml to a 1000 ml capacity, consequently affecting the heat and mass transfer processes during extraction. Thus, scale-up factors need to be considered for effective design during the scaling up of the SWE process to obtain higher mass transfer efficiency.



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sciforum-104150: A Comprehensive Review on the Drying Kinetics of Common Corn (*Zea mays*) Crops in the Philippines

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Drying agricultural crops is essential for preserving them and extending their shelf life. Incorporating drying technology in food production has improved product quality and helped meet increasing food demands. Corn (*Zea mays*) is a major crop grown in Southeast Asia, used for food and livestock. The preservation of crop grains, such as rice and corn, heavily relies on efficient drying processes. Common corn varieties like sweet corn, wild violet corn, waxy corn, white corn, purple corn, and young corn are cereal grains that are often dried for various food products. The study of the drying kinetics of these crops is crucial, because drying parameters significantly impact the drying process. This review article discusses various factors affecting drying, including airflow, temperature, relative humidity, sample size, and initial moisture content. Understanding these parameters helps optimize the drying process to achieve better quality and efficiency. The review also examines several mathematical models that are used to describe drying kinetics. Models such as the Weibull and Peleg models, Midilli Kucuk model, and Page and Modified Page models are analyzed for their effectiveness in evaluating design parameters. These models provide a scientific basis for improving drying techniques and ensuring consistency in food production. By presenting a comprehensive review of these aspects, this review aims to enhance the understanding of how to utilize drying technology effectively in food manufacturing and preservation, which can be vital for developing better preservation methods, improving product quality, and ultimately meeting the growing food demands.



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sciforum-100544: A patent analysis on 2D-materials in active food packaging

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Introduction

Active food packaging technology encompasses systems that incorporate active substances into the polymeric matrix.

The embedded components exhibit antimicrobial, antifungal, antioxidant properties and are able to absorb or reduce oxygen, carbon dioxide or ethylene, thereby enhancing the quality and safety of food products.[1]

The utilization of two-dimensional materials, such as graphene, has facilitated the advent of novel avenues for the advancement of active packaging (AP). The integration of these materials with polymers has the potential to enhance the barrier, thermal, and mechanical properties of packaging.[2,3]

The objective of this paper is to provide a comprehensive overview of patented two-dimensional materials in the field of active packaging.

Methods

Patent searches were carried out using Espacenet, a database provided by the European Patent Office using a combination of keywords in the title/abstract/claims search fields with Boolean and proximity operators and classification codes.

Results

China is the country with the highest number of patent applications filed for 2D-materials in AP technology, followed by the United States, and Japan. A significant number of applicants opted to utilize the PCT procedure, which permits the postponement of entry into the national phases.

The number of patent applications filed has increased significantly from 2016 to 2022.

Graphene and graphene oxide are the most frequently claimed compounds in patents, followed by layered double hydroxides and hexagonal boron nitride.

Other two-dimensional materials, such as transition metal dichalcogenides, reduced graphene oxide, MXenes and graphitic carbon nitrides (g-C₃N₄), have been the subject of fewer patent applications.

Conclusions

China, the USA and Japan are the countries with the highest number of filings. In terms of the materials most frequently claimed in patent applications, carbon allotropes are the most prevalent.



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sciforum-104290: An overview of food science's use of nanostructured applications

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Modern advances in nanoscience and nanotechnology offer innovative applications in the food sector, a relatively new field compared to biological and pharmaceutical uses. Nanostructured materials, including nanosensors, packaging materials, and encapsulated components, enhance food science. Nanostructured food systems, such as polymeric nanoparticles and liposomes, improve solubility, bioavailability, and controlled release, safeguarding bioactive components. Organic molecules (proteins, lipids, and saccharides) and inorganics (metal and metal oxides, carbon-based materials, and clays) make up the building blocks of food nanostructures. Nanostructured colloids in food include fat globules in homogenised milk, casein micelles, and β -lactoglobulin fibres in milk. Synthetic nanostructures are commonly used in food to increase solubility, improve bioavailability, preserve biologically active chemicals from degradation, extend shelf life, colour, and flavour, and provide nutritional value. These materials, which comprise nanoparticles, nanocomposites, and nanoemulsions, have increased solubility, stability, and other unique properties. Nanostructured materials detect contaminants like Salmonella or E. coli in food, ensuring consumer safety. Nanostructured materials reduce the energy consumption and environmental impact of food processing. This study aims to provide insights into nanotechnology's benefits and risks, informing the development of novel, functional food products with improved attributes and prolonged shelf life. By exploring the potential of nanostructured materials, we can enhance food safety, quality control, and consumer acceptance.



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sciforum-103500: Analysis of European wines before and after activated carbon treatment: total, active and volatile acidity; free and total sulfites; total polyphenols; color intensity and shade

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The use of activated carbon to remove colorants and odors from wine is a common practice in the wine industry. However, its use for the removal of heavy metals is at a research stage. The use of any additive must not negatively affect the original quality of the wine and it must not alter its organoleptic characteristics, as well as its appearance. In this research, we focused on the physicochemical characteristics of wine after the use of two activated carbons from potato peel (AC-Pot) and from banana peel (AC-Ban) that we prepared and characterized in our laboratories. In order to reach safe conclusions, we chose to focus on the measurement of specific measurements and indicators in ten wine samples before and after the application of the two active carbons. After selecting ten wine samples from all over Europe, before the addition of active carbons, we measured the following parameters: total acidity, active acidity, volatile acidity, free sulfites, total sulfites, total polyphenols, color intensity and color shade. We repeated the measurements a few days after adding the activated carbons to the wine samples, and the same procedure was performed three more times over a period of 2 years on the same wine samples. The results obtained were quite satisfactory and the conclusions drawn were very useful for further study.



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sciforum-107675: Apple-Based Biodegradable Film Packaging: A Zero-Waste Solution

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Conventional packaging, often reliant on synthetic preservatives and non-biodegradable materials, is incompatible with the EU's Green Deal and Farm to Fork Strategy, which promote a reduced dependence on chemically based components for single-use plastics. As a result, there is a growing need for eco-friendly packaging alternatives that preserve fresh produce while minimizing their environmental impact. Sustainable packaging, particularly bio-based and biodegradable materials, presents a promising solution by reducing waste and enhancing food preservation. In line with zero-waste principles, food industry by-products, such as dried apple by-products, can be repurposed into innovative packaging materials. Combined with natural polymers like pectin, these by-products can create functional absorbent pads that reduce moisture and prevent spoilage in strawberries. The present study aimed to develop a biodegradable packaging film based on apple by-products to be applied as a controller of strawberry degradation. Apple by-products (30% w/v) were incorporated into a pectin matrix (5% w/v) with sorbitol, forming the primary components of the films. The films were evaluated for microbiological stability, water solubility, water absorption, colour properties, and biodegradability in soil. A response surface methodology was employed to optimize the production conditions of the films, varying the pectin concentrations (0.5% to 5%), by-product content (5% to 30%), and solid-to-area ratios (0.33 to 0.132 g/cm²). The results demonstrated that the pectin concentration and by-product content significantly influenced the films' water absorption capacity and microbiological stability. Over a 38-day period, the films exhibited biodegradation rates ranging from 62.3% to 98.51%. More than 50% of the material disintegrated during the assay period, highlighting the rapid and environmentally safe degradation potential of these pads. The use of agrifood by-products aligns with zero-waste policies and promotes sustainable consumption, providing an eco-friendly solution for extending the shelf-life of fresh fruits.



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sciforum-103574: Bread enriched with bioactive compounds from plant-based additives: antioxidant properties

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Background: The use of plant-based additives with high nutritional value in the bakery technologies is an important trend in the development of functional foods.

Objective: The aim of this study was to develop the technology of wheat and rye breads as functional foods with antioxidant properties using plant-based by-products of oil industry. The inclusion of additives such as wheat germ and rosehip cake meal was carried out by partially replacing flour in the wheat and rye bread formulation in the range of 3-20% (depending on the type of additive).

Methods: The total antioxidant capacity (TAC) and the total polyphenol content (TPC) of the samples were determined by galvanostatic coulometry with electrogenerated bromine as a model oxidant and a spectrophotometric Folin–Ciocalteu method, respectively. The TAC and TPC values of the samples were classified using multivariate statistical methodology techniques such as cluster and principal component analysis.

Results: It was found that the inclusion of plant-based additives increased both the antioxidant properties of TAC and TPC of both wheat and rye bread. The greatest effect of an increase in TAC at the level of 10% was observed in samples of wheat bread with the inclusion of rosehip meal. The TAC of rye bread samples was higher than wheat bread samples. There is a positive correlation between TAC and TPC values for samples with a Pearson correlation coefficient of 0.898. This confirms the possibility of using TAC as a preliminary characteristic of the antioxidant properties of samples. The use of cluster analysis methodology allowed us to classify the effect of additives on increasing antioxidant properties in the form of two clusters. The results of multivariate analysis were discussed.

Conclusion: The inclusion of wheat germ flour and rosehip cake in the bread formulation develops a functional food with increased antioxidant properties.



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sciforum-103305: Chemistry Behind Lactose Intolerance And Recent Developments In Producing Lactose Free Dairy Alternatives

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Lactose, or milk sugar, is the most essential and essential carbohydrate found in mammalian milk. Aside from fat and protein, it is the most important component of milk solids in cow's milk. Due to low levels of intestinal lactase, also known as lactase-phlorizin hydrolase (LPH), a β -D-galactosidase present in the apical surface of the intestine microvilli, around 70% of the global adult population is lactose intolerant. This might be brought on by the adult loss of intestinal lactase, a disorder caused by a recessive autosomal gene that varies in racial populations in humans. These days, a lot of goods are sold to people who are lactose intolerant as dairy substitutes. A lactose-free diet is a crucial part of treatment for people with lactose intolerance thus those who are impacted must avoid certain dairy foods and non-dairy items that have lactose. To mitigate lactose sensitivity and enhance human health and well-being, lactose-free dairy products are suggested as substitutes. Probiotics and fermented dairy products have been shown in recent research to alter the metabolic processes of the intestinal microbiota and perhaps reduce lactose intolerance symptoms. According to studies, sweet kefir has a microbial diversity that is comparable to that of typical milk kefir, suggesting that it could be a viable probiotic substitute. Nonetheless, it has been demonstrated that sweet kefir contains probiotic qualities, including the ability to adhere to mucosa by penetrating its lumen and allow microorganisms to colonize the mucosa. Thus, clinical investigations have indicated possible health effects such immunomodulation, anticancer, anti-obesity, inhibition of inflammatory agents, decrease of oxidative stress, and antibacterial activity. Plant based milk has recently been developed with sorghum seeds, sesame seeds, cantaloupe seeds. The highest fat contents were found in coconut milk, sesame milk, and cantaloupe seed milk respectively.



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sciforum-107341: Complex electrochemical assessment of the antioxidant properties of essential oils

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Essential oils are one of the sources of natural antioxidants in food industry. Their major representatives are phenolic compounds, whose composition is strongly dependent on the type of plant material, the geographical conditions of its growth, the vegetation stage, and the processing method. Therefore, the characterization of the antioxidant properties of essential oils is in demand today. The total antioxidant parameters obtained by electrochemical methods were shown as an effective approach for the sample characterization. In current work, the commercial essential oils from basil, ylang-ylang, bergamot, marjoram, clove, jasmine, neroli, cinnamon, lavender, rosemary, ginger, nutmeg, thyme, anise, and clary sage were studied. Galvanostatic coulometry with electrogenerated Br_2 and $[\text{Fe}(\text{CN})_6]^{3-}$ ions and chronoamperometry were used for the assessment of total antioxidant capacity (TAC), ferric reducing power (FRP), and antioxidant capacity, respectively. TAC reflects the impact of both phenolic antioxidants and terpenes, while FRP indicates the content of phenolic antioxidants only. Chronoamperometry at glassy carbon electrode covered with carboxylated multi-walled carbon nanotubes makes it possible to differentiate the impact of phenolic compounds and terpenes applying various potentials, i.e., 800 and 1400 mV, respectively. The sufficient electrolysis time was 75 s on each step. The total antioxidant parameters screening was performed, and positive correlations with the standard spectrophotometric methods (Folin–Ciocalteu for clove, cinnamon, nutmeg, and thyme essential oils only and the DPPH test for all samples) were found. Electrochemical approaches are express, cost-effective, simple, reliable, and have no limitations typical for spectrophotometry. Therefore, electrochemical assessment of the antioxidant properties of essential oils is a perspective for practice.



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sciforum-107503: Determination of *Escherichia coli* in raw and pasteurized milk using a piezoelectric gas sensor array

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The importance of assessing the microbiological safety of food products is beyond doubt, which is also true for milk and dairy products. They are very important in the diet and contain nutrients necessary for the human body in well-balanced proportions and in an easily digestible form. Therefore, the goal of this work was to evaluate the changes in the composition of the gas phase over milk based on signals from chemical sensors to predict the quantity of the coliform bacteria group in the milk samples. The gas phase over raw milk samples and samples after pasteurization, as well as for a standard (a model aqua solution of macronutrients and minerals), was studied using an array of sensors with polycomposite coatings, including those contaminated with *E. coli* bacteria. Assessment of microbiological indicators was carried out according to GOST in parallel with the gas-phase analysis. The patterns of the sensor signals, the calculation parameters, and calibration graphs with an error of ± 100 CFU/ml were established based on the results of analyzing the standard samples. The adequacy of the calibration graphs was tested on seven raw milk samples, including those containing other types of pathogenic microorganisms (*Staphylococcus aureus*, *Klebsiella* spp., etc.). Thus, the proposed approaches to quantitative assessments of coliform bacteria in raw and pasteurized milk using gas-phase analysis with an array of sensors make it possible to significantly reduce the analysis time to 2-3 hours (including the sample collection and data processing) and thereby intensify the production of safe dairy products.



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sciforum-104325: Determination of Properties of Meat Products with Plant Supplements

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One way to implement the global program for sustainable development and ensure adequate nutrition for the population is by creating mass-consumption products, minced meat products utilizing sources of various biologically active compounds. Polyunsaturated fatty acids of sunflower oil, polyphenolic complexes, antioxidants, dietary fibers of fenugreek (*Trigonella foenum-graecum* L.) and dried leaves of black currant (*Ribes nigrum* L.) (DLBC) not only significantly increased the nutritional and biological value of the products but also improved their functional and technological properties, organoleptic characteristics, reduced losses after heat treatment, and extended the shelf life of the products. The stability of minced meat emulsions (SE) with sunflower oil and fenugreek or sunflower oil and DLBC was evaluated based on the mass fraction of the intact emulsion, which lost a certain amount of moisture and fat after heat treatment at a temperature of 75–80°C for 60 minutes. The SE index for minced meat with a mass fraction of fenugreek of 1.7% and 3.4% exceeded the SE of the sample without fenugreek by 3.0% and 4.9%, respectively. The SE for minced meat with a mass fraction of DLBC of 0.75% and 1.85% exceeded the results of the sample without DLBC by 7.5% and 8.9%, respectively. The indicators of fat-holding capacity and water-holding capacity of minced meat with the addition of fenugreek or DLBC exceeded the results of samples without supplements by 6.3%, 3.2%, and 14.5%, 20.6%, respectively. The protein content of ready-made meat products with plant supplements was 16.5–18.5%. The products contained vitamins E, A, β -carotene, and minerals such as sodium, potassium, calcium, magnesium, phosphorus, zinc, copper, and iron. Due to the use of fenugreek, the iron content increased from 1.27 ± 0.03 mg% to 1.71 ± 0.04 mg% and 2.14 ± 0.04 mg%. The created products can be characterized as health products that can be recommended for adjusting the diet of the population.



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sciforum-102837: Development and characterization of jams produced from the pomace of different fruits

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Fruit pomace, which is the pulp and peels leftover from processing or juicing fruit, is a nutrient-rich and adaptable waste that can be made into useful goods like natural colours, biofuels, and dietary supplements, or it can be utilized as compost and animal feed. The goal of the current study was to create and evaluate fruit pomace jam using various juice waste leftovers in terms of its rheological and biochemical characteristics. Four types of pomace jams were made: mixed-fruit pomace jam (MFPJ), guava pomace jam (GPJ), pineapple pomace jam (PPJ), and apple pomace jam (APJ). In prepared pomace jams, surface morphology showed heterogeneous ultrastructure with pocket formation, with KPJ exhibiting the best 3D gel network. PPJ additionally exhibited the maximum values of the colour coordinates (L^* , a^* , and b^*). When dietary fibre amounts were compared to other pomace jams and commercial fruit jams, GPJ had the highest, at 7.21 g/100 g. The highest amount of phenolic content (343.22 mg GAE/100 g) was found in MFPJ. There were noticeable levels of carotenoids in GPJ (6.86 mg/100 g) and MFPJ (4.21 mg/100 g). The antioxidant capacity of pomace jams shows the following trend for radical scavenging activity (%) and reducing power potential (PPJ) according to the ABTS and FRAP assays: GPJ > APJ > MFPJ > PPJ. The research effectively produced and identified fruit pomace jams with favourable rheological, biochemical, and antioxidant characteristics, emphasizing their potential as wholesome and environmentally friendly substitutes for conventional fruit jams.



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sciforum-107851: Development of technology for candy caramel with barberry powder and sugar substitute isomaltitol

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Background: Confectionery products and in particular caramel have a low nutritional value and a high glycemic index. Overcoming these shortcomings is possible by including new generation sugar substitutes such as polyols and fortifying agents based on dried plant powders in the formulation of candy caramel.

Object: The purpose of this study was to develop the technology of candy caramel as a functional product with a lower glycemic index. The index reduction was achieved by including sugar substitute such as isomaltitol in the caramel formulation. As a fortifying agent with a significant amount of bioactive compounds and at the same time a natural colorant, the dried powder of the wild plant *Berberis vulgaris* L. was used in an amount of 1, 2.5, 5 and 10% (w/w).

Methods: The microstructural characteristics of the powder were determined by laser diffraction. The elemental composition was confirmed by atomic adsorption spectroscopy. Physicochemical methods and sensory analysis were used to evaluate candy caramel samples.

Results: The technology for the production of candy caramel using isomaltitol, invert syrup and barberry powder was developed. Dry barberry powder was used to prepare the samples, characterized by an optimal average particle size of 37.4 µm and a width of the SPAN particle distribution curve of 2.94 µm. The addition of barberry powder in quantity made it possible to enrich candies with trace elements such as sodium, potassium, iron, manganese and zinc. When the amount of barberry in the caramel recipe is increased, the acidity increases significantly from 1.02 to 10.2 mg/100 g of the sample in the equivalent of citric acid and changes the pH from 3.45 to 3.12. Sensory analysis allowed us to establish that the optimal amount of barberry powder inclusion in caramel formulations is 2.5-5%.

Conclusion: The result was a candy caramel with a potential functional food.



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sciforum-105223: Effect Of Extraction Method On The Yield And Physicochemical Properties Of Cashew Nut

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This study was conducted with the aim of identifying the most effective extraction technique and evaluating the suitability of the extracted oils for ingestion and other potential applications by extracting oils from cashew kernels using three different methods: cold press, mechanical, and Soxhlet extraction. The research focused on comparing the yield and physicochemical properties of the oils obtained through each of these methods. The cold press extraction was performed using a traditional local method, which has been passed down through generations; the mechanical extraction method was carried out using hydraulic presses, which apply significant pressure to the kernels; and the Soxhlet extraction was conducted using Soxhlet apparatus, a well-established method in which n-hexane is used as the solvent to facilitate the extraction process. The study found that the percentage of oil extracted from the cashew kernel was highest with the Soxhlet extraction method, yielding 40%, followed by the mechanical method with a 27% yield, and the cold press method with a 12% yield. Cashew kernel oil (CKO), as observed through physical analysis, is light yellow in color. The physical and chemical characterization of the oil revealed a pH of 5.65 for Soxhlet extraction, 5.4 for mechanical extraction, and 5.4 for cold press extraction. The acid value was found to be 8.25 mg KOH/g for Soxhlet extraction, 8.43 mg KOH/g for mechanical extraction, and 8.697 mg KOH/g for cold press extraction. The density of the oils was measured at 0.91g/cm³, 0.909g/cm³, and 0.907g/cm³, and the free fatty acid content was 4.125, 4.215, and 4.348 for the Soxhlet, mechanical, and cold press extractions, respectively. Given that cashew kernel oil is non-toxic, this suggests its potential for use in the food and cosmetic industries.



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sciforum-102883: Ensuring Food Safety in Workers' Compounds: Addressing Challenges and Implementing Best Practices"

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This study explores food safety measures in workers' living compounds, focusing on the entire food handling process from receiving, inspecting, storing, preparing, cooking, and presenting food. . The research emphasizes the implementation of food safety protocols at each stage, using a case study approach at project sites. Employing both qualitative and quantitative methods, data was collected through questionnaires and interviews with workers in onsite canteens. Findings indicate that while most food safety protocols are followed during food handling, significant issues were identified in storage practices, leading to a higher risk of contamination. These issues are often due to site conditions and resource limitations. Practical implications of the study highlight the need for improved storage solutions and ongoing training for food handlers to enhance overall food safety. By addressing these challenges, project sites can better protect workers from foodborne illnesses and improve health outcomes. However, the study's limitations include its focus on a single company and geographical area, which may affect the generalizability of the findings. Future research should consider a broader range of companies and locations to validate these results and provide more comprehensive recommendations. This research underscores the importance of rigorous food safety protocols in maintaining health and productivity in workers' living compounds.



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sciforum-099996: Essential mineral content and vanadium in a popular Spanish brand of alcoholic and non-alcoholic beer

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Cereals, water, hops and adjuncts have been described as the major contributors to the mineral content in beer, in contrast yeast, industrial processes and containers will have a minor contribution. Beer mineral content contributes to the quality and flavour of the commercially produced beer. We have studied the content of Fe, Cu, Cr, Mg, Mn, V and Zn in nine different bottles of a popular brand of beer (5 alcoholic, 4 non-alcoholic) from the Madrid Region in Spain. Elements were monitored by ICP-MS following appropriate methods. Fe was detected only in the samples of non-alcoholic beer, meanwhile traces of V were detected in the samples of the alcoholic version. Except for Fe, levels were higher in the alcoholic beer, which could be attributed to differences in the brewing and manufacturing processes, such as reverse osmosis and filtration. Levels of Cu and Zn were below the permissible limit in wine (1 and 5 mg/L; respectively) set by the international organisation for grapes and wine. The daily dietary intakes for each element were (in µg/person, respectively) as follows, for alcoholic (0, 3.225, 3.036, 4244.81, 4.495, 28.255, 7.016) and non-alcoholic (72.937, 2.137, 2.094, 2434.63, 3.036, 20.064, 0) beer. The percentages that they would cover of the established RDAs for Fe, Cu, Cr, Mg, Mn, Zn for males (0.01; 900; 35; 420,000; 2,300 and 11,000 µg day⁻¹ person⁻¹) for consumers of alcoholic beer would be low: 0, 0.358, 8.674, 1.011, 0.195, 0.257%. Moreover, the intake of V from alcoholic beer would not represent a significant risk as a daily intake of 10-100 mg/day is considered safe from food sources. Our results would suggest that beer would not constitute an important source of these essential minerals.



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sciforum-091223: Exploring the Efficacy of Various Preservative Methods in Extending the Shelf Life of Sugarcane Juice

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Sugarcane, a member of the Poaceae family, is a significant cash crop globally, valued for its refreshing taste and nutritional benefits. However, its commercialization faces challenges due to rapid decay and a short shelf life caused by harmful microorganisms. This study aimed to develop safe, long-lasting sugarcane juice suitable for human consumption during off-season periods. It focused on enhancing the storage stability of bottled sugarcane juice through various treatments (T_0 – T_5), including microwave pasteurization at temperatures of 80°C and 90°C for 15–20 min and the addition of the preservatives sodium benzoate and citric acid at a ratio of 1:2 g/L, as well as their combination. Sugarcane juice samples were stored in 120 mL PET bottles at refrigeration ($5 \pm 1^\circ\text{C}$) and analyzed every 10 days over a 40-day storage period for physicochemical, color, microbial, antioxidant, and sensory attributes. The results revealed a decrease in titratable acidity, total soluble solids, L^* value, and microbial content during storage. However, pH, color (a^* and b^* values), and total phenolic content increased significantly. The sensory attributes notably changed in later storage stages. Sugarcane juice treated with sodium benzoate, citric acid, and heat treatment (referred to as treatments T_4 and T_5) exhibited minimal sensory changes during storage. Furthermore, the study successfully produced high-quality, ready-to-drink bottled sugarcane juice with satisfactory storage stability for 40 days, ensuring its quality and safety for consumption.



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sciforum-107745: Extraction Of Tannins From Chestnut By-Products For Incorporation Into Chestnut Flour

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Based on the concepts of a circular economy and sustainability, this research aims to enrich foods by incorporating extracts from food by-products into them.

As the south of Galicia and the north of Portugal are major producers of *Castanea sativa* Miller chestnuts, it is imperative to devise sustainable uses for the by-products generated during their processing.

Chestnuts' consumption is widely promoted for its nutritional value and health benefits. It is a starchy fruit that is rich in vitamin C and minerals and gluten-free, making it great for people with coeliac disease, as well as being low in fat. There are several studies that describe the shells and hedgehogs of chestnuts as promising sources of bioactive compounds and fibre. Taking the nutritional advantages associated with both chestnut flour and chestnut by-products by various authors as a starting point, the aim is to extract tannins from the shells and hedgehogs for future incorporation into the flour. The shells will be heat-treated, dried, roasted, and boiled in thermal water. The hedgehogs will only be freeze-dried before being extracted. It is also hoped that we will ascertain the feasibility of incorporating the extracts of these by-products into chestnut flour, which is also made using different thermal processes, including drying, roasting, and boiling in thermal water, and is rich in minerals. The main aim of this study is to optimise a food product, chestnut flour, with added value by incorporating extracts from chestnut shells and hedgehogs. The aim is to produce a nutritionally enriched product with greater antioxidant capacity, thereby increasing the shelf life of chestnut flour.



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sciforum-104299: From azo dyes to natural colors: evaluating safety and regulatory standards

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Azo dyes are synthetic chemicals added to food products to enhance color and increase consumer appeal. Compounds such as Tartrazine, Sunset Yellow, and Carmoisine fall into this category, offering no nutritional benefits, health advantages, or preservative qualities. These dyes are favored in the food industry for their cost-effectiveness, stability, and availability, despite ongoing safety concerns. Health risks associated with azo dyes primarily stem from the breakdown of the azo bond, which can release aromatic amines, which are compounds known to be carcinogenic and allergenic. This review provides an extensive analysis of azo dyes, their classification, and the current regulations and toxicity issues associated with them. It also investigates potential natural alternatives that could effectively replace azo dyes, such as anthocyanins, curcumin, red beet betalains, and lycopene, which offer safer and often nutritionally beneficial options. Following the PRISMA (Preferred Reporting Items for Systematic Reviews and Meta-Analyses) guidelines, a systematic review was conducted using PubMed and ScienceDirect with the search terms “Azo dyes,” “Food dyes,” and “Food safety,” without restricting publication years but focusing on the most recent references available. The review aims to present a understanding of the implications of azo dye use in the food industry and to highlight viable natural alternatives that ensure consumer safety without compromising product appeal.



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sciforum-106721: From Sea to Farm: Using Seaweed Extracts for Sustainable Control of Fungal Diseases in Rocha Pear

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Rocha pear, a well-known Portuguese fruit, faces significant pre- and post-harvest challenges due to fungal infections. *Stemphylium vesicarium* is a phytopathogenic fungus that causes brown spot disease and has been responsible for significant economic losses. The available synthetic treatments are not fully effective and can negatively impact the environment, highlighting the need for sustainable alternatives. Several seaweeds are known for their antimicrobial properties, showing potential in this context. Pre-harvest trials investigated the effects of *Fucus vesiculosus* and *Sargassum muticum* extracts on pear trees. The seaweed extracts were applied both before and after inoculation with the pathogen *S. vesicarium*. The continuous application of *S. muticum* extract effectively prevented disease symptoms, possibly due to bioactive compounds including phytohormones, fatty acids, among others, suggesting the potential of seaweeds as natural priming agents to boost plant defenses.

Following the value-chain process of Rocha pear, post-harvest fungal infections, caused by pathogens such as *Alternaria alternata*, *Botrytis cinerea*, *Fusarium oxysporum*, and *Penicillium expansum*, also result in substantial losses, ranging from 20 to 25% of total fruit industry output. Seaweed extracts from *Asparagopsis armata*, *Codium* sp., *F. vesiculosus*, and *S. muticum* were evaluated for their antifungal properties. *In vitro* tests revealed that *A. armata* extracts strongly inhibited fungal growth, and promising *in vivo* results against *B. cinerea* were obtained using *S. muticum*.

These studies highlight the potential of seaweed-derived compounds in managing both pre- and post-harvest fungal diseases in Rocha pear, offering a more sustainable and ecofriendly approach to agricultural practices and fostering a bioeconomy that links the sea to the farm.



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sciforum-107677: Functional Characterization of novel synbiotic drink developed using kefir and basil seed mucilage

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Introduction: The growing demand for different dietary interventions including synbiotics that promote gut health benefits. We characterized the novel formulation of a synbiotic drink (SD) combination of Kefir (probiotic) and basil seed mucilage (prebiotic). Kefir, a milk-based fermented beverage, contains beneficial microorganisms and basil seed, a natural polysaccharide, and acts as prebiotic and fat-replacer agent.

Methodology: Kefir grains (3% w/v) and basil seed mucilage extract (BSME, 0.3% w/v) were inoculated with cow-milk and further allowed to ferment at 25°C for 24 hours. Stability and zeta-potential of SD was analysed using Zetasizer. Formulation of SD was estimated using Fourier-Transform Infrared Spectroscopy (FTIR). Micronutrient analyses were performed using AOAC methods. Amino acid profiling and fatty acid content was estimated using LC-MS and GC-FID, respectively. Antioxidant potential was evaluated through DPPH radical-scavenging activity, total phenolic compounds (TPC), total flavonoid content (TFC), and Ferric reducing antioxidant power (FRAP) assay.

Results: Zetasizer showed that the Zeta potential of 15 mV indicated towards substantial stability of synthesized SD. FTIR analysis confirms that the physicochemical properties of the milk changed during the fermentation process, due to addition of BSME. Micronutrient profiling revealed iron 3.5mg, calcium 29.3mg, potassium 120.6mg, and sodium 59.3mg per 100mL. Amino acid and fatty acid analysis revealed notable concentrations of essential amino acids and unsaturated fatty acids. Antioxidant assays indicated DPPH inhibition at 82%, TPC at 24 mgGAE/100mL, TFC at 61mg QE/100ml, and FRAP at 31mgTE/100mL

Conclusion: Novel SD formulation showed noble stability and micronutrient content and significant antioxidant potential. These findings suggest that this novel SD could serve as a beneficial dietary intervention for gut health.



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sciforum-104310: Harnessing Rosmarinus officinalis: A Dual Approach to Antioxidant and Antifungal Activity in Food Preservation

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Food is an essential part of human life, serving as a fundamental source of nutrition and energy. But has limited shelf life, so in order to increase the the latest and maintain it's quality certain preservatives are used , they prevent poisoning, illnesses, increase the shelf life and maintain its nutritional values[1]. As much as synthetic preservatives are effective they have significant disadvantages. Health risks include allergic reactions, hormonal disruptions, and potential carcinogenic effects. Environmentally, they are often non-biodegradable, contributing to pollution and ecotoxicity, harming wildlife and ecosystems. Extracts from medicinal plants are promising alternative natural preservatives cause of Their biological properties (antioxidant and antimicrobial) due to the presence of several active aromatic compounds [2]In this work, the antimicrobial capacities of extracts from *Rosmarinus officinalis* are measured. They were chosen for their beneficial effects for human health and their notable properties and richness with phenolic compounds. The extract was obtained by the maceration method with a yield equal 14.34%, measuring the antifungal activity of *Rosmarinus officinalis* extract using three different concentration 250,200 and 150 mg/L, the extract showed activity against FOL *Fusarium oxysporum* f. sp. *lycopersici* varies depending on the concentration, it showed highest inhibition percentage at 250 mg/L with $\tau=30.5\%$, as for the antioxidant activity the total phenolic compounds was measured , and several test been made ,by 2,2-diphenyl-1-picrylhydrazyl (DPPH), 2,2-Azinobis (3-ethylbenzothiazolin) -6-sulphonic acid (ABTS), Ferric Reducing Antioxidant Power (FRAP), and phenanthroline, the results showed that *Rosmarinus officinalis* extract exhibits an excellent antioxidant capacity.



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sciforum-103543: Impact of Individual Cow Milk Quality Measurement on Accuracy of Calibration Models Using Near-infrared Spectroscopy

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The purpose of this study was to use a near-infrared (NIR) spectroscopic sensing system to monitor each cow's milk quality accuracy every 20 seconds and every time the cow was milked. We used the milk fat, lactose, milk urea nitrogen (MUN), and somatic cell count (SCC) as four indices of milk quality. Raw milk samples were obtained from four Holstein cows belonging to Hokkaido University. Using an NIR sensing system, raw milk's NIR spectra were recorded every 20 seconds while the cows were being milked. The wavelengths of the spectra ranged from 700 to 1050 nm. Using the MilkoScan instrument, milk fat, lactose, and MUN were measured while a Fossomatic instrument was used to measure SCC. Partial least squares regression analysis was used to generate calibration models in order to verify the precision and accuracy of the models. The obtained results demonstrated that the accuracy of each cow's milk quality measurement every 20 seconds and at one milking time during the milking process was outstanding for milk fat and comparable for milk lactose. For every cow, the MUN and SCC findings showed a considerable difference. These findings showed that the measurement of each cow's milk quality could have an effect on the calibration models' precision and accuracy.



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sciforum-103090: Liquid and supercritical carbon dioxide extraction of bioactive components from pomegranate peel

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Rich and underutilized, pomegranate peel is a powerful source of nutrients with significant concentrations of dietary fibre, antioxidants, vitamins C and E, potassium, and punicalagin, among other bioactive substances. This study investigated the process of extracting bioactive substances from pomegranate peel, an agricultural food waste. Pomegranate peel extractions were carried out under liquid and supercritical conditions using carbon dioxide (CO₂), an environmentally acceptable solvent. We also investigated whether ethanol might be used as a cosolvent in tiny amounts of up to 30%. The extracts' antiradical activity, volatile organic chemicals, total polyphenolic levels, and individual polyphenolic profiles were assessed. When 30% ethanol was utilized as a cosolvent in both liquid (at 25 MPa and 30 °C) and supercritical (at 40 MPa and 50 °C) CO₂ extraction, the best yields were obtained. Furthermore, the extracts made with liquid CO₂ plus 30% ethanol had the highest concentrations of terpenes, specifically limonene, and naringin (36.41) among pomegranate peel extracts. According to ABTS+ and DPPH measurements, this extract type exhibited the highest antiradical activity (32.33–6–3.78 µmolTE g⁻¹). These results indicate that the extraction using a liquid CO₂ and ethanol mixture may be a good substitute for conventional solvent extraction, which uses 70% less organic solvent, and yields extracts rich in volatile organic chemicals and with strong antiradical activity.



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sciforum-107532: Microbial and Chemical properties of household-based water kefir fermented drink.

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Water kefir is a fermented probiotic-rich beverage that has potential health benefits, which include improving digestive health and preventing chronic disorders like obesity, irritable bowel syndrome, hyperlipidaemia, and hypertension. It is also a very good alternative for someone who is lactose intolerance and cannot have milk-based fermented drinks. This study aims to formulate and examine the microbial and chemical properties of three samples (A, B and C) of fermented drinks made from water kefir grains. For the development of the water kefir-based fermented drinks, a concentration of 2-6 gm of water kefir grains (WKG) was inoculated into 100 ml of mineral water containing 10 gm of brown sugar in aerobic conditions. The samples' pH, titratable acidity, water activity, color, total soluble solids, total bacterial count (TPC), antioxidant activity, and total phenolic content were assessed using AOAC methods. The sensory evaluation of the water kefir samples was examined using a nine-point hedonic scale.

The chemical and microbiological examination revealed that sample C was more desirable in all aspects as compared to samples A and B, with a pH level of 3.86; a TA of 0.04 meq/mL; water activity=0.9273±0.04 AW Aw; TPC= 3.1×10^7 ; DPPH= 78.75%; phenolic compounds= 40.755 mg/100 GAE; and an overall acceptability score of 7.29. The colour parameters of sample C were L* (lightness) = 20.29, a* (reddish/greenish) = -2.38, b* (yellowish/bluish) = 5.61, C** (saturation/vividness) = 6.01, and h° (hue angle) = 112.93. The overall results show that this concentration of water kefir fermented drink could be a great source of vegan fermented drink as well as a good alternative for preventing many diseases, including gut health issues.



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sciforum-103065: Natural Polymers and Their Applications in Fast Dissolving Tablets: A Comprehensive Review

Meet Vijaykumar Naliyadhara ^{1,*}, Riyaben Bharatbhai Chovatiya ¹, Shyam Rameshbhai Vekariya ¹, Deep Dineshbhai Undhad ¹ and Sheetal Sandip Buddhadev ²

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The oral route is the most preferred method of pharmaceutical delivery across all age groups due to its safety, convenience, and cost-effectiveness. This preference has driven innovation in fast-dissolving tablets (FDTs), or mouth-dissolving tablets (MDTs), which dissolve rapidly in the mouth without water, addressing issues faced by patients with swallowing difficulties, including pediatric and geriatric populations.

FDTs offer significant advantages over traditional dosage forms, enabling rapid breakdown in the buccal cavity for direct absorption through the buccal mucosa, ensuring quick therapeutic effects. This rapid disintegration and absorption enhances bioavailability and hastens drug effects by bypassing the gastrointestinal tract and first-pass metabolism.

This review examines the formulation, mechanism, advantages, and challenges associated with FDTs, including their properties and various preparation methods like freeze-drying, tablet molding, and spray drying. Special emphasis is placed on natural polymers, such as starch, chitin, chitosan, alginates, and xanthan gum, and various mucilages, derived from plants, animals, and microorganisms. These polymers are valued for their biocompatibility, biodegradability, and non-toxic properties, serving as binders, disintegrants, taste-masking agents, and stabilizers.

The review also explores regulatory considerations, emphasizing safety, efficacy, and quality control when using natural polymers. This review highlights recent advances in developing new natural polymers, sustainable sourcing practices, and improvements in extraction and purification technologies.

In conclusion, natural polymers significantly enhance FDT formulations, improving patient compliance and therapeutic outcomes. This review underscores their critical role in the evolving landscape of fast-dissolving drug delivery systems.



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sciforum-104614: Nutritious horticulture crops for malnutrition alleviation

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Malnutrition, including undernutrition, micronutrient deficiencies, and the rising incidence of overweight and obesity, remains a significant global health challenge. Horticulture crops, such as fruits, vegetables, roots, tubers, and legumes, have the potential to alleviate various forms of malnutrition through their nutrient-dense profiles. This investigation studies the nutritional compositions and health benefits of selected horticulture crops and their role in combating malnutrition. The data show that horticulture crops are rich sources of essential vitamins, minerals, dietary fiber, and phytochemicals. For example, spinach and kale are excellent sources of vitamins A (472 µg RAE and 565 µg RAE, respectively), C (28.1 mg and 93.4 mg), and K, as well as folate (179 µg) and iron (2.7 mg and 1.1 mg). Sweet potatoes are particularly high in vitamin A (835 µg RAE), while legumes like lentils provide substantial amounts of protein (9.0 g), fiber (7.9 g), folate (179 µg), iron (3.3 mg), and zinc (1.1 mg). Horticulture crops have demonstrated their ability to alleviate micronutrient deficiencies, reduce the risk of chronic diseases, and improve maternal and child health. However, challenges such as access, affordability, seasonality, and knowledge gaps must be addressed. Leveraging opportunities like biofortification, home/community gardening, value chain development, and nutrition education can transform the nutritious bounty of horticulture crops into sustainable solutions for combating malnutrition globally.



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sciforum-098881: Optimisation of microbiological, physicochemical and textural quality attributes of goat milk kefir

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Kefir is a popular probiotic drink known for its fermented, acidic, and slightly alcoholic properties. This study aimed to determine key processing variables, namely, the ratio of kefir grains/milk, the incubation temperature, and the incubation time, that optimise the quality of pasteurised goat milk kefir. Fourteen kefir treatments built upon three grain/milk ratios (0.5%, 1%, and 1.5%), three incubation times (16 h, 20 h, and 24 h), and three incubation temperatures (15 °C, 20 °C, and 25 °C) were carried out, according to a Box–Behnken design with three central points, to determine the best triplet variables regarding the following properties: pH, acidity (% of lactic acid), syneresis (%), mesophile and lactic acid bacteria concentrations, firmness, consistency, cohesiveness, and viscosity index. Response surface analysis was applied to each of the quality attributes. It was found that all the quality properties were affected by the three factors, with the factors having, in all cases, significant effects ($p < 0.05$) for the first-order estimation. Kefir acidity was maximised at 0.66%, 25.3 °C, and 22.8 h, although the temperature had a much greater effect than time, and in turn, the latter had a greater effect than the grains/milk ratio. In terms of the textural properties, the firmness and viscosity index were maximised under conditions of 1.07%, 19.9 °C, and 17.4 h and 1.28%, 18.5 °C, and 20.4 h, respectively. At an incubation temperature of 25 °C, syneresis was found to be between 38.5 and 39.9%; lower values (4.46 – 4.49%) were attained at 15 °C. Lower incubation temperatures or longer incubation times can also produce kefir with the desired acidity and textural quality regarding hardness and consistency, but only if the ratio is increased ($>1.0\%$). Thus, this study has been very valuable in understanding the effects of these three key processing variables and helping in the determination of the variables necessary to obtain goat milk kefir of good technological quality for subsequent studies.



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sciforum-104297: Optimization and characterization of olive leaf (*olea europaea*) obtained ultrasonic stimulations and vacuum by response surface methodology

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INTRODUCTION

Olive leaves, a byproduct of olive tree pruning, are considered an industrial residue with significant potential due to their content of bioactive compounds, such as oleuropein and hydroxytyrosol, which exhibit antioxidant, anti-inflammatory, and antimicrobial properties. Traditional extraction methods for these compounds typically require large volumes of solvents, prompting the need for innovative technologies that minimize solvent use and reduce processing times. Conventional methods often involve the use of heat and agitation to enhance the transfer of compounds from olive leaves into the solvent. A new extraction technique has been developed, using high temperature, ultrasound, and vacuum to improve the efficiency of compound extraction.

METHODS

To optimize the process, response surface methodology was employed, evaluating the influence of key variables (% EtOH, temperature, and number of cycles) at three levels (low, medium, high). A total of 27 assays were conducted. The samples were analyzed by HPLC-DAD and Folin-Cocolteau method for the assay of total phenols; DPPH and FRAP methods for antioxidant activity methods.

RESULTS

The highest yield of the extractions of oleuropein and hydroxytyrosol was observed at medium level of temperature, high level of hydroalcoholic solution, and medium level of number of cycles obtaining 43.53 mg/g and 2.73 mg/g for oleuropein and hydroxytyrosol, respectively. In contrast, samples processed without the new technology, yielded 35.08 mg/g and 2.70 mg/g for oleuropein and hydroxytyrosol, respectively. The antioxidant activity, assessed by the FRAP and DPPH methods, showed that untreated samples yielded 1.5 mg TE/g, which increased to 3.31 mg TE/g under conditions of high % EtOH, low temperature, and high flash cycles.

CONCLUSIONS

The optimal combination of variables enhanced the extraction yield by up to 24% for bioactive compounds like oleuropein, compared to unprocessed samples.



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sciforum-107846: Soluble fibers from persimmon by-product promote the growth of anti-inflammatory beneficial bacteria and display anti-inflammatory properties

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Persimmon by-product serves as a good source of bioactive compounds like polyphenols, carotenoids or polysaccharides. The revalorisation of these by products could offer different venues to develop new functional ingredients that promote the health and well-being. Here we determined the potential of soluble polysaccharides from persimmon by-product to promote the growth of specific beneficial bacteria from the human gut that are implicated in anti-inflammatory properties. Our results suggest that persimmon polysaccharides promote the growth of Firmicutes species that display anti inflammatory properties, especially due to their stimulation in the production of short chain fatty acids like butyrate, showcasing a noted effect with beneficial fermentation profile stimulation than the control (glucose). These fractions also generated anti inflammatory properties in RAW 264.7 cells (macrophages), by reducing the levels of IL-6 and TNF- α . Also, the samples showed to promote the production of antioxidant enzymes such as catalase and superoxide dismutase. In this sense, the samples have displayed anti inflammatory properties by both, regulating the inflammatory response of stressed cells, as well as by promoting the growth of specific beneficial bacteria. These results suggest a noted potential of persimmon fractions to be used as functional ingredients, especially for diseases related to uncontrolled pro-inflammatory that require supplements.



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sciforum-104187: Sour beer fermentation without using bacteria

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For a lot of microbrewers, the use of lactic acid bacteria for sour beer production could be an interesting product differentiation strategy. However, the subsequent difficulties in containing contaminations between products could lead to problems regarding product stability and batch reproducibility. The potential use of non-*Saccharomyces* yeast for sour beer production can be an interesting alternative. In this study, the strain *L. thermotolerans* was used for its ability to lower the pH during fermentation. The yeast was tested with an all-grain wort of an original gravity (O.G.) of 12 °P and 5.1 pH, under different conditions like temperature (13, 18, 24, 30) °C and supplemented with glucose (at 16, 20 °P). It was shown that *L. thermotolerans* has a great ability to ferment at different conditions (albeit slower than *S. cerevisiae*, up to ~14 days at 12 °P O.G.) and could lower the pH at ~3.5 by day three. It completed the fermentations in all different temperatures and original gravities. Lower temperatures resulted in longer fermentation periods (~30 days) and higher pH levels (~4.0). Furthermore, higher original gravities did not slow the fermentation rate; to the contrary, the addition of higher amounts of glucose resulted in a more rapid pH drop by day two and lower overall pH (~3.0). In conclusion, *L. thermotolerans* seems to be a very capable souring yeast that had no negative effect on color, turbidity, foam stability and other beer characteristics. The sensory profile of the produced beers was different depending on the O.G. and fermentation temperatures, but did not exhibit any sensory faults.



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sciforum-107764: The impact of gas micro/nano-bubbles on the fermentation pattern and rheology of stirred yoghurt

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Micro/nano-bubbles (MNBs) are tiny gas-filled cavities in bulk liquids. Recently, MNBs have drawn a lot of attention due to their industrial applications, such as in wastewater treatment, cleaning, disinfection, and other agriculture- and food-related applications due to their low cost, eco-friendliness, and ease of scale-up. Fermentation is an age-old practice adopted for the preservation of food and dairy products. Stirred yoghurt is one such product prepared by adding yoghurt starter culture and breaking the clumps after incubation. The present study attempted to understand the impact of the incorporation of MNBs on the fermentation pattern of yoghurt starter culture (YSC), i.e., *Streptococcus thermophilus* and *Lactobacillus bulgaricus*, and its rheological attributes when thus prepared. Different types of MNBs were prepared using compressed purified air, CO₂, O₂, and N₂ gas in water and milk systems using a bulk nanobubble generator. It was observed that the types of MNBs had a significant impact on the metabolism and microbial growth of the starter culture. Among the four different types of MNBs, the CO₂-MNBs had a significantly positive effect on bacterial growth besides increasing the viability of the fermented milk. Our findings suggest that MNBs in general and CO₂-MNBs specifically have the potential for applications in altering fermentation patterns. Furthermore, concerning the quality attributes of the MNBs incorporated into the stirred yoghurt, notable changes were observed in terms of its viscosity, mouthfeel, and shelf life. A significant rise in the viscosity of the stirred yoghurt with MNBs incorporated was observed as compared to that of the control sample, which may be attributed to the milk protein-polysaccharide interaction at the interface of the MNBs. It is therefore concluded that MNB technology has the potential to be used as a new processing tool to easily adjust the fermentation pattern and the rheological properties of fermented dairy products to fulfil growing consumer demand for innovative products with adjustable consistency and functionality.



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sciforum-102988: The Influence of Oregano powder on the chemical, microbiological and sensorial quality of bun-bread

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The influence of the incorporation of oregano powder (1.5 and 3% of flour) on the chemical, microbiological and sensorial quality of bun-bread were investigated. Oregano powder, known for its antioxidant and antimicrobial properties, was added to bun-bread at varying concentrations to assess its effectiveness in enhancing bread quality. The chemical composition, microbiological, and sensory analysis of the supplemented bun-bread were measured. Sensory evaluation involved a panel of trained judges who assessed attributes such as flavor, texture, aroma, and overall acceptability. Results showed that the lowest amount of oregano powder (1.5%) revealed the best value of sensorial scores, in terms of its color and nature of crust, crumb color, texture, aroma, and taste. The results revealed that 1.5% of oregano powder can be involved in bun-bread preparation without modifying dough processing and bun-bread overall features, where this ratio approximates chemical compositions, microbiological stability, and shelf-life of bun-bread. Among the explored samples, bun-bread with 1.5% of oregano powder could be utilized industrially with acceptable properties and shelf-life stability. This study suggests that oregano powder is a valuable natural additive for improving the nutritional quality, safety, and sensory attributes of bun-bread, making it a viable option for consumers seeking functional and preservative-free baked goods. The findings highlight the potential of incorporating oregano powder in bread production to deliver health benefits and extend shelf life, aligning with growing consumer demands for healthier and more sustainable food options.



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sciforum-103498: The use of activated carbons to remove heavy metals and N-phosphonomethyl)glycine from European wines

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The pollution of the planet has exceeded all limits. One aspect of concern is the environmental burden caused by heavy metals. The issue with these metals is that they tend to accumulate in the environment, leading to adverse effects. In the present work, we deal with the detection and removal of specific heavy metals (Lead, Cadmium, Mercury, Zinc, Chromium, Cobalt, Copper, Iron, Nickel, Selenium, Silver and Arsenic) from European wines with activated carbon from potato peels (AC-Pot) and banana peels (AC-Ban). In addition to heavy metals, we use the same activated carbon to remove (N-phosphonomethyl)glycine. Activated carbon derived from potato peels (AC-Pot) and from banana peels (AC-Ban) was prepared and characterized. Then, we selected ten wine samples of various European countries such as Greece, Italy, Austria, France, Portugal, etc., and measured their content of the above heavy metals as well as the chemical substance (N-phosphonomethyl)glycine. We repeated the measurements a few days after the addition of the activated carbons in the wine samples; the same procedure was carried out three more times over 2 years on the same wine samples. The results obtained were quite satisfactory, and the conclusions drawn were very useful for further study. Some metals were more present in the samples, while others had higher rates of removal after the activated carbon treatment.



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sciforum-107336: Application of image analysis in the assessment of '*Mejhou*' date fruit quality under freezing storage

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The emergence of new technologies focusing on “image analysis” contributes significantly to the assessment of fruit quality based on objective and non-destructive features. In this investigation, the '*Mejhou*' date fruit cultivar was subjected to freezing at -10°C and -18°C and stored for 6 months. Its quality was evaluated according to texture features extracted from images acquired using a digital camera and flatbed scanner. The extraction process was carried out according to an internal procedure using MaZda software. Then, the extracted features were used as inputs for pre-established algorithm groups within WEKA software to classify frozen date fruit after 0, 2, 4, and 6 months of storage. Accordingly, reducing these features using the “Best-First” method allowed for a selective ranking of about twenty accurate features that were submitted to four classifier groups of algorithms: Bayes, Functions, Lazy, and Trees.

The results allowed for the extraction of a hundred texture features that differ depending on “storage temperature” and “storage period”. Furthermore, high accuracy levels for the classification of '*Mejhou*' date fruit were obtained for each storage period based on the selected features, and slight differences were noted between the algorithms used. In future, physicochemical attributes will be added to the developed models to correlate with image features and predict the behaviour of date fruit under storage.



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sciforum-107680: Bioactive Potential of *Castanea sativa* Hedgehog Extracts for Sustainable Packaging Solutions

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Bioactive packaging is a term that has become increasingly widespread in society. This packaging enhances the effectiveness against food deterioration and inhibiting microbial growth, which is often associated with food loss and waste (1). Natural extracts from agro-industrial by-products have been shown to improve packaging properties, including physical and mechanical characteristics, while also potentially providing antioxidant and antimicrobial effects. Which can extend food shelf life and reduce dependence on synthetic additives (2). This research focuses on *Castanea sativa* hedgehog extracts obtained from northeastern Portugal. This by-product extract is rich in bioactive components, including both condensed and hydrolysable tannins, phenolic acids (such as ellagic and gallic acids), and flavonoids (including catechin, epicatechin, apigenin, quercetin, and rutin), all of which exhibit important antioxidant and antimicrobial activities (3,4). The purpose of this study is to evaluate the possibility of incorporating *C. sativa* hedgehog extracts as bioactive compounds in composite films. The biological properties of this extract, such as its antibiofilm, antimicrobial, and antioxidant characteristics, were assessed. The results obtained show high antioxidant activity, with free radical scavenging values of 0.17 mMTrolox/g and 0.43 mMTrolox/g, as determined by the Ferric Reducing Antioxidant Power and 2,2'-azinobis (3-ethylbenzothiazoline-6-sulfonic acid) assays, respectively. In terms of antimicrobial assays against key pathogens, the extracts demonstrated broad-spectrum efficacy, achieving activity rates of 78% against *Staphylococcus aureus*, 75% against *Escherichia coli*, and 51% against *Klebsiella pneumoniae*. Furthermore, biofilm reduction was observed, with decreases of 75% for *S. aureus*, 54% for *E. coli*, and 36% for *K. pneumoniae*. These results support the statement that *C. sativa* hedgehog extracts represent a promising natural source of bioactive compounds for future applications in bioactive packaging materials.



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sciforum-107822: Electrochemical techniques for monitoring analytes dissolved in acidic solutions for the food industry

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Introduction

Real-time monitoring of liquid solutions has several critical applications in the food industry, where detecting and quantifying several analytes is essential for preventing health hazards, guarantying quality control and reducing production costs. The wine industry is presenting an increasing interest in monitoring different analytes, like sulfites, leading to studies regarding different materials and monitoring techniques. Electrochemical solutions present significant advantages for industrial applications due to their straightforward instrumentation. Nevertheless, when dealing with complex chemical solutions, like wine, one must find methods that allow for simple calibration curves and reutilization and can effectively account for many interfering molecules.

Methods

In this work, we applied different electrochemical techniques for monitoring sulfites in acidic solutions. Electrodes made from different materials were used to perform the techniques of amperometry and cyclic voltammetry for sulfite detection. DC potential and pulsed amperometry techniques were compared. Cyclic voltammetry was used for detecting sulfites and identifying different solutions.

Results

The results show that amperometry can be used to monitor different concentrations of sulfites, using pulsed potential waveforms (PAD) to prevent signal decay, and provide a more stable response. Cyclic voltammetry can also monitor sulfites but one great application is in identifying different solutions, analytes and electrodes, thus adding layers of information with features present in the respective voltammograms.

Conclusions

The information gathered from these electrochemical techniques can be fed into different models that allow for the separation of interfering molecules from our desired target analyte. This suggests the potential of using amperometry and CV together as applicable methods for real-time analyte monitoring in the food industry.

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sciforum-104551: Estimation of Lod of Detection of *Proteus* spp. In Surface Samples

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Microbiological contamination of surfaces in food production facilities and food-handling areas represents a major challenge in preventing cross-contamination and selecting biocidal products. Consequently, examining the microbiology purity of surfaces that come into contact with food requires a serious methodological approach.

This paper presents the method of determination of *Proteus* spp. from surface samples (5x5 cm²). The three levels of artificial soiled aluminium foil were prepared using bacterial suspensions of *Proteus hauseri* ATCC 13315. After the surface swabbing method for determination of *Proteus* spp. was applied. The swab was homogenized with Eugon LT 100 broth and 1 mL was transferred to enrichment broth. After incubation of the enrichment broth, streaking on the Brilliant green agar and SS agar was performed. The characteristic colonies were confirmed by biochemical reactions.

The number of positive findings of *Proteus hauseri* on the applied level of contamination was used for calculation by the PODLOD_ver12.xls ECEL program by Wirlich and Wilrich. This program estimates the probability of detection (POD) function and the limit of detection (LOD) of qualitative microbiological methods.

The results of the detection of *Proteus hauseri* in surface samples showed a LOD_{50%} = 48.957 [24.596; 97.446] CFU in 1 ml of swab rinse, and LOD_{95%} = 211.589 [106.303; 421.155] CFU in 1 mL of swab rinse.

These results open a discussion about the performance of the applied method. Also, they provide ideas for further research related to the type of surface, the type of used swab sticks and the type of microorganisms tested.



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sciforum-107642: Evaluating the Antibiofilm and Antibacterial Properties of Diverse Honeys on Chronic Wound Pathogens

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Honey is an inexpensive, food-based option for treating diabetic foot ulcers (DFUs) due to its anti-inflammatory and antibacterial properties. It has proven effective against bacterial biofilms and multidrug-resistant bacteria, positioning honey as a promising candidate for DFU management. However, honey's physicochemical properties and concentration variations can lead to differing bacterial responses. This study aimed to assess the effects of various honey types and concentrations on bacterial biofilms. Seven honey types were tested at concentrations of 1x, 5x, and 10x the minimum inhibitory concentration (MIC) against biofilms of *Staphylococcus aureus*, *Escherichia coli*, *Klebsiella pneumoniae*, *Pseudomonas aeruginosa*, and *Candida albicans*.

Results indicated that honey types 3 and 4 achieved significantly higher biofilm removal for *C. albicans* compared to types 5 ($p = 0.008$; $p = 0.001$), 8 ($p = 0.022$; $p = 0.003$), and 9 ($p = 0.009$; $p = 0.001$) at the same concentrations. Similarly, honey types 2 and 4 were more effective against *E. coli* than type 9 ($p = 0.016$; $p = 0.004$). Higher honey concentrations resulted in greater biofilm removal for *C. albicans* and *E. coli* ($p = 0.004$, both), and more pronounced biofilm metabolic inactivation for *C. albicans*, *K. pneumoniae* ($p = 0.004$, both), and *P. aeruginosa* ($p = 0.048$). Principal Component Analysis suggested a correlation between pollen content and antimicrobial activity. Overall, honey demonstrated significant potential in removing bacterial biofilms and inhibiting metabolic activity, particularly at higher concentrations. The differences in bacterial responses to honey treatments may be attributed to variations in the honeys' physicochemical properties and bacterial strain sensitivity.



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sciforum-104432: Innovative Use of Spent Brewer's Yeast for Tannin Adsorption from Treatment Solution

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This study aimed to evaluate the capacity of spent brewer's yeast (BSY) to adsorb tannins and other phenolic compounds from an alkaline-extracted chestnut shell tannin solution (CS tannin extract). The alkaline extraction process used 5% NaOH (v/v), a method commonly employed to extract cellulosic material from chestnut shells (CSs). The findings of this research contribute to the development of more sustainable laboratory practices and enhance the economic viability of cellulosic material extraction from CS.

Various treatments—lyophilization, immobilization in calcium alginate beads, and both alkaline and acid treatments—were applied to BSY to determine which method resulted in the highest tannin adsorption capacity from the CS tannin extract. Kinetic and equilibrium adsorption studies were performed to identify the best adsorption approach. The tannin content was analyzed using the Folin–Ciocalteu method, with results expressed as milligrams of tannic acid equivalents (TAEs) per milliliter of extract solution. The adsorbent material was characterized before and after the experiments; the characterization methods included the determination of the point of zero charge (pH_{PZC}), Fourier Transform Infrared (FT-IR) Spectroscopy, and Scanning Electron Microscopy with Energy Dispersive Spectroscopy (SEM/EDS).

Equilibrium was reached within 10 minutes, with the highest ($p < 0.05$) biosorption capacity of tannins from the CS tannin extract observed in lyophilized BSY (35.51 ± 0.97 mg TAE per gram of BSY). The Sips models provided an adequate description of the adsorption process, indicating that tannin biosorption by BSY is driven by chemisorption. FTIR analysis identified various functional groups in BSY, with carboxyl, amino/hydroxyl, and amide groups playing a significant role in the biosorption process.

Overall, these findings suggest that BSY has potential as a delivery system for the valorization of tannins from treatment solutions.



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sciforum-104345: Strong antioxidant activity of the probiotic *Bifidobacterium animalis* subsp. *lactis* on HeLa cells - in 2D co-culture system: a promising approach to the use of probiotics in anticancer activity

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Cancer cells contain higher levels of ROS (Reactive Oxygen Species) and RNS (Reactive Nitrogen Species) than normal cells. The increased levels of ROS/RNS in cancer cells stimulate proliferation as well as metastasis processes. Therefore, maintaining the level of these reactive species is an important factor in antitumor therapy. *Bifidobacterium animalis* subsp. *lactis* (BAL) probiotics have been attracting much attention for the last few years due to the increasingly noticeable results in the field of anticancer activity. These live microbes in combination with food products, such as mushrooms, have great potential in cancer therapy.

This study aimed to examine the individual antioxidant effect of the probiotic BAL on HeLa cells (cervical cancer cell line), as well as its activity in co-treatment with the ethyl acetate extract of the mushroom *L. sulphureus* (EALS – concentration 10 µg/mL). NBT assay was used to quantify superoxide anion radicals' level (O_2^-), Griess assay for NO_2^- , and glutathione test for GSH according to standard procedures. Cervical cancer cells were incubated with treatments in a modified 2D co-culture system, and the results were evaluated after 12 and 24 h.

Our results suggest a strong antioxidant activity of BAL probiotics on HeLa cells. The levels of ROS and RNS, as well as GSH, remained at significantly low levels compared to the control. This is especially important if we consider that it is favorable for cancer cells to have reactive species elevated. On the other hand, in the BAL/EALS 10 µg/mL treatment, the parameters of oxidative status were higher compared to BAL, which indicates that the EALS extract slightly reduced the antioxidant activity of the tested probiotic. Overall, the results of this study indicate that BAL and BAL/EALS 10 µg/mL treatments are valuable subjects for future studies of antioxidative activity in HeLa cells.



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sciforum-104445: Transforming *Citrus* Peel Waste: Innovative Green Extraction and Multi-Functional Applications of Pectin and Essential Oils

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The present study focuses on the green extraction methods and the evaluation of the biological properties of pectin and essential oils derived from *citrus* peel waste, aiming to both add value to these byproducts and manage waste effectively. *Citrus* peels are abundant in bioactive compounds, rendering them an innovative resource for transforming waste into value-added products. Pectin, a non-starch polysaccharide, and essential oils, consisting of volatile aromatic compounds, present opportunities for diverse industrial applications, depending on the extraction methods and raw material sources. This research integrates recent advancements in sustainable extraction technologies with a comprehensive review of peer-reviewed literature to compare the physicochemical properties and biological activities of pectin and essential oils from diverse *citrus* species. Key aspects investigated include the efficiency of different green extraction methods, the impact of raw material variation on product quality, and the potential for novel applications in functional foods, natural preservatives, and therapeutic agents. The systematic review highlights how the synergy between the physicochemical attributes and biological activities of *citrus* peel derivatives can drive their applications in functional foods, natural preservatives, therapeutic agents, and other industrial applications. By integrating recent advancements in sustainable extraction technologies, the importance of leveraging waste-derived compounds to achieve both economic and environmental goals, thus supporting the development of environmentally sustainable practices within the citrus industry.



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Session 8. Applied Physical Science

sciforum-104458: Thermo-optic discrimination of aqueous solution composition using a multimodal interference fiber optic sensor

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The precise optical identification of aqueous solutions with different compositions is challenging for samples that have a similar refractive index at a certain temperature. However, their thermo-optic response, which describes how the refractive index varies with temperature, provides simple means for discrimination. We report on the use of a conventional fiber optic sensor based on multimodal interference to distinguish aqueous solutions of Tris and fructose based on thermo-optic effects. At room temperature, aqueous solutions of these components have indistinguishable properties. In fact, our sensor exhibited a linear dependence on concentration in both cases, with similar sensitivities of 0.2179 nm/% for Tris and 0.2264 nm/% for fructose, indicating that their discrimination is hindered based on concentration. On the other hand, by changing the temperature controllably, from 25°C to 45°C in increments of 2.5°C, we were able to change the refractive index enough to clearly discriminate between the samples at the same concentration. The thermal sensitivity measured was 0.14433 nm/°C for Tris and 0.1852 nm/°C for fructose, allowing for evident differentiation among samples in the range of 35°C to 45°C. Our findings demonstrate that the proposed thermo-optic discrimination approach is effective and offers a promising practical solution; the optical fibers do not need to be prepared in a special way and the temperature control can be carried out with general-purpose laboratory equipment, like a hot plate, over a temperature range that is easily attainable. Overall, the results presented are relevant to industrial and research applications involving advanced monitoring and fine processing control.



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sciforum-104268: Unveiling the Binding Dynamics of two organic compounds with Human Serum Albumin: Integrating Computational, Spectroscopic, and Preliminary Single-Crystal X-ray Diffraction (SCXRD) Insights

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This study investigates the interactions between human serum albumin (HSA) and two detergents, propylene carbonate (PC) and decyl glucoside (DG), using a combination of experimental and computational approaches. Albumin, a highly abundant and multifunctional non-glycosylated protein, plays a crucial role in various physiological processes and exhibits significant changes in plasma levels in response to inflammation. To understand the binding affinity and stability of these detergents with HSA, we employed molecular docking, molecular dynamics (MD) simulations, UV-visible spectroscopy, and preliminary single-crystal X-ray diffraction (SCXRD) analysis. Molecular docking studies revealed that DG binds more effectively to HSA than PC, as indicated by lower free energy of binding (FEB) values. MD simulations provided insights into the stability of the HSA-detergent complexes, showing that while the ligand remained relatively stable, a slight repositioning occurred during the simulation. UV-visible absorption spectroscopy confirmed the interaction of both PC and DG with HSA, evidenced by changes in the absorption spectrum, particularly around 280 nm. Preliminary SCXRD analysis of HSA crystals indicated successful crystallization, though attempts to crystallize the HSA-PC complex were unsuccessful. Overall, this study highlights the binding affinities and interaction dynamics of PC and DG with HSA, emphasizing the impact of these interactions on albumin's functionality. The integration of experimental data and computational modeling offers a comprehensive understanding of these molecular interactions, potentially guiding future research and applications in biological and industrial contexts.



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sciforum-107189: Convergence of The Mann Iteration For Hardy–Rogers Contraction Mappings In Convex G_b : Metric Spaces With An Application To Fredolm-Type Integral Equations

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The convergence of the Mann iteration scheme to fixed points of any class of mappings in any space is guaranteed only on the existence of a convexity structure defined therein.

For metric spaces, one notion of convexity is that propounded by Takahashi, and it has been generalized to the framework of metric spaces, establishing convex metric spaces as defined by Takahashi. For these particular spaces, a result has been published that establishes the condition for which the Mann iteration converges to fixed points of Banach contraction mappings defined therein.

On consideration of this result, the author of this work was inspired to formulate an analogous result that establishes the condition for which the Mann iteration converges to fixed points of Hardy–Rogers contraction mappings in the same framework. This result is novel in the sense that no such result has been published by any author. Additionally, it extends the cited existing result to a bigger class of contraction mappings.

Also, since Banach contraction mappings, Kennan contraction mappings and Chatterjee contraction mappings are special cases of Hardy–Rogers contraction mappings, this result produces three corollaries, each establishing a condition for the convergence of the Mann iteration for only one of the mentioned classes of contraction mappings.

Finally, this result is applied to the existence and approximation of solutions of Fredolm-type integral equations of the second kind; these equations arise in many problems in signal processing, theory of imaging and fluid mechanics, among other fields in the physical sciences and engineering.

In sum, the result to be presented extends a result on the convergence of the Mann iteration in convex G_b metric spaces and is applied to the existence and approximation of solutions of Fredolm integral equations, which find expressions in many models in science and engineering.



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sciforum-105976: Correlation Between Nutrient Concentration and Leaf Extinction Coefficient of *Brassica Rapa* (Pechay) as Measured by Time Domain Optical Coherence Tomography System

Tristan Dave Taeza ^{1,*}, Mark Emmanuel Witongco ¹, Maria Cecilia Galvez ¹, Edgar Vallar ¹, Mark Nickole Tabafa ¹, James Roy Lesidan ¹, Jumar Cadondon ¹, Jejomar Bulan ¹ and Tatsuo Shiina ²

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This study explores the relationship between nutrient concentration (**NC**) and epidermal thickness(**d**) of the leaves of hydroponically grown *Brassica rapa* and its attenuation coefficients (**m**) using a portable Time-Domain Optical Coherence Tomography (TD-OCT), which is a non-invasive imaging technique that uses low-coherence interferometry to generate axial scans of plants leaves by measuring the time delay and intensity of backscattered light. The portable TD-OCT system in this study has an axial and lateral resolution of 7 μm and 3 μm , respectively, a scanning depth of 12 mm, and a 1310 nm Super Luminescent Diode (SLD). Several studies suggest that the differences in **d**, and **m** indicate the status of plant health. The study used the Kratky method, a simple non-circulating hydroponic system, to cultivate *Brassica rapa* with varying **NC** (25%, 50%, 75%, 100% (control), and 125%). Each treatment group used two plants. The TD-OCT sample probe was placed on a fixed holder and was oriented vertically so that light was directed downward onto the leaf's surface to obtain the depth profile (A-scan). The distance between the probe and the leaf was adjusted to get the optimum interference signal. Five averaged A-scans were obtained per leaf on the 7th, 18th, and 21st days post-nutrient exposure. The logarithm of the averaged A-scan is linearly fitted to extract **m**. Results showed a positive correlation between **NC** and **m** which suggest that plants produce more chlorophyll and develop denser cells and increase **m**. There was no correlation obtained between **NC** and **d**. The study demonstrates the potential of TD-OCT as a non-destructive tool for assessing plant health and monitoring growth dynamics in hydroponic systems and **m** as a sensitive indicator of plant health as compared to **d**. Continued exploration of TD-OCT applications in agriculture can contribute to improving crop management strategies and promoting sustainable food production practices



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sciforum-104539: Extension of the Log-Logistic Distribution for Groundwater Analysis and Potability Prediction Using Machine Learning Models

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Groundwater quality analysis and potability prediction are essential for public health and sustainable environmental management. This study adopts a two-part approach, integrating statistical modeling and machine learning classification to analyze groundwater data. In the modeling phase, we introduced the Inverse Power Log-Logistic (IPLL) distribution, specifically designed to capture the unique characteristics of groundwater quality data, focusing on pH and sulfate concentrations due to their significant impact on water potability and health. pH levels are critical as they affect water acidity and the potential for heavy metal dissolution, while sulfate concentrations are commonly associated with water taste and health risks when present in excess. We derived key structural properties of the IPLL distribution, including its moments, hazard, and survival functions, with parameters estimated using maximum likelihood estimation. Compared to conventional models, the IPLL distribution shows enhanced flexibility and accuracy, as measured by metrics such as AIC, BIC, and RMSE. In the classification phase, we applied machine learning algorithms—logistic regression, K-Nearest Neighbors (KNN), Support Vector Classifier (SVC), and Random Forest—to predict groundwater potability. Performance was evaluated using accuracy, F1-score, and ROC-AUC. Random Forest achieved the highest accuracy (92.3%), F1-score (0.89), and ROC-AUC (0.94), with SVC following closely at 89.7% accuracy, 0.87 F1-score, and 0.92 ROC-AUC. Both KNN and logistic regression models also performed well, achieving accuracy scores of 87.5% and 85.2%, respectively. This study offers a comprehensive framework for groundwater analysis, combining advanced statistical modeling with effective machine learning classification. The IPLL distribution's adaptability to environmental data and the machine learning models' predictive strength in potability assessment provide valuable insights for public health officials and environmental policymakers. This dual approach has broad potential applications in fields that require reliable data modeling and prediction.



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sciforum-103526: Green Synthesis of Carbon-Based Aerogels for Sustainable Applications

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Aerogels, with low density and high porosity, are promising materials for applications in food packaging, energy storage, thermal insulation, and water treatment [1]. This study introduces a sustainable method for producing carbon-based aerogels via hydrothermal carbonization of accessible precursors. Samples with CaCl_2 and glucose at mass ratios 2 were placed in PTFE-lined autoclaves and heated to 220°C . After cooling, the solid products were recovered and analyzed using XRD, SEM-EDX, FTIR, and UV-VIS DRS. At temperatures above 146°C , glucose liquefies, dissolving CaCl_2 and forming a viscous mass that decomposes above 200°C , releasing water vapor and CO_2 , which expands the melt. The aerogel's volume remains stable unless bubble coalescence collapses the foam. Experiments show that without CaCl_2 , the carbon structure is nearly non-porous. Adding CaCl_2 creates a porous structure with a maximum pore size of ~ 40 micrometers at a CaCl_2 /glucose ratio of 0.5. The average pore size decreases by over 50% as this ratio exceeds 1.8. XRD spectra also reveal CaCO_3 formation from CO_2 reacting with molten CaCl_2 , with solid particles reducing pore coalescence by increasing viscosity. The study presents a novel method for producing carbon aerogels in a closed environment through thermal decomposition of glucose–calcium chloride mixtures. By adjusting the CaCl_2 : glucose ratio, the average pore size can be controlled, enabling formation of either non-porous amorphous carbon or closed-cell aerogels. Higher CaCl_2 concentrations result in smaller pores due to increased viscosity and enhanced surface tension of the melt. In conclusion, the development of tunable pore size aerogels through the controlled synthesis of carbon aerogels offers significant potential for a wide range of applications. These materials have the potential to revolutionize fields like energy storage, catalysis, environmental remediation, and biomedical engineering. This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CCCDI-UEFISCDI, project number PN-IV-P8-8.3-PM-RO-BE-2024-0004 within PNCDI IV.



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sciforum-105399: Variable Angle Spectroscopic Ellipsometry of thick TiO₂-P25 films: graded-layer modeling for depth-dependent optical analysis

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Titanium dioxide (TiO₂) is a highly versatile material extensively used due to its non-toxic nature, chemical stability and high photocatalytic activity. These features make TiO₂ particularly promising for a wide range of applications, especially as a film coating on various substrates. TiO₂ is commercially available in many forms, including pure anatase and mixed-phase products like P25, which is a mixture of anatase (80%) and rutile (approximately $\leq 20\%$), ideal for photocatalysis.

In this study, TiO₂-P25 films on FTO substrates were synthesized using the sol-gel process and studied using Variable Angle Spectroscopy Ellipsometry (VASE) to determine their optical constants and thickness. The measurements were carried out at room temperature in the wavelength range (300–900) nm at incident angles varying from 55° to 70°. The resulting thicknesses were found to be ranging from 1000 nm to 10000 nm.

Scanning Electron Microscope (SEM) measurements confirmed the porous nature of the films, suggesting an inhomogeneous structure with depth-dependent compositional gradients. The novelty of this study lies in the structural complexity of these films that presented unique challenges for VASE measurements, which are typically straightforward for thinner films under a few hundred nanometers.

A graded layer model, which allowed for an accurate representation of the depth-dependent optical variations, was employed to model the properties of these TiO₂-P25 films. This advanced modeling approach provided deeper insights into the internal structure of the films, particularly how the graded structural characteristics impact the overall optical behavior. The bottom layers of the films typically exhibited a significant increase in both refractive index and extinction coefficient, indicating greater density and higher absorbance compared to the top layers. Understanding these depth-dependent variations is essential for optimizing the use of TiO₂-P25 films in technologies such as solar cells and optical devices, where precise control over material properties is critical.



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