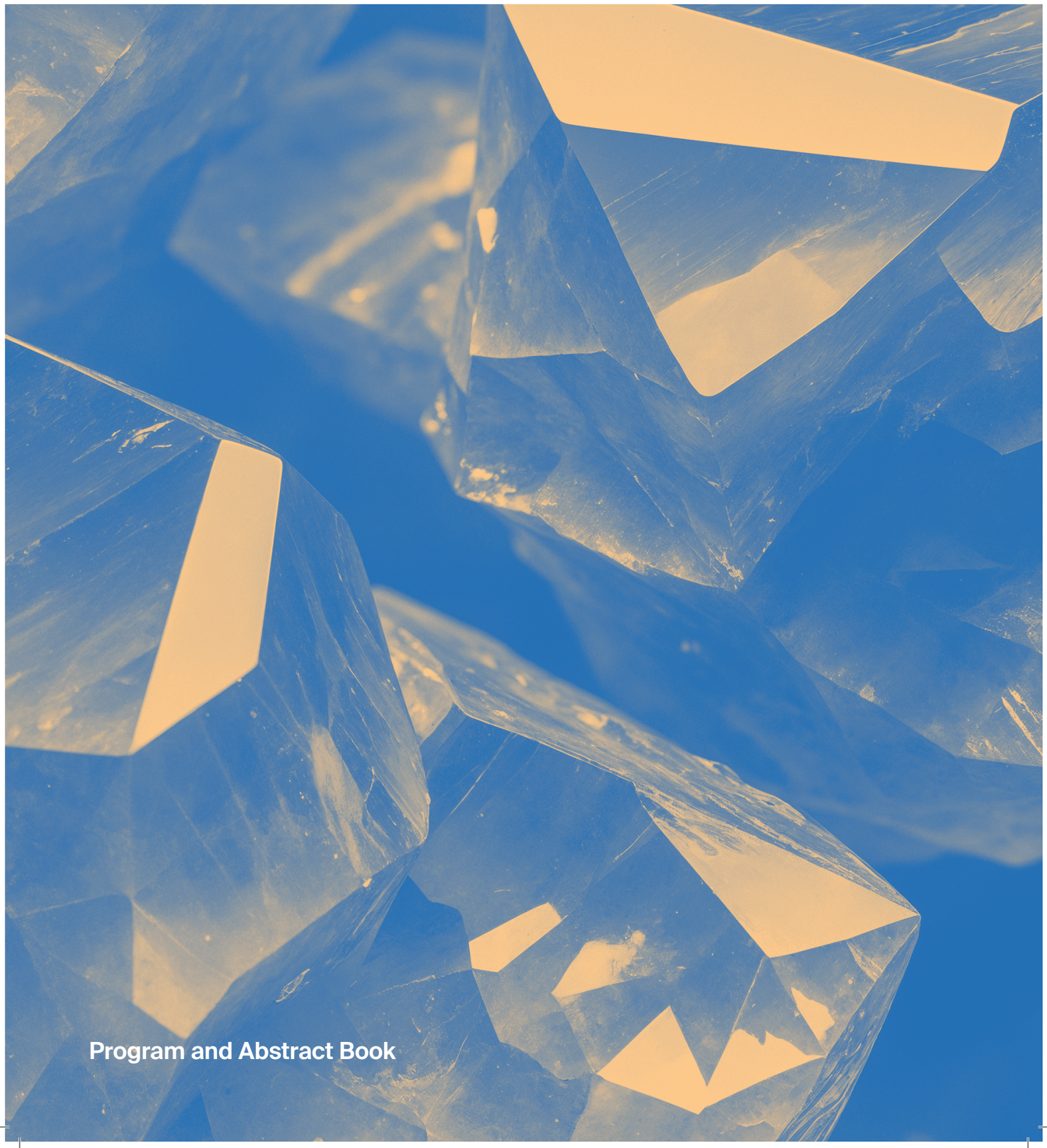
IOCC
2026
Conference

The 5th International Online Conference on Crystals

15–17 June 2026 | Online



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MDPI

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Welcome from the Chair

Dear Colleagues,

It is our great pleasure to announce the **5th International Online Conference on Crystals (IOCC 2026)**, a premier online event dedicated to the latest advancements in research about crystalline materials, sponsored by the MDPI open access journal *Crystals*. Over the years, this conference has grown into a dynamic platform for researchers, industry professionals, and students to share insights, discuss emerging trends, and foster collaboration in this ever-evolving field.

This year's conference will focus on the following topics and related themes.

S1. Inorganic Crystalline Materials;
S2. Liquid Crystals;
S3. Organic Crystalline Materials;
S4. Hybrid and Composite Crystalline Materials;
S5. Materials for Energy Applications;
S6. Crystal Engineering;
S7. Crystalline Metals and Alloys.

This edition promises an exciting lineup of presentations covering recent breakthroughs in the synthesis, characterization, and applications of crystalline materials. We encourage you to engage actively in the sessions, participate in Q&As, and take advantage of networking opportunities that our virtual format offers. Your contributions and enthusiasm will make this conference a success, and we look forward to an inspiring exchange of knowledge.

Thank you for joining us on this journey of discovery and innovation. Let's make the Fifth Edition of the International Online Conference on Crystals a memorable and fruitful experience!

Prof. Dr. Alessandra Toncelli
Conference Chair
Department of Physics, University of Pisa, Pisa, Italy

crystals
an Open Access Journal by MDPI

Crystals (ISSN 2073-4352) is an open access journal that covers all aspects of crystalline material research in different sections: https://www.mdpi.com/journal/crystals/sections. *Crystals* provides a forum for the advancement of our understanding of the nucleation, growth, processing, and characterization of crystalline and liquid crystalline materials. Their mechanical, chemical, electronic, magnetic, and optical properties, and their diverse applications, are all considered to be of importance. Additionally, we encourage contributors to send articles focused on crystals research (of small and high molecular weight). Their characterization by using modern techniques for crystal growth and high resolution characterization such as synchrotron radiation and modern methods for the growth of crystals for X-ray free electron lasers (XFELS) would also be welcome.

Crystals can be used as a reference and publication source for the crystalline research community. *Crystals* publishes reviews, regular research articles, short communications and perspectives et al. Our aim is to encourage scientists to publish their experimental, theoretical and computational results in as much detail as possible so that results can be reproduced. Therefore, there is no restriction on article length.

Impact Factor: 2.4 (2024); 5-Year Impact Factor: 2.4 (2024)

Keynote Speakers

Dr. Ingo Dierking

School of Physics and Astronomy of the University of Manchester, Manchester, United Kingdom

Dr. Stanislav Ferdov

Physics Centre of Minho and Porto Universities, University of Minho, Guimarães, Portugal

Prof. Dr. Željka Antić

Vinca Institute of Nuclear Sciences: Belgrade, Serbia

Invited Speakers

Dr. Ramzi Maalej

University of Sfax, Sfax, Tunisia

Dr. Robert Jackson

Keele University, School of Chemical and Physical Sciences, Keele, United Kingdom

Assoc. Prof. Zhengqing Liu

Institute of Flexible Electronics, Northwest University of Technology, Xi'an, China

Professor Mark Wilson

Department of Chemistry, University of Durham, Durham, United Kingdom

Prof. Dr. Dušan Dimić

Faculty of Physical Chemistry, University of Belgrade, Belgrade, Serbia

Prof. Dr. Sen Lin

State Key Laboratory of Photocatalysis on Energy and Environment, College of Chemistry, Fuzhou University, Fuzhou, China

Program at a Glance

	Day 1	Day 2	Day 3
Morning	**Session 1.** Inorganic Crystalline Materials	**Session 4.** Hybrid and Composite Materials	**Session 5.** Materials For Energy Applications
Afternoon	**Session 2.** Liquid Crystals	**Session 6.** Crystal Engineering	**Session 3.** Organic Crystalline Materials **Session 7.** Crystalline Metals and Alloys

IOCC 2026 Program

15 June 2026 (Monday)

Session 1. Inorganic Crystalline Materials

Time: 9:00 (CEST, Basel) / 03:00 (EDT, New York) / 15:00 (CST Asia, Beijing)

Time (CEST)	Speaker	Title
09:00–09:10	**Prof. Dr. Alessandra Toncelli** Event Chair	*Welcome & Opening Remarks*
09:10–09:20	**Dr. Zongyou Yin** **Prof. Dr. John Parthenios** Session Chairs	*Welcome from the Session Chairs*
09:20–09:45	**Prof. Dr. Željka Antić** Keynote Speaker	Pr3+ Visible to Ultraviolet Upconversion for Antimicrobial Applications
09:45–10:05	**Prof. Zhengqing Liu** Invited Speaker	Phase engineering of transition metal dichalcogenides
10:05–10:25	**Prof. Dr. Sen Lin** Invited Speaker	Single-Atom Catalysis: Mechanism and Dynamics
10:25–10:45	**Dr. Ramzi Maalej** Invited Speaker	TBA
10:45–11:00	**Pietro Lenzi** Selected Speaker	Er-activated nanoparticles as probes in biothermal imaging
11:00–11:15	**Gábor Mandula** Selected Speaker	Photorefraction and photochromism in bismuth–magnesium-codoped stoichiometric lithium niobate
11:15–11:30	**Monica Pavel** Selected Speaker	Synthesis, characterization, and physicochemical properties of copper halide-intercalated RbLaTa2O7 layered inorganic material
11:30–11:45	**Alexander Kanibolotskiy** Selected Speaker	Layered chalcogenides of the FeGa2S4 structure type: synthesis, crystal structure, and magnetic properties
11:45–14:00		**BREAK**

S2. Liquid Crystals

Time: 14:00 (CEST, Basel) / 08:00 (EDT, New York) / 20:00 (CST Asia, Beijing)

Time (CEST)	Speaker	Title
14:00–14:10	**Prof. Dr. Vladimir Chigrinov** Session Chair	*Welcome from the Session Chair*
14:10–14:35	**Dr. Ingo Dierking** Keynote Speaker	The Use of Convolutional Neural Networks to Characterise Liquid Crystals
14:35–14:55	**Professor Mark Wilson** Invited Speaker	Molecular simulation insights into the stability of the ferroelectric nematic phase
14:55–15:10	**Ivan Simdyankin** Selected Speaker	Selective Reflection Zones in modulated Flexoelectric Structures induced by a Planar Electric Field
15:10–15:25	**Dorota Dardas** Selected Speaker	Evaluation of applied methods for the determination of viscoelastic effects in chiral liquid crystals
15:25–15:40	**Mateusz Mrukiewicz** Selected Speaker	Electric Permittivity Behavior in Highly Polar Liquid Crystals: From Paraelectricity through Ferroelectricity to Superparaelectricity
15:40–15:55	**Stanisław Różański** Selected Speaker	The effect of the presence of 5CB liquid crystal molecules in the electrolyte on the current–voltage parameters of the DSSC cell

16 June 2026 (Tuesday)

Session 4. Hybrid and Composite Materials

Time: 9:00 (CEST, Basel) | 03:00 (EDT, New York) | 15:00 (CST Asia, Beijing)

Time (CEST)	Speaker	Title
09:00–09:10	**Prof. Dr. Ferdinando Costantino** Session Chair	*Welcome from the Session Chair*
09:10–09:30	**Prof. Dr. Dušan Dimić** Invited Speaker	Structural Diversity of Hybrid Metal–Semicarbazone and Thiosemicarbazone Crystalline Materials and Their Interactions with Biomolecular Targets
09:30–09:45	**Marzia Pentimalli** Selected Speaker	MOF-Based Composites for Sustainable Processes
09:45–10:10	**Fabio Manna** Selected Speaker	An Ultramicroporous Fe(II)-Anilato MOF for CO2 Capture and Environmental Applications
10:10–10:25	**Pietro Rassu** Selected Speaker	Multivariate Anilate-Based Metal–Organic Frameworks: Exploring Assembly and Linker Exchange Pathways
10:25–10:40	**George Marian Ispas** Selected Speaker	Polypyrrole-Functionalized Magnetic Zeolite for Efficient Recovery of Waste Oil from Water Surfaces
10:40–10:55	**Izabella Crăciunescu** Selected Speaker	Flexible Polypyrrole Composite Films with Organic and Inorganic Fillers for Electrocardiographic Sensing Applications
10:55–11:10	**Emilia Crăciun** Selected Speaker	Chiral Redox-Active Metal–Organic Frameworks Based on Benzoquinone-Derived Linkers
11:10–14:00		**BREAK**

S6. Crystal Engineering

Time: 14:00 (CEST, Basel) | 08:00 (EDT, New York) | 20:00 (CST Asia, Beijing)

Time (CEST)	Speaker	Title
14:00–14:10	**Prof. Dr. Tandabany Dinadayalane** Session Chair	*Welcome from the Session Chair*
14:10–14:35	**Dr. Stanislav Ferdov** Keynote Speaker	From Collapse to Creation: How Zeolites Reinvent Themselves
14:35–14:50	**Chittran Roy** Selected Speaker	Crystallization behaviour of phage shock protein: morphological analysis and growth mechanisms
14:50–15:05	**Kevinkumar Garala** Selected Speaker	Crystallo-Co-Agglomeration as a Crystal Engineering Strategy for Tailoring Pharmaceutical Crystal Properties and Enhancing Drug Processability
15:05–15:20	**Arijit Mukherjee** Selected Speaker	Control of photoreactivity in organic solids through large synthons
15:20–15:35	**Youssef Smayou** Selected Speaker	Coupling Between Br-Hexahelicene Molecules through Br···Br and Br···H Bonds
	Flash Poster Session	
15:35–15:40	**Jayant Kumar Sahoo** Poster Presenter	Crystallography and Structural Evolution of Iron Ore Minerals in Banded Iron Formations: Implications for Geometallurgy
15:40–15:45	**Akmaljon Tojiboev** Poster Presenter	Crystal Engineering of Quinazoline Derivatives: Impact of Chalcogen Substitution and Substituent Bulk on 3D Architecture and Intermolecular Interaction

15:45–15:50	**Christos Michail** Poster Presenter	X-ray luminescence performance of a BGO single crystal under the influence of external temperatures: Comparison with BaF2
15:50–15:55	**Madalina Bold** Poster Presenter	Antimicrobial activity of Iron oxide nanoparticles (IONPs) functionalized with anthocyanin extracted from blackcurrants (Ribes nigrum)
15:55–16:00	**Huma Amber** Poster Presenter	Electrolessly Deposited Transition Metal Phosphide Catalysts for Hydrogen Generation from Hydrolysis of Sodium Borohydride
16:00–16:05	**Ivan Yakovkin** Poster Presenter	Plasmonic Poynting vector vortices for uniform coupling to photocatalytic coatings
16:05–16:10	**Irina Kaurova** Poster Presenter	Scaling of HKUST-1 metal–organic framework polymer with catalytic and adsorption properties
16:10–16:15	**Kristijan Živković** Poster Presenter	Design of Mono- and Multimetal Oxide Nanoparticles for Enhanced Antimicrobial Surface Application
16:15–16:20	**Tomislav Balic** Poster Presenter	Crystal structure of novel 22- and 23-membered acylhydrazone-based macrocycles
16:20–16:25	**Mane Sahakyan** Poster Presenter	Optical properties of non-centrosymmetric Th-based superconductors: a density functional theory study
16:25–16:30	**Abdelkader Boutaleb** Poster Presenter	Design and Crystal Engineering of a Photonic Crystal Fiber for Optical Pressure Sensing
16:30–16:35	**Beynor-Antonio Paez-Sierra** Poster Presenter	Quantitative Raman Spectroscopic Analysis of Crystallographic and Molecular Orientation in Rubrene Film

17 June 2026 (Wednesday)

Session 5. Materials for Energy Applications

Time: 9:00 (CEST, Basel) | 03:00 (EDT, New York) | 15:00 (CST Asia, Beijing)

Time (CEST)	Speaker	Title
09:00–09:10	**Dr. Jasmina Grbović Novaković** Session Chair	*Welcome from the Session Chair*
09:10–09:30	**Dr. Robert Jackson** Invited Speaker	Computer modelling of materials for energy applications
09:30–09:45	**Muhammad Faheem Maqsood** Selected Speaker	Thickness-Driven Crystallization and Structural Evolution of Ultra-Thin p+ Poly-Si Passivated Contacts
09:45–10:00	**Adam Roślak** Selected Speaker	Characterization of the mechanical performance of epoxy resin composites containing graphene powder
10:00–10:15	**Hamza Wardi** Selected Speaker	Strontium Hydrides for Hydrogen Storage and Strain-Enhanced Hydrogen Desorption near Room Temperature
10:15–10:30	**Maycol F. Mena** Selected Speaker	Effect of crystal structure on the electrochemical performance of LLTO perovskite-type solid electrolytes for lithium-ion batteries
10:30–10:45	**Fausto Secci** Selected Speaker	Mesoporous CeO_2-Supported Ni Catalysts: Tuning Nickel Dispersion for CO_2 Methanation
10:45–11:00	**Hector David Agudelo Arias** Selected Speaker	Microwave-Assisted rGO Coupling for Stabilizing a V-Doped Co-Free Li-Rich Layered Cathode with High Discharge Capacity at 5C and 10C
11:00–11:15	**Ilyas Jalafi** Selected Speaker	Improved Dielectric and Nonlinear Properties of Doped $CaCu_3Ti_4O_{12}$ Ceramics for High-Efficiency Energy Storage Applications
11:15–14:00		**BREAK**

Session 3. Organic Crystalline Materials
Session 7. Crystalline Metals and Alloys

Time: 14:00 (CEST, Basel) | 08:00 (EDT, New York) | 20:00 (CST Asia, Beijing)

Time (CEST)	Speaker	Title
14:00–14:10	**Dr. Stanislav Ferdov** Session Chair	*Welcome from the Session Chair*
14:10–14:25	**Saravanan Kandasamy** Selected Speaker	Deciphering Intermolecular Interactions in Molecular Crystals through Quantum Crystallography and Non-Covalent Interaction Analysis
14:25–14:40	**Alexander P. Voronin** Selected Speaker	Complete the circle: cocrystal formation thermodynamics derived from congruent sublimation and solution cycles
14:40–14:55	**Ines Benzitouni** Selected Speaker	Novel Sulfanilamide-Derived Schiff Base: Synthesis, FT-IR spectroscopy, Crystal Structure, Hirshfeld Surface Analysis, and in silico ADME investigation
14:55–15:10	**Prof. Dr. Shouxun Ji** Session Chair	*Welcome from the Session Chair*
15:10–15:25	**Salah Uddin** Selected Speaker	Investigation of Crystal Deformation by X-ray Diffraction Method
15:25–15:40	**Hassane MES-ADI** Selected Speaker	Effect of heterogeneous interfaces on the mechanical characteristic and deformation behavior of metal Bilayers
15:40–15:55	**János György Bátorfi** Selected Speaker	Simulation of recrystallization in polycrystalline materials

Session 1. Inorganic Crystalline Materials

sciforum-176832: Crystal scintillators for high precision beta spectroscopy: the GAIAS experiment

Alice Leoncini [1,2,*], Aagrah Agnihotri [3], Mattia Atzori Corona [2], Pierluigi Belli [1,2], Fabio Cappella [4,5], Vincenzo Caracciolo [1,2], Riccardo Cerulli [2], Alessio Giarnetti [4], Fedor Danevich [2,6,7,8], Jouni Suhonen [3,9], Dymtro Kasperovych [6], Volodymyr Klavdiienko [10], Vladislav Kobychev [10], Jenni Kotila [3], Vittorio Merlo [2], Marlom Ramalho [11], Antonella Incicchitti [4,5] and Volodymyr Tretyak [10]

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3 Department of Physics, University of Jyväskylä, Jyväskylä P.O. Box 35, 40014 Finland
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11 School of Physics, Engineering and Technology, University of York, Heslington, York YO10 5DD, United Kingdom

The effective value of the axial-vector coupling constant g_A in nuclear media represents one of the dominant sources of uncertainty in the interpretation of neutrinoless double beta decay ($0\nu\beta\beta$) experiments. Its quenching relative to the free-nucleon value significantly impacts nuclear matrix element calculations and, consequently, the inferred values (limits) of the Majorana neutrino mass.

The GAIAS (GAxIaI Analysis with Scintillators) project proposes a crystal-scintillator-based strategy to probe the g_A through high-precision measurements of forbidden non-unique beta decays. These transitions exhibit strong sensitivity of the beta spectral shape to the axial coupling constant, particularly in the low-energy region.

The method exploits key properties of scintillating crystals: high light yield, low energy threshold (5–20 keV), good energy resolution, high radiopurity, stable operation over a long time to accumulate large enough statistic and the possibility of incorporating beta-emitting isotopes directly into the crystal bulk. Materials under investigation include $CdWO_4$, $^{106}CdWO_4$, CsI(Na,Rb), NaI(Tl,Tc), and $CeCl_3$, hosting isotopes such as ^{113}Cd, ^{113m}Cd, ^{87}Rb, and ^{99}Tc either intrinsically or as controlled dopants.

The experiment is being installed in the low-background environment of the INFN Gran Sasso National Laboratory (LNGS), enabling high-statistics beta spectroscopy under stable and well-controlled conditions. Particular emphasis is placed on crystal growth strategies, isotope incorporation, control of scintillation non-proportionality below 100 keV, and long-term energy scale stability.

By combining optimized crystal engineering, optimized electronic read-out, precision spectroscopy, Monte Carlo simulations, and nuclear-structure modeling, GAIAS aims to extract g_A with high accuracy, strengthening the role of functional crystalline materials in fundamental physics.

sciforum-176783: Crystal structure of tetraaqua(κ²-N,N′-8-aminoquinoline)nickel(II) sulfate

Gulnora Abdurahmonova Umirova *, Abdurasul Erkin ugli Toshtemirov and Khayit Khudaynazarovich Turaev

Department of Physical Chemistry, Faculty of Chemistry, Termez State University, Termez 190111, Uzbekistan

This study reports on the synthesis, crystal structure, and Hirshfeld surface investigation of the nickel(II) complex $[Ni(C_6H_2N_2)(H_2O)_4]SO_4$. $NiSO_4{\cdot}6H_2O$ and 8-aminoquinoline were reacted in ethanol under reflux conditions at 60 °C for 30 minutes to create the complex. Slow evaporation of the reaction solution at room temperature yielded light-green single crystals suitable for X-ray diffraction investigation (75% yield). The results of the elemental analysis are in good agreement with the proposed molecular formula $[Ni(C_9H_8N_2)(H_2O)_4]SO_4$. The compound crystallizes in the monoclinic crystal system with the space group P21/c, according to single-crystal X-ray diffraction study. The unit-cell volume is 1473.33(14) Å^3, Z = 4, a = 12.0672(6) Å, b = 9.2001(4) Å, c = 14.4120(8) Å, and β = 112.953°.

The nickel(II) ion possesses a six-coordination number and a deformed octahedral shape generated by one nitrogen atom from the 8-aminoquinoline ligand and four coordinated water molecules, according to structural analysis. The Ni-N and Ni-O bonds measure 2.106 Å and 2.081(3) Å, respectively.

An large hydrogen-bonding network including coordinated water molecules, the ligand's amino group, and the sulfate anion helps to maintain the crystal packing. The cationic complex and sulfate anion form layered supramolecular structures through twelve hydrogen bonds of the N-H···O and O-H···O kinds, with sulfate oxygen atoms acting as acceptors.

Hirshfeld surface analysis was used to explore intermolecular interactions in the crystal structure. The findings show that H···O/O·· ·H interactions account for 45.0% of total contacts in crystal packing, followed by H···H (34.4%) and H···C/C···H (14.3%) interactions. Hydrogen bonding plays a crucial role in crystal structure stabilization, as evidenced by minor contributions from C···C (4.3%) and H···N/N···H (0.8%) contacts, which, although small, indicate that these interactions still contribute to the overall stability of the crystal structure.

sciforum-177315: Equitable Partitions in Inorganic Nanoclusters

Vasilios Raptis [1,*], Ioannis Michos [1] and Theophanes Raptis [2]

[1] Department of Computer Science and Engineering, School of Sciences, European University Cyprus, 6 Diogenes str., Nicosia 2404, Cyprus
[2] Independent Researcher, Athens, Greece

Introduction. Graph-theoretical concepts allow an alternative understanding of the role of symmetry in inorganic nanomaterials and offer a fine-grained look at the relative importance of their constituent atoms. Here, a link is shown between the concept of Equitable Partitions (EP) of chemical graphs [1–3] and the distribution of local properties of nanoparticles.

Methods. The study focused on the geometrical and physical properties of idealised spherical and polyhedral nanoclusters of iron and cobalt. Clusters extracted from bulk lattices of the corresponding chemical elements, were modeled as graphs based on nearest-neighbor adjacency, and their EPs were determined. The clusters were subjected to classical force-field modeling, as well as DFT calculations using the SIESTA software package [4].

Results. The following properties were determined: atom radial distances from cluster center; measure of forces on atoms; local charge densities; local magnetic moments. Their values were found to be distributed according to the graph's equitable partition; in other words, all atoms in a given partition cell, share the exact same properties.

Conclusions. Our method sheds new light on the symmetries of inorganic nanomaterials and the role of individual atoms therein. Our findings can have implications in the understanding, design, and engineering of magnetic nanoparticles, catalyst materials, and other applications at the nanoscale.

References

1. I. Michos, V. Raptis. Graph Partitions in Chemistry. *Entropy* **2023,** *25,* 1504.
2. V. Raptis, A. Kaltzoglou. Graph Theoretical Analysis as an Aid in the Elucidation of Structure-Property Relations of Perovskite Materials. AIP Conf Proc **2024,** *3030,* 110005.
3. V. Raptis, I. Michos. Chemical Equitable Partitions: A new Perspective on Molecular Symmetries and Its Implications for the Study of Structure–Property Relationships. *MDPI Proceedings* **2025,** *123,* 6.
4. José M. Soler *et al*. The SIESTA method for *ab initio* order-*N* materials simulation. *J. Phys.: Condens. Matter* **2002,** *14,* 2745.

sciforum-176938: New Solid Solutions Based on Barium Borates Incorporating Bismuth and Rare Earth Elements: Thermal Expansion, Crystal Structures, and Photoluminescence

Sofya Vladimirovna Demina [1,*], Andrey Pavlovich Shablinskii [1], Rimma Sergeevna Bubnova [1], Alexey Valerievich Povolotskiy [2] and Stanislav Konstantinovich Filatov [3]

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[2] Institute of Chemistry, St. Petersburg State University, 7/9 Universitetskaya Emb., St. Petersburg, 199034, Russian Federation
[3] Institute of Earth Science, St. Petersburg State University, 7/9 Universitetskaya Emb., St. Petersburg, 199034, Russian Federation

Seven new series of solid solutions (42 compositions total), doped with REE^{3+} ions, were synthesized based on two barium borate matrices: $BaBi_2B_2O_7$ and $Ba_3REE_2(BO_3)_4$ (*REE* = Y, Eu). Nine crystal structures were refined using single-crystal X-ray diffraction. Additional characterization included Raman spectroscopy, IR spectroscopy, thermal analysis , and high-temperature powder X-ray diffraction. Photoluminescence spectra were recorded for all series, and the temperature dependence of photoluminescence intensity was examined.

For the $BaBi_2B_2O_7$ matrix, solid solutions doped with REE^{3+} were obtained. The compositional ranges of continuous solid solutions were determined. Co-doping of the $BaBi_2B_2O_7$ lattice was found to expand the miscibility regions of the solid solutions. Eight crystal structures were refined from single-crystal data for $BaBi_{2-x}Eu_xB_2O_7$ (x = 0.1, 0.2, 0.4), $BaBi_{2-x}Sm_xB_2O_7$ (x = 0.05, 0.3), $BaBi_{2-x}Tb_xB_2O_7$ (x = 0.1, 0.3, 0.4). All compounds crystallize in the $BaBi_2B_2O_7$structure type (hexagonal system, space group $P6_3$). The structure contains three independent crystallographic sites for large cations, each split into Ba and Bi subsites. REE^{3+} ions occupy the Bi subsites. Upon REE^{3+}activation, the larger Sm and Eu ions preferentially occupy the *M*1 and *M*2 sites (largest coordination polyhedra volumes), whereas Tb^{3+}, with the smallest ionic radius, occupies the *M*3 site (smallest polyhedral volume).

A new solid-solution series $Ba_3Y_{2-x}Er_x(BO_3)_4$ (x = 0.01—0.3), along with end-member borates $Ba_3Y_2(BO_3)_4$, $Ba_3Eu_2(BO_3)$, was synthesized via melt crystallization. Thermal expansion was studied for $Ba_3Eu_2(BO_3)$ and $Ba_3Y_2(BO_3)_4$, and the crystal structure of $Ba_3Y_2(BO_3)_4$ was refined across a wide temperature range (40 data points). Photoluminescence spectra and their temperature dependence were investigated for the $Ba_3Y_{2-x}Er_x(BO_3)_4$ series. The optimal activator concentration was determined to be x = 0.1.

This work was supported by the RSF (No. 22-13-00317-P) and utilized equipment from the "RDMI" and "OLMIV" of the Scientific Park of SPbSU.

sciforum-179389: PHASE FORMATION IN THE $Ag_2S–Sb_2S_3–GeS_2$ SYSTEM

Lyudmyla Piskach *, Vitalia Semenyuk, Orysia Berezniuk, Yuri M Kogut and Lubomir D Gulay

Department of Inorganic and Physical Chemistry, Lesya Ukrainka Volyn National University, Lutsk, 43025, Ukraine

The quasi-ternary system $Ag_2S–Sb_2S_3–GeS_2$ is of interest since the initial binary compounds and ternary compounds Ag_3SbS_3, $AgSbS_2$, Ag_8GeS_6, $Ag_{10}Ge_3S_{11}$ and Ag_2GeS_3 of the limiting quasi-binary systems exhibit promising properties for applications in solar energy, thermoelectricity, optoelectronics and biomedicine.

The samples for the study of the $Ag_2S–Sb_2S_3–GeS_2$ system were obtained by direct single-temperature synthesis from high purity (at least 99.99 wt.%) elements silver, antimony, germanium and sulfur in evacuated quartz containers. The ampoules were heated to the maximum synthesis temperature of 1220 K, cooled to 500 K, annealed at 500 K for 500 h, then quenched in air.

The identification of the synthesized samples employed X-ray phase analysis, microstructure analysis, and differential thermal analysis.

Two compounds are formed in the $Ag_2S–Sb_2S_3–GeS_2$ system at 500 K, $Ag_{11}Sb_3GeS_{12}$ (intersection of $AgSbS_2–Ag_8GeS_6$ and $Ag_3SbS_3–Ag_2GeS_3$ sections) and $Ag_{23}Sb_3Ge_7S_{30}$ (intersection of $Sb_2S_3–Ag_{10}Ge_3S_{11}$ and $Ag_3SbS_3–Ag_2GeS_3$ sections). The isothermal section thus consists of eight two-phase equilibria on the boundary sides, and eleven in the middle of the quasi-ternary system, separating ten three-phase fields.

Vertical section $Ag_3SbS_3–Ag_2GeS_3$ was investigated which is a quasi-binary system. Both quaternary compounds $Ag_{11}Sb_3GeS_{12}$ and $Ag_{23}Sb_3Ge_7S_{30}$ form at this section at 25 mol.% Ag_2GeS_3 and 70 mol.% Ag_2GeS_3, respectively, and melt congruently at 1047 K and 1077 K, respectively. $Ag_{11}Sb_3GeS_{12}$ has two polymorphous transitions at 527 K and 605 K; $Ag_{23}Sb_3Ge_7S_{30}$ has a polymorphous transition at 880 K.

The crystal structure of both compounds was determined by powder XRD. $Ag_{11}Sb_3GeS_{12}$ ($Ag_{0.917}Ge_{0.083}Sb_{0.250}S$) crystallizes in cubic space group *F*-43*m*, and $Ag_{23}Sb_3Ge_7S_{30}$ ($Ag_{1.600}Ge_{0.400}Sb_{0.268}S_2$) crystallizes in tetragonal space group *I*-42*d*.

sciforum-176157: X-ray luminescence performance of a BGO single crystal under the influence of external temperatures. Comparison with BaF_2

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Background. Scintillators are employed in a wide range of applications, spanning from medical imaging to radiation detectors operating under extreme temperature conditions or high radiation flux. In this context, systematic investigation of their luminescence response as a function of temperature and or radiation flux is of significant importance. In this sense, this study examined the influence of temperature on the luminescence efficiency of a bismuth germanate ($Bi_4Ge_3O_{12}$-BGO) single crystal. Results were compared with a barium fluoride (BaF_2) single-crystal scintillator.

Materials and Methods. The experimental setup, comprised of a medical X-ray unit, for crystal irradiation, that was set to a voltage of 90 kVp. Crystal's light output measurements were performed under temperatures ranging from 19 to 174 °C. The BGO crystal under investigation has a light yield of 8.2-8.9 × 10^3 photons/MeV, a decay time of 300 ns and a timing resolution of 2500-6000 ps @ FWHM.

Results. The luminescence efficiency values of BGO are 2.96 EU at 21.0 °C and 0.37 EU at 172.4 °C. The corresponding values for BaF_2 decreases with increasing temperature, ranging from 1.56 EU at 19.5 °C, to 0.32 EU at 174.2 °C. BGO appears with clearly higher luminescence efficiency values across the examined temperature range, however for temperatures reaching 174 °C the efficiencies of BaF_2 and BGO scintillators converge with each other, despite their initial differences.

Conclusion. Despite the higher luminescence efficiency values of BGO an interesting finding of this work is that BaF_2 maintains a performance profile that is comparable to BGO, especially as temperatures approach 174°C where the differences between the two materials minimizes. This combination of economic accessibility and thermal stability, at high temperatures renders it an good choice for harsh environments and large-scale applications where budget and durability are as critical as performance.

sciforum-178342: Crystal Structure and Thermal Conductivity of Al-Doped β-$FeSi_2$

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Iron silicide (β-$FeSi_2$) is an important semiconductor that has attracted significant attention for optoelectronic, photovoltaic, and thermoelectric applications. Its conductivity can be tuned to either n-type or p-type through doping, providing flexibility for device design. In thermoelectric (TE) applications, however, the introduction of dopants often leads to the formation of secondary metallic phases, which can degrade TE performance. The thermoelectric performance of p-type β-$FeSi_2$ is generally inferior to that of n-type material. Therefore, it is necessary to investigate the crystal structures and transport properties of p-type Al-doped β-$FeSi_2$.

The polycrystalline $FeSi_{2-x}Al_x$ samples were prepared by arc melting followed by a heat treatment process to obtain the β-phase. The crystal structures were identified using X-ray diffraction, and the phase fractions were quantified by Rietveld refinement. The electrical resistivity and Seebeck coefficient were measured using both a Hall effect measurement system (ResiTest8300) and a homemade device. Thermal conductivity was measured using a power efficiency measurement system.

As a result, undoped $FeSi_2$ samples were initially crystallized in the ε and α-phases and transformed into a semiconducting β-phase (~97%) after heat treatment, confirming the essential role of thermal processing in β-phase formation. The unit cell volume increases with increasing Al doping level, which can be attributed to the larger atomic radius of Al compared to Si, indicating substitutional incorporation of Al into the Si sublattice. It is found that Al incorporation significantly affected secondary phase formation, reducing the β-phase fraction to below 70% for $x \geq 0.04$. This result reveals a strong destabilization effect of Al on β-$FeSi_2$, which has not been clearly quantified in previous studies. Meanwhile, thermal conductivity decreased with increasing Al content, likely due to enhanced phonon scattering from point defects caused by Al substitution, consistent with previous reports. This study provides useful insights for material design and thermal-to-energy conversion applications.

sciforum-177198: Crystallographic Insight and Functional Properties of Zn-Modified $Sr_5CaTi_2Nb_8O_{30}$ Tungsten Bronze Ceramics

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This work reports a comprehensive investigation of the structural, dielectric, electrical, optical, and energy storage properties of $Sr_5CaTi_{2-x}Zn_xNb_8O_{30}$ (x = 0–0.08) tetragonal tungsten bronze ceramics synthesized via the solid-state reaction method. Rietveld refinement of X-ray diffraction data confirms the formation of a single-phase tetragonal tungsten bronze structure with Im2a space group, highlighting the successful incorporation of Zn ions into the lattice and the resulting modifications in crystallographic parameters. Microstructural analysis reveals dense ceramics with low porosity and uniformly distributed grains, with average grain sizes ranging from 15.01 to 17.16 µm. Dielectric measurements performed over a temperature range of 30–400 °C and frequencies from 1 kHz to 1 MHz exhibit two distinct anomalies corresponding to the ferroelectric phase transition (Tc) and a relaxation process (Ts), indicating diffuse phase transition behavior. Impedance spectroscopy, Nyquist plots, and electric modulus analysis demonstrate the significant contribution of grain and grain boundary effects to the electrical response, while activation energy calculations confirm thermally activated conduction mechanisms. The polarization–electric field hysteresis loops exhibit slim shapes, characteristic of relaxor ferroelectrics, which are favorable for energy storage applications. Compared to previous studies, this work provides deeper insight into the relationship between crystallographic structure and multifunctional properties, emphasizing the role of Zn substitution in tuning dielectric relaxation and enhancing energy storage performance in tungsten bronze ceramics.

sciforum-179374: Design of Mono- and Multimetal Oxide Nanoparticles for Enhanced Antimicrobial Surface Applications

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Rapid rise of antimicrobial resistance poses a critical threat to global health, accounting for more than 35,000 deaths annually across the EU, Iceland, and Norway alone. This escalating burden necessitates the development of innovative antimicrobial materials that can overcome the limitations of conventional approaches. Unlike antibiotic-releasing coatings, metal oxide nanoparticles (NPs) offer durable, long-term antimicrobial activity without inducing resistance, positioning them as a promising next-generation solution. Their high physicochemical stability, robustness, and low cytotoxicity further support their integration into biomedical and surface-coating applications. Among these, copper oxide (CuO) and zinc oxide (ZnO) nanoparticles stand out due to their strong intrinsic antimicrobial activity and biological relevance as essential trace elements [1,2].

In this work, we present a systematic investigation of mono- and multicomponent nanoparticle systems, including CuO, ZnO, Y_2O_3, and multimetallic Cu–Zn–Y oxide nanoparticles. The nanomaterials were synthesised using a controlled approach based on different anionic precursors, with tannic acid acting as a stabilising and structure-directing agent.

The antibacterial performance of the prepared nanoparticles was evaluated against *Staphylococcus aureus*, revealing pronounced antimicrobial activity across all systems, with clear differences linked to structural and compositional variations. The results demonstrate that nanoparticle size, morphology, and surface chemistry are key determinants of antibacterial efficiency, while multimetallic Cu–Zn–Y nanoparticles exhibit enhanced tunability and potential for synergistic effects.

Overall, this study provides new insights into the structure, activity relationships governing nanoparticle-mediated antibacterial effects, and establishes a rational framework for the design of advanced, biocompatible antimicrobial coatings. The findings highlight the potential of multimetallic nanoparticle systems as versatile platforms for next-generation biomedical and surface-engineering applications.

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sciforum-175957: Enhancement in the crystallinity of ZnO nanostructures induced by rapid thermal annealing

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ZnO is a multifunctional semiconductor material, with a wide band gap (~3.37eV), high coupling energy (60 meV), excellent chemical and thermal stability, and enhanced optical, electronic and structural properties, enabling its wide range of applications. In this study, crystalline ZnO films were deposited on silicon substrates, obtained by a chemical method, using $Zn(NO_3)_2$ as the Zn precursor, NaOH as the precipitating agent, and SDS as the surfactant. The deposited ZnO films were initially treated at 150°C, followed by RTA at 550 and 900°C, for 300 sec. Morphological and structural analyses were compared with conventionally treated samples to highlight the changes induced by RTA. SEM analysis showed that temperature influenced the morphology of ZnO NPs, obtaining particles with spherical shapes and sizes between 15 and 60 nm in a short time. In addition, the tendency agglomeration increases with increasing temperature. Structural analysis indicated a high degree of crystallinity and a hexagonal wurtzite structure; the size of the surface boundaries decreased as the temperature increased from 550°C to 900°C. The FTIR spectra show absorption bands that can be associated with the vibration mode of the Zn-O bonds, and confirm the improvement of crystallinity by enhancing the intensity of the peaks. The surface properties exhibit high wetting capacity, through contact angles with an average value of 45°, regardless of the RTA applied. The results obtained highlight the potential of the RTA process as an efficient alternative to classical thermal methods for improving the quality of crystalline ZnO films, increasing their potential for various technological applications, by controlling the thermal cycle parameters.

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sciforum-175374: Environmentally friendly route for synthesis of Nd-doped Y_2O_3 nanocrystalline phosphor with applicability in imaging

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Rare earth-doped Y_2O_3 phosphors represent a class of fluorescent materials that with unique optical characteristics and properties, which are reflected in high color purity and long lifetime, with the possibility of covering the entire electromagnetic spectrum, along with low cytotoxicity. In this paper, we propose the synthesis of crystalline Nd^{3+}doped Y_2O_3 nanoparticles for the development of fluorescent labels with applicability in imaging. The nitrates of the two main cations, urea as a precipitating agent, and sea buckthorn *(Hippophae rhamnoides)* extract are the raw materials used in the precipitation procedure to obtain the oxide precursor. Thermal decomposition of the precursor occurs at 600°C in the presence of glycerin used as a combustion agent. By controlling the parameters, we oriented the process towards obtaining with sufficiently small dimensions for efficient visualization of the distributions of target molecules in imaging, but no smaller than 10 nm to avoid the problem of cytotoxicity. SEM analysis shows well-defined particles with a spherical shape, smooth surface, no defects, and an average size of 50 nm. Analysis by X-ray diffraction, FTIR and EDX spectroscopy demonstrates the purity and high degree of crystallinity of the developed fluorescent labels and the possibility of using these types of materials in the field of biotechnology, as a result of meeting structural requirements. The study of the optical properties of doped phosphor shows red-shifted absorption spectra relative to Y_2O_3, and by excitation at 980 nm, multiple emission peaks in the NIR region were observed. The synthesis of NIR-emitting phosphors for biomedical applications is the main objective of this work, as they are less absorbed and scattered by tissue structures, and can achieve high penetration efficiency.

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sciforum-176951: Er-activated nanoparticles as probes in biothermal imaging

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YF3:Er^{3+} nanoparticles (NP) are characterized as possible intracellular nanoprobes for temperature measurements at the nanoscale. First, their spectral emission in the visible range is characterized and the excitation mechanism is studied through the observation of emitted intensity as a function of the excitation power. A slightly sub-linear excitation mechanism is observed. Then, their temperature-sensing ability in the typical biological temperature range is investigated by means of luminescence intensity ratio (LIR) measurements between two thermally coupled levels. We obtained a maximum relative sensitivity of 0.009 K^{-1} at 24 °C with an uncertainty associated with the temperature measurements that ranges from 0.2 °C to 0.4 °C. Luminescence lifetime of the NPs embedded in various mounting media (air, agarose and ProLong) is measured from images acquired using a confocal time-gated microscope. Mean lifetimes observed are in agreement with the measured lifetime of this composition. Moreover, given the impact of the environment on the photophysical properties, we compared the measured lifetime of NPs embedded in different mounting media. The highest lifetime is measured when ProLong is used as a mounting medium, probably because of the hindered vibrational motion of water which can act as a quencher molecule for NP luminescence. Luminescence lifetime in ProLong is ~40% higher compared with the ones obtained in agarose and air, while lifetime in agarose is slightly higher than the one in air. NPs are then functionalized with poly (acrylic acid) (PAA), to improve both their water dispersibility and their uptake in cancer cells (HeLa). Cells are incubated with NPs and imaged by the time-gated confocal microscopy, that takes advantage of the long luminescence lifetimes of these NP to temporally separate their emission from cellular autofluorescence. We demonstrated that PAA functionalization strongly improved cell internalization of the NP and yielded smaller aggregates in solution with respect to non-functionalized NP.

sciforum-176685: Evaluation of biomolecular interaction, catecholase activity and *in vitro* cytotoxic activity of a mononuclear and a dinuclear cobalt(II) complexes

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A mononuclear and a dinuclear cobalt(II) complexes **C1** and **C2** were synthesized, characterized and examined for their potential biological studies. The structural validation of **C1** and **C2** was ascertained by various analytical and spectral methods which corroborated well with single crystal X–ray diffraction studies. The DFT/TD–DFT investigations of **C1** and **C2** were performed to understand their electronic and structural properties. *In vitro* DNA/BSA interactions of synthesized complexes were conducted by a range of biophysical techniques including UV–vis, fluorescence, circular dichroism (CD), cyclic voltammetry (CV) and electron paramagnetic resonance (EPR). The binding strength of complexes **C1** and **C2** with DNA was calculated to be 8.06(±0.84) × 10^4 and 8.63(±1.03) × 10^5 M^{-1} and with BSA was found to be 2.8(±0.31) × 10^4 and 6.7(±0.54) × 10^4 M^{-1}, respectively. Catechol oxidase activity of complexes **C1** and **C2** were explored employing 3,5–di–tert–butylcatechol (3,5–DTBC) as a substrate and its subsequent conversion to 3,5–di–tert–butylquinone (3,5–DTBQ) product was validated. We have also validated the antioxidant potential of **C1** and **C2** *via* DPPH assay. Furthermore, cytotoxic activity of **C1** and **C2** was carried out against A549 (lung), MCF–7 & MDA–MB–231 (breast), MIA–Pa–Ca–2 (pancreas) and Hep–G2 (liver) employing ADR (adriamycin) as a standard and the results specified that the complexes **C1** and **C2** demonstrated cytotoxicity against A549 cell lines with a relatively low GI_{50} values (8–10 μg mL^{-1}).

sciforum-152896: Fabrication and Optimization of Low-Cost Clay–Marble Membranes for Textile Effluent Microfiltration

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This study presents the development of an innovative flat ceramic microfiltration membrane produced from low-cost and environmentally friendly raw materials. The approach is based on the valorization of marble waste powder in combination with natural clay, thereby addressing both the need for effective wastewater treatment and the sustainable reuse of industrial by-products. The fabrication process was carefully optimized through a statistical strategy using the Doehlert experimental design within the response surface methodology framework. This allowed for the systematic evaluation of key synthesis parameters, including marble waste content, sintering temperature, and dwell time, in order to identify conditions leading to high-performance membranes.

The optimized membranes exhibited a well-balanced combination of structural, mechanical, and functional characteristics, making them suitable for microfiltration applications. Their porosity and microstructural uniformity ensured efficient liquid–solid separation, while their mechanical strength provided stability under operating conditions. In addition, the materials demonstrated strong resistance to aggressive chemical environments, particularly under alkaline conditions, thus confirming their durability for long-term use.

Performance tests with real industrial wastewater further confirmed the effectiveness of the membranes. Substantial improvements in water clarity and notable reductions in organic load indicators were observed, highlighting their ability to remove suspended solids and partially reduce dissolved contaminants.

Overall, this research demonstrates the potential of sustainable ceramic membranes based on natural clay and marble waste as viable, eco-friendly alternatives to conventional filtration materials. By combining waste valorization, low production costs, and efficient water purification capacity, these membranes represent a promising solution for industrial wastewater treatment and resource-efficient water management.

sciforum-176799: Formation and characterization of hollow spherical Al_2O_3 granules synthesized by plasma-assisted spray pyrolysis

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Plasma spray pyrolysis is an advanced technique for the synthesis of ceramic and metallic particles through the interaction of powder precursors with a high-temperature gas flow. In this research, the process was implemented using an experimental plasma-chemical reactor operated with a direct current (DC) plasma torch to generate an atmospheric-pressure air plasma jet. Aluminum hydroxide ($Al(OH)_3$) was used as a precursor material. Under plasma heating, $Al(OH)_3$ decomposes into Al_2O_3 after the melting, drying, and crystallization processes within the reactor, resulting in the production of aluminum oxide particles. Experiments were carried out with plasma torch powers ranging from 30 to 35 kW, when the gas temperature was sufficient to induce Al_2O_3 melting. The formed particles were analyzed using scanning electron microscopy (SEM) to determine their morphology and X-ray diffraction (XRD) to identify their crystalline phases and structural composition. The obtained Al_2O_3 particles exhibited a narrow size distribution (50–150 μm), spherical shape, and predominantly hollow internal structure with smooth hexagonal surfaces. Plasma spray technology enables the controlled formation of uniform, spherical granules: the morphology and size of the produced Al2O3 particles can be controlled by adjusting flow parameters, residence time, and injection geometry. Al2O3 particles prepared by this method exhibit excellent characteristics, including a fine size, narrow size distribution, pure phase, and hollow spherical morphology. The morphological analysis demonstrates the ability to manufacture powders with controlled characteristics for specific applications. The produced hollow spherical Al_2O_3 granules are promising as lightweight ceramic fillers, high-temperature insulators, catalyst supports, and feedstock materials for plasma spraying or thermal barrier coatings, where controlled particle morphology and narrow size distribution are essential.

sciforum-176027: Geometry of the Adsorption Sites in Metal Nanoparticles and Surfaces

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We present a study of 18 adsorption sites found on metal nanoparticles and surfaces that have either Face-Centred Cubic (FCC) or Hexagonal Close-Packed (HCP) structure. Most metals of the periodic table have these structures and we determine using a geometric approach the adsorption site geometry on a nanoparticle made using physical magnetic ball-and-stick models. These geometric models include the existence of an octahedral or tetrahedral hole beneath the adsorption site as these can affect the adsorption site strengths of adsorbates. Furthermore, these adsorption sites are a combination of the three-fold hollows and four-fold hollows that are adsorption sites known to activate diatomic molecules (e.g. N2, CO). In addition, adsorption of larger molecular weight adsorbates can be defined on these sites as they provide multiple contact points in contrast to the typical, four-fold hollow, three-fold hollow, bridge and atop adsorption. We find that there are 9 geometrically distinct adsorption site topologies that are composed of square (i.e. 100) and triangular (i.e. 111) motifs. These adsorption site topologies when combined with a characteristic angle (ζ) result in 18 distinct adsorption site geometries that can be found on metal nanoparticles and surfaces. A systematic naming system for these adsorption sites is provided that defines explicitly the adsorption site geometry. Using this approach we find that there are five different type of B5 sites, an adsorption site that has been previously found to activate dinitrogen on ruthenium for the ammonia synthesis reaction.

sciforum-178681: Governing growth and performance of Fe(Se,Te) epitaxial superconductors on TiN buffered metal substrates

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Epitaxial thin films assume nowadays the leading role as functional material in several applications: among these, the deposition of cuprates High Temperature Superconductors (HTS) as modern Coated Conductors (CCs), where the epitaxial growth of the material is enabled through multiple oxide buffer layers, led to huge advancements in the high field magnet sector and thus fusion technology.

Iron-based superconductors (IBS) constitute a novel class of superconducting materials, with critical temperatures in the 10 – 60 K range and extremely high critical magnetic fields. For IBS CC, the materials characteristics reduce the need for strict texturing and deposition conditions are less demanding than those required for HTS. Recently, we showed that a thin TiN film can represent an effective single buffer layer for the Fe(Se,Te) superconductor, enabling the oriented growth of high-performance films on biaxially textured Ni-W. This single buffer layer is furthermore appealing because TiN is electrically conductive. The resulting structure, fabricated by pulsed laser deposition, is characterized by simplicity ang good performance.

However, several aspects require careful control, with a multi-layered system characterized by several critical interfaces: the chalcogenide and TiN are characterized by a high lattice mismatch (26 %). High Resolution TEM images highlight however the epitaxy of Fe(Se,Te) on TiN, showing how a domain matching epitaxy mechanism drives the film orientation. Moreover, the performance of the superconducting film is influenced by the structure and the presence of secondary phases inclusions at grain boundaries, affecting the regularity of the layered chalcogenide, as observed by TEM and diffraction analyses.

The results here shown unveil how different parameters influence the microstructural properties down to the atomic scale and how these are reflected on the superconducting behaviour, providing guidelines for the optimization of the Fe(Se,Te) growth on simplified coated conductor architectures for a novel generation of superconducting tapes.

sciforum-176752: Growing single crystals of sodium tungstate by the low-gradient Czochralski method

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Abstract

Crystals of alkali metal tungstates are widely used as photonic materials due to their physico-chemical stability, wide transmission range, and relatively low cost. Since bulk boules with a size of 40 mm are required for the creation of scintillators, it is necessary to develop new approaches to crystal growth under conditions of low temperature gradients. This method is the low-gradient Czochralski method, which allows for the production of homogeneous crystals with a lower number of structural defects and thermoelastic stresses.

Method

The feedstock was loaded into a crucible, then melted in a sealed chamber with a thermoinsulation installed above the crucible with a pipe. Immediately before the crystal growth process, the melt was kept at a temperature slightly above the melting point to homogenize the melt. The seed is a single crystal of high structural perfection with a minimum density of dislocations, which is cut in a strictly defined crystallographic direction. The seed was immersed in the melt. The process of crystal stretching began with the formation of a monocrystalline neck, immersing the seed into the melt. The neck was formed by simultaneously lowering the melt temperature at a high linear velocity and large axial temperature gradients. Once the crystal reaches the desired diameter, the growing conditions should be stabilized to ensure a constant crystal diameter and high structural perfection.

Results

We have successfully grown $Na_2W_2O_7$ crystals using the low-temperature gradient Chochralski method and measured the excitation and emission spectra of the crystal.

Conclusion

Growing crystals of alkali metal tungstates using the Chochralski method with low temperature gradients is a effective method for growing single crystals. The advantages of this method include the ability to change the crystal's geometric shape and the reduction of temperature gradients, which allows for the production of larger crystals with high optical quality.

sciforum-176835: Growth and Correlated Structural-Mechanical-Optical Study of Yb^{3+} activated $Y_{0.7}Gd_{0.3}VO_{-4}$ Single Crystal

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Disordered laser host materials have attracted significant attention due to their favorable spectroscopic properties, making them promising candidates for ultrafast laser gain medium applications [1,2]. In particular, disordered rare-earth orthovanadates provide an effective route for tailoring structural and optical properties through controlled cation substitution [2]. In this work, a 2.5 at% Yb^{3+} doped $Y_{0.7}Gd_{0.3}VO_4$ single crystal was grown along the [100] direction using the optical floating zone technique. Its structural, mechanical, and optical properties were systematically investigated and correlated. The selected composition introduces controlled Y/Gd substitutional disorder while preserving the structural stability of the zircon-type lattice.

Powder XRD confirm single-phase crystallization in the tetragonal structure (space group $I4_1/amd$) with refined lattice parameters a = b = 7.143 Å and c = 6.306 Å. High-resolution rocking-curve analysis of the (200) plane shows a narrow FWHM of 63.7 arc-sec, corresponding to a threading dislocation density of approximately 4.2×10^6 cm^{-2}, indicating excellent crystalline perfection. Williamson–Hall analysis reveals microstrain of the order of 10^{-4}, attributed to ionic radius mismatch and substitution-induced lattice distortion. Vickers microhardness measurements demonstrate good mechanical robustness, with a hardness of about 4.8 Mohs, suitable for post-growth processing.

Polarized UV-Vis-NIR spectroscopy confirms strong optical anisotropy in the tetragonal zircon structure. The optical bandgap estimated is about 3.53 eV for π-polarization and 3.60 eV for σ-polarization. The absorption coefficient reaches ~16.47 cm^{-1} under π-polarization compared to ~5.56 cm^{-1} under σ polarization, with corresponding absorption cross-sections of ~5.47×10^{-20} cm^2 (π) and ~1.82×10^{-20} cm^2 (σ), confirming dominant π-oriented transitions. Photoluminescence spectra shows broad emission near 1020 nm under 985 nm excitation, corresponding to the $^2F_{5/2} \rightarrow {}^2F_{7/2}$ transition of Yb^{3+}.

Overall, the $Yb_{0.025}Y_{0.7}Gd_{0.275}VO_4$ combines high crystalline quality with disorder-induced spectral broadening, highlighting the novelty of disorder-engineered orthovanadate hosts for broadband ultrafast solid-state laser gain media.

sciforum-176812: Growth Conditions and the Effect of Partial Substitution of Tungsten with Molybdenum on the Luminescent Properties of a Li2wo4 Single Crystal

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Abstract

Crystals of tungstates and molybdates are widely used to create scintillation detectors of ionizing radiation and are of interest for the search and study of neutrinoless double beta decay. Such experiments require high precision and impose strict requirements on the optical quality and purity of scintillator crystals.

Single crystals Li_2WO_4 and $Li_2W_{1-x}Mo_xO_4$ doped with molybdenum (x = 0.0125, 0.05) were grown by the Chokhralsky method with a low temperature gradient, which allows obtaining the required crystals.

Method

The Czochralski method with a low temperature gradient was developed for growing large oxide crystals for use in scintillators (LTG Cz).

During melting of the charge, the temperature in the growth furnace was elevated at a rate of 100 degrees/hour to a value of 760 °C and was kept at this temperature for 5 hours until the melt was completely homogenized. Before seeding, the temperature was decreased to 733 °C. The first growth experiments were carried out on a platinum seed holder, and subsequently on monocrystalline seeds cut from the obtained Li_2WO_4 crystals.

Results

The crystal, in which 1.25% of tungsten was replaced by molybdenum, visually completely repeated the appearance of pure Li_2WO_4: it was transparent, optically homogeneous, without visible defects and was characterized by a convex shape of the crystallization front.

A single crystal with a molybdenum content of 5 mol.% reached 65 mm in length and 40 mm in diameter. Its upper part remained transparent, however, at a distance of 25 mm from the seed, macroscopic structural defects began to form, the crystal acquired a yellowish tint, and a general deterioration in its optical quality was recorded.

Conclusion

The LTG Cz method has successfully grown a series of visually defect-free single crystals of Li_2WO_4, both unalloyed and with partial replacement of $[WO_4]^{2-}$ by $[MoO_4]^{2-}$ (1.25 mol.% and 5 mol.%, respectively).

sciforum-176992: Hafnium-Substituted Magnetite with Tunable Heating Performance for Hyperthermia Therapy

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Spinel ferrite crystals are widely explored for magnetic hyperthermia, yet the design of crystal-chemistry "thermal brakes" that prevent overheating remains underdeveloped. Here we report a crystal-structure–driven strategy to tune heating performance in hafnium-substituted magnetite nanocrystals, $Hf_xFe_{3-x}O_4$ (x = 0.4, 0.6), synthesized by a scalable reverse co-precipitation route. X-ray diffraction confirms the cubic spinel structure across the series and reveals a systematic shift of the (311) reflection toward lower 2θ with increasing Hf content, consistent with lattice expansion and distortion induced by aliovalent substitution. The lattice parameter increases monotonically with , while the coherent crystallite size decreases (≈10.6 → 7.9 nm), indicating enhanced microstructural disorder at higher substitution levels. Transmission electron microscopy shows quasi-spherical particles with comparable physical sizes (~12–14 nm), supporting a model where a reduced crystalline coherence length (rather than gross particle growth) governs structure–property changes. Magnetization measurements evidence a progressive decrease in saturation magnetization with Hf incorporation, consistent with modified cation distribution and increased surface/spin disorder. Under alternating magnetic field excitation, the specific absorption rate (SAR) decreases from pristine magnetite to Hf-doped (e.g., ~39.4 to ~8.1 W g^{-1}), yielding a controllable heating response that mitigates the risk of surpassing the therapeutic window. Baseline *in vitro* assays in MDA-MB-231 breast cancer cells (without AMF) support cytocompatibility within the tested concentration range, complementing prior ISO-guided viability results in non-tumor cells. Overall, these results establish lattice distortion and crystalline coherence as practical design knobs to engineer safer, dose-controlled hyperthermia agents based on spinel nanocrystals.

sciforum-179421: Interaction Between Phthalate Plasticizers and Calcium Oxalate: Impacts on Precipitation Behavior

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Introduction:

Calcium oxalate (CaOx) is the dominant mineral phase in human kidney stones, making the understanding of its nucleation, growth, and phase selection essential for elucidating urolithiasis mechanisms. Phthalate esters are ubiquitous plasticizers with diverse hydrophobic and steric properties, and rising human exposure has increased interest in their potential interactions with urinary constituents. This study investigates how structurally distinct phthalates (DIDP, DINP, DEHP, DNOP, BBP, DBP, DIBP) influence CaOx precipitation under physiologically relevant conditions.

Methods:

CaOx was precipitated in aqueous media in the presence or absence of individual phthalates under controlled conditions (pH 6.5, ionic strength 0.05 M, 37 °C). Crystal morphology was assessed using light microscopy, and phase composition was determined by PXRD and FTIR.

Results:

In the additive-free system, crystallization yielded exclusively COT, with crystals uniformly dispersed throughout the solution. In contrast, all phthalate-containing systems exhibited pronounced aggregation of crystals around hydrophobic additive domains. This aggregation was accompanied by clear morphological alterations, including variations in crystal dimensions and habit. While most phthalates had no measurable impact on phase composition, DINP uniquely induced partial transformation from COT to the thermodynamically more stable calcium oxalate monohydrate, indicating a structure-dependent effect on CaOx stability.

Conclusions:

Phthalate esters consistently promoted crystal aggregation and induced morphology changes, supporting predominantly surface-mediated interactions influenced by molecular size, hydrophobicity, and chain branching. DINP was the only compound capable of modifying CaOx phase stability, likely due to its branched isononyl structure perturbing the hydration environment of COT. These findings indicate that aggregation is a common response to all tested phthalates. However, more detailed investigations are required to fully clarify the underlying mechanisms.

Funding:

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sciforum-176839: Investigation of detector technology alternatives in Cone beam CT- A Simulation study

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Introduction: Cone beam CT (CBCT) is an excellent alternative in breast imaging since the breast is uncompressed while CBCT image quality is adequate, even in dense breast. CBCT detector technology is based on CsI:Tl material but recent research explores photon counting detectors' technology adapted from nuclear medicine. A key question is whether an optimum detector configuration exists in terms of MTF (Modulation transfer function), which reflects spatial resolution, and DQE (Detective quantum efficiency), reflecting the overall image quality.

Methods: A micro-CBCT system was simulated in GATE (GEANT4 Application for Tomographic Emission) v.9.2 incorporating seven different detector configurations. The scintillators evaluated were BGO (light yield: 8000-10000 photoms/MeV), LSO (25000-30000 photons/MeV), LYSO (30000-38000 photons/MeV), $LaBr_3$ (60000-70000 photons/MeV), GAGG (40000-60000 photons/MeV) and LuAG (18000-25000 photons/MeV) along with CZT as a semiconductor. These materials were selected due to their higher density and effective atomic number (Z_{eff}) compared to CsI, which can enhance DQE. Each scintillator (50x50x1 mm^3) was discretized in 100x100 pixels and coupled to a generic SiPM (Silicon photomultiplier) with pixelated readout. A 40 keV X-ray spectrum was used. A 1mm aluminum capillary and a cylindrical water phantom (20 mm height and 16 mm diameter) were simulated.

Results: GAGG demonstrated a 4% increase in spatial resolution and an 11% increase in DQE compared to CsI. Similar results were obtained from FBP (Filtered backprojection algorithm) and OS-SIRT (Ordered subsets simultaneous iterative reconstruction technique) reconstructed images. GAGG's high light yield (40000-60000 photons/MeV), high density (6.6-6.7 g/cm^3) and high Z_{eff}, contribute to improved signal to noise ratio (SNR). Additionally, it offers fast decay time (80-100 ns) and a low afterglow, good energy resolution, and robust mechanical properties.

Conclusions: GAGG is a strong candidate for CBCT detectors, offering improved spatial resolution, image quality and matched well in SiPM readout systems.

sciforum-178965: Layered chalcogenides of the $FeGa2S_4$ structure type: synthesis, crystal structure, and magnetic properties

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A 2D material is a crystalline substance consisting of a single layer of atomic thickness. If any magnetically ordered material is exfoliated down to a single crystal lattice layer, its magnetic properties are likely to disappear at room temperature. This occurs due to thermal fluctuations, which readily destroy the magnetic order. The first magnetic 2D materials have recently been obtained, but most of them are unstable in air, hindering their practical application. These compounds exhibit novel magnetoelectric and magneto-optical properties, which are extremely important for spintronics. Layered chalcogenides of the $FeGa2S_4$ structure type represent a promising class of materials for the discovery of new two-dimensional systems.

The objective of the present work is to synthesize new layered magnetic compounds of the $FeGa_2S4$ structure type: $FeAl_2S_4$, $FeAl_2Se_4$, VGa_2S_4, and $CrGa_2S_4$, and to investigate their structure and magnetic properties. Bulk crystals of the target compounds can be used to obtain 2D materials via mechanical exfoliation, since the structural layers, bounded by sulfur or selenium atoms, are linked only by weak van der Waals interactions. This report will present the conditions for the synthesis of polycrystalline samples, as well as the growth of large bulk crystals using chemical vapor transport reactions. The crystal structure of the isostructural compounds has been studied by powder X-ray diffraction. The iron-containing compounds were also investigated by Mössbauer spectroscopy, and the selenide compound was examined by high-resolution transmission electron microscopy. The composition of the crystals was characterized by electron-probe microanalysis. The work presents measurements of the magnetic properties of the samples.

sciforum-179672: Nanostructured CuO, ZnO, and ZnO/CuO thin films synthesized by SILAR method and their enhanced photocatalytic activity for methylene blue degradation

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Thin films of ZnO, CuO, and ZnO/CuO heterostructures were synthesized using the SILAR (Successive Ionic Layer Adsorption and Reaction) method with 50 deposition cycles, ensuring controlled thickness and uniform growth. The structural, morphological, and optical properties of the thin films were systematically characterized. X-ray diffraction (XRD) analysis confirmed the crystalline nature and phase purity of ZnO and CuO, as well as the successful formation of the heterostructure. Scanning electron microscopy (SEM) revealed uniform surface morphology with well-distributed grains, indicating good film quality. UV–Vis spectroscopy showed that ZnO films mainly absorb in the ultraviolet region, while CuO extends absorption into the visible region. The ZnO/CuO heterostructure exhibited improved optical absorption over a broader spectral range, thereby enhancing its photocatalytic potential. The photocatalytic performance of the films was evaluated through the degradation of methylene blue under UV–Vis light irradiation (λ = 310 nm). A 5 ppm methylene blue solution was used as a model pollutant. The results showed that the ZnO/CuO heterostructure film exhibited 17% methylene blue degradation compared to the individual ZnO (12%) and CuO (15%) films. This improvement is attributed to enhanced charge separation and reduced electron–hole recombination at the ZnO-CuO interface. Overall, the study highlights the potential of SILAR-fabricated ZnO/CuO thin films as efficient photocatalysts for environmental remediation applications.

sciforum-179588: Optical and thermal properties of tin disulphide Single Crystals

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Single crystals of SnS_2 were grown using the direct vapor transport (DVT) technique in a dual-zone muffle furnace. Initially, an elemental stoichiometric proportion totaling 10 g was used to prepare the SnS_2 compound at 550 K for 24 hours. This as-prepared compound was then used for the subsequent growth of single-crystalline SnS_2 via the DVT method. The resulting crystals are thin, shining, orange-colored, wafer-like flakes with maximum dimensions of 20 mm × 20 mm × 0.015 mm. The grown crystals were characterized to evaluate their microstructure, optical, and thermal properties. The growth mechanism observed on the as-grown single-crystal surfaces consists of growth layers originating from growth islands. No cracks or pinholes were observed in the grown crystals. Optical absorbance was recorded in the 200 nm to 3500 nm range. The grown SnS_2 single crystals show high optical absorption between 382 nm and 570 nm. The direct optical bandgap was evaluated using a Tauc plot ($(\alpha h\nu)^2$ versus $h\nu$) and was determined to be 2.2 eV. The thermal properties of the grown SnS_2 single crystals were evaluated in the temperature range of 307 K to 1230 K using thermogravimetric analysis (TGA), differential thermal analysis (DTA), and derivative thermogravimetric (DTG) analysis in an inert N_2 atmosphere with a heating rate of 5 °C/min. showed a total weight loss of 59.84%. Total decomposition occurred in two distinct steps: the first and second decomposition phases occurred from 855 K to 985.13 K and 1083 K to 1207 K, with weight losses of 14.85% and 40.68%, respectively. Two DTG peaks observed at 948.28 K and 1192.91 K corroborate these thermal decompositions. DTA analysis revealed two peaks at 948.80 K and 1140.67 K with an increase in negative potential, indicating endothermic behavior. Activation energy and other thermodynamic parameters were evaluated and are discussed in detail.

sciforum-176893: Petrography and Geochemistry of Gold-Like Rocks from Battambang, Mondulkiri, Kratie, and Takeo Provinces, Cambodia: A Scientific Evaluation of Local Beliefs

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Rocks commonly referred to as Meas Sruoy in Cambodia resemble “fool’s gold,” a mineral that is frequently mistaken for real gold due to its similar appearance. In many Cambodian communities, these rocks are believed not only to contain gold but also to possess spiritual qualities that can ward off evil and bring prosperity, health, and happiness. To investigate the composition of these materials, Meas Sruoy samples collected from Battambang, Mondulkiri, Kratie, and Takeo provinces were analyzed using hand-held X-ray fluorescence (XRF), energy-dispersive X-ray spectroscopy (EDS), and X-ray diffraction (XRD). The intact samples were first cleaned using an ultrasonic cleaner to remove surface contaminants and then dried prior to elemental characterization using a handheld XRF (X-MET8000). Elemental distribution was further examined using EDS. For elemental composition, the samples were ground into powders to improve homogeneity and subsequently analyzed by XRD (Malvern Panalytical Aeris, λ = 0.15406 nm), with diffraction patterns analyzed using MDI Jade 6 software. The analytical results revealed no detectable gold in any of the examined samples. Instead, the rocks exhibited diverse mineralogical compositions dominated by silica, iron, sulfur, and aluminum, along with trace levels of heavy metals, including arsenic, lead, chromium, and copper. Mineral phase analysis consistently identified quartz and pyrite, indicating a complex geological origin and confirming the visual resemblance to pyrite, commonly known as fool’s gold. These findings provide scientific evidence that contrasts with traditional beliefs surrounding Meas Sruoy while contributing valuable information regarding the mineralogical characteristics of rocks from different regions of Cambodia. Additionally, the detection of pyrite and trace heavy metals suggests potential environmental and public health considerations, particularly with prolonged exposure to these materials.

sciforum-176930: Photorefraction and photochromism in bismuth-magnesium-codoped stoichiometric lithium niobate

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Introduction

Lithium niobate (LN) is a work-horse of photorefractive holography. Recently outstanding results on (Bi,Mg)-codoped congruent LN have been reported. As the photochromic effect often degrades the quality of photorefractive devices, our aim is to investigate the dynamics and mechanism of photochromism and photorefraction in (Bi,Mg)-codoped stoichiometric LN, separating their effects on the diffraction efficiency in two-wave mixing experiments.

Methods

Czochralski-grown samples with a Li/Nb ratio of 1.38:1, Bi concentrations of 2 or 4 mol%, and Mg concentrations of 1 or 2 mol% (all data in the melt) were used to investigate both photochromic and photorefractive effects at 405 and 443nm at temperatures between 10 and 45°C. A two-wave mixing simulator program was developed based on a one-center model involving photochromic and various photorefracive mechanisms.

Results

Apart from persistent light-induced absorption reported earlier [1] and small transients on the ms timescale, an important photochromic component was found to be saturating on a subsecond and decaying on a subminute timescale, the recovery governed by an activation energy of ~0.6eV. Photorefractive response was faster with $\tau \approx 30$ms. The ratio of the photorefractive and photochromic diffraction efficiencies was determined as a function of the input intensity showing the domination of the photorefractive one for total input intensities above some tens of mW/cm^2. Estimates of the recombination coefficient and the effective cross section for electron excitation by photon absorption could be derived.

Conclusions

Despite its pronounced photochromism, LN:(Bi,Mg) is an efficient and fast photorefractive material, even at low intensities. This is due to various Bi-defect complexes promoted by Mg-codoping, introducing localized ground and higher pinned-exciton (exciton-polaronic) levels in the gap both serving as potential donors [1]. The results are helpful for optimizing holographic systems and a better understanding of the microscopic behavior of LN:(Bi,Mg).

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sciforum-179431: Preparation and Characterization of Zinc(II) Complexes with Coumalic Acid

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Introduction:

Coumalic acid (2H-pyran-2-one-5-carboxylic acid) is an oxygen-rich heterocyclic compound containing both carboxylic and lactone functional groups, making it a suitable ligand for coordination with metal ions. Zinc(II), a d^{10} metal center with a preference for oxygen donor atoms, readily forms stable complexes with carboxylate-containing ligands. Studying Zn(II)–coumalic acid interactions provides insight into coordination behavior, ligand binding modes, and structural diversity. This study investigates the formation of zinc(II) complexes using nitrate and acetate precursors.

Methods:

Zinc(II) complexes were synthesized by reacting aqueous solutions of zinc(II) nitrate hexahydrate and zinc(II) acetate dihydrate with coumalic acid under ambient conditions. The resulting solids were isolated and characterized by FTIR, PXRD, TGA/DSC, and UV–Vis spectroscopy. These techniques were used to evaluate coordination modes, structural features, thermal stability, and solution behavior. A comparative analysis of nitrate- and acetate-derived systems was conducted.

Results:

Complex formation was confirmed in both systems, indicating effective coordination through oxygen donor atoms. Spectroscopic data suggest that coordination primarily involves the deprotonated carboxylate group, with possible participation of the lactone carbonyl oxygen. Coumalic acid may act as a mono- or bidentate ligand, enabling the formation of stable coordination motifs. The obtained solids exhibit characteristic spectroscopic features and thermal behavior consistent with coordinated zinc(II) systems.

Conclusions:

Zinc(II) forms stable complexes with coumalic acid through coordination involving oxygen donor atoms, predominantly from the carboxylate group. The results highlight the ligand's versatility and its ability to support different coordination modes, contributing to the structural diversity of Zn(II) complexes.

Funding:

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sciforum-179429: Preparation and Structural Characterization of Copper(II) Complex with Maltol

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Maltol (3-hydroxy-2-methyl-4*H*-pyran-4-one) is a bidentate ligand that coordinates transition metal ions via its hydroxyl and carbonyl groups. Copper(II) forms stable complexes with oxygen-donor ligands due to its flexible coordination geometry and biological relevance. This study investigates the complexation of copper(II) nitrate trihydrate with maltol, forming a stable complex with distinct structural characteristics. The copper(II)-maltol complex was synthesized by reacting copper(II) nitrate trihydrate with maltol in aqueous solution under ambient conditions. The resulting solid was characterized using FT-IR, PXRD, TGA/DSC to evaluate coordination modes, structure, thermal stability, and solution behavior. FT-IR analysis showed the absence of the C–OH stretching vibration at 3255 cm^{-1}, indicating deprotonation of maltol and coordination to the copper ion. The C=O stretching vibration shifted from 1616 cm^{-1} in free maltol to 1568 cm^{-1} in the complex, confirming chelation. A weak Cu–O band at 719 cm^{-1} was observed, with no nitrate ions detected. Thermal analysis revealed a single-step degradation, with 70% mass loss attributed to the removal of maltol, and a sharp exothermic peak at 220°C in the DSC curve, consistent with CuO. X-ray diffraction confirmed the monoclinic crystal system (space group C2/c) with square-planar coordination around the copper ion, exhibiting Jahn-Teller distortion. This study successfully synthesized and characterized the copper(II)-maltol complex. FT-IR confirmed maltol coordination to copper, forming a stable chelate. Thermal analysis indicated good stability, and X-ray diffraction revealed a monoclinic structure with Jahn-Teller distortion. These findings enhance understanding of copper(II) coordination chemistry with maltol.

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sciforum-179263: Rapid Microwave-Assisted Hydrothermal Growth of ZTO Nanowires through Systematic Parameter Optimization

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Zinc-tin oxide (ZTO) is a ternary metal oxide that offers promising properties for applications in electronics, energy harvesting and sensing devices due to its high electron mobility, chemical stability and tunable optical properties [1]. Among the different synthesis techniques, microwave-assisted hydrothermal synthesis has emerged as an efficient approach for producing nanostructured materials due to its fast and homogeneous heating [2]. However, the morphology and crystalline phases obtained are strongly influenced by the synthesis parameters employed [3]. In this work, the influence of solution volume, microwave power and synthesis time on the formation of ZTO nanowires was systematically investigated. Two solution volumes (7.5 mL and 15 mL), two microwave powers (75 W and 100 W) and synthesis times ranging from 2 to 4 h were evaluated to identify optimal synthesis conditions. The resulting nanostructures were characterized using scanning electron microscopy (SEM), X-ray diffraction (XRD) and Fourier transform infrared spectroscopy (FTIR) to assess morphology, crystalline structure and chemical bonding. Overall, the results demonstrate that synthesis time, microwave power and solution volume play critical roles in controlling ZTO nanowire morphology and growth. By optimizing these parameters, $ZnSnO_3$ nanowires with comparable morphological and crystallinity quality to those obtained via conventional oven-based hydrothermal synthesis [4] were successfully produced in only 4 h, corresponding to a reduction of 20 h in synthesis time.

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sciforum-179523: Simple TiO_2-based photocatalyst for HMF transformation under UV irradiation

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5-hydroxymethylfurfural (HMF), a six-carbon heterocyclic organic compound containing both aldehyde and alcohol functional groups, is produced from dehydration of hexose sugars under acidic conditions. The hydroxymethyl and carbonyl groups of HMF can be oxidized to form various important furanic chemicals, which serve as platform molecules for further transformations. During the last years, research in the field of photocatalysis expanded from degradation of harmful compounds to synthesis as a green chemistry tool to replace the dangerous and polluting routes. Different catalysts were already reported as active in the selective oxidation of HMF under UV or visible light irradiation. Doping of TiO_2 with rare earth metals is a very efficient way to improve its photocatalytic performance as result of different factors. In our work, TiO_2 containing different amounts of Er and Yb was prepared using the sol-gel method and then calcined at 500 and 750°C, respectively. The characterization of these samples showed that the phase distribution of these is different than that of the pristine TiO_2. While the pristine TiO_2 calcined at 500°C contained about 5% anatase along with the predominant rutile phase, the doped samples contained 100% anatase. The increased calcination temperature led to a content of about 66% in rutile for TiO_2, compared the doped samples contained a maximum of 28% rutile for 1%Yb-TiO_2. These catalysts were active under UV irradiation, more active than the pristine TiO_2, but most of them oxidized HMF to lactic acid (LA, major product) and glycolic acid (GA). The activity increased with the amount of dopant, and decreased with the increase of the calcination temperature. The only catalysts who led to 2,5-hydroxymethylfurancarboxylic acid (HMFCA) as reaction product were 1%Er-TiO_2 calcined at 750^0C and 1%Er-1%Yb-TiO_2 calcined at 500^0C, the samples with the smallest amount of rutile. No base was added in our experiments.

sciforum-178081: Structural analysis of DMF cocrystalization as a quantitative stabilization strategy for metastable N, N'-bis(4-chlorophenyl)thiourea

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Metastability is a challenging problem in crystallization, where the metastable in a crystalline phase is usually thermodynamically unfavourable and unstable, but kinetically favourable and stable [1]. The aim of this study was to assess synthensized metastable *N*, *N*'-bis(4-chlorophenyl)thiourea for its stability status [2-4]. In line with this, *N*, *N*'-Dimethylformamide was used in slow evaporation process. In this process, *N*, *N*'-Dimethylformamide formed a cocrystal ($C_{16}H_{17}Cl_2N_3OS$) witth *N*, *N*'-bis(4-chlorophenyl)thiourea via network of classical N-H....O to avoid voids. Characterization technique of Single X-ray crystallography confirmed the structure of th cocrystal, ShelXT solution program solved the structure, while Gauss-Newton version 2017/1 of olex2 refined the structure. Results revealed that $C_{16}H_{17}Cl_2N_3OS$ (cocrystal) with Mr (370.30) and crystal size of 0.17 x 0.12 x 0.10 mm, appeared as a white crystal in a polygon-like shape in the $P2_{1/c}$ monoclinic space group. Additional results revealed are cell parameters of a = 92.360 (4) Å, b = 7.2232 (3) Å, c = 25.2555 (11) Å, β = 91.376 (3), $\alpha = \gamma = 90°$, V= 1684.40 (12) Å3, T = 119. 94 (13) K, Z = 4, Z' = 1, and calculated density (gcm-1). The significance of this study is the application of cocrystal as desolution blocker in the active pharmaceutical ingredients (API) and materials science.

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sciforum-176548: Structural characterization of novel 1H-1,2,3-triazole copper(II) complex: insight from experiment and quantum chemistry

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Carrently, 3d-metal complexes are of great importance in modern research and industrial processes of organic synthesis, allowing for the efficient and sustainable synthesis of organometallic compounds. Most metals with acceptor properties has become a pressing issue. Also, copper (Cu) stands out as a promising method due to its low cost, relatively low toxicity, and rich redox properties [1]. Copper ions are widely used in catalysis and coordination chemistry because they exhibit different oxidation states, have flexible coordination geometries, and form stable complexes with donor atoms of ligands [2]. In recent years, the synthesis of new derivatives of 1,2,3-triazole derivatives is rapidly developing due to their pharmacological and biological activity, because of this, ligands containing a 1,2,3-triazole fragment, one of the 5-membered heterocyclic compounds, have attracted particular interest in the synthesis of Cu-based complexes due to their strong N-donor properties [3]. In this study, we synthesized the Cu-based compound $C_{34}H_{26}Br_4Cl_2CuN_6O_6$ **(1)** with (1-(2-bromophenyl)-1H-1,2,3-triazol-4-yl)methyl 2-(4-bromophenoxy)acetate and characterized it by single-crystal X-ray diffraction, and performed conformational calculations based on quantum chemical analyses. For this complex compound, supramolecular and Hirshfeld surface analysis were performed to determine the intermolecular interactions. According to our results, intermolecular and intramolecular hydrogen bonds: C—H···O and C—H···N and C—Br···π stacking interactions are associated. Three-dimensional Hirshfeld surface analysis and two-dimensional fingerprint plots showed that the structures are dominated by H···H, H···C/C···H and H···O/O···H contacts, these interactions present in the determined molecular structure were characterized as stabilizing factors in the unit cell. Quantum chemical analysis revealed that the N atom located at the 3rd position in the triazole ring of the ligands has electron-rich donor properties in this complex.

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sciforum-176778: Structural insights, *in vitro* biomolecular interactions, biosensing and cytotoxic activity of two novel one–dimensional coordination polymers

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In this work, two novel zigzag one–dimensional Co(II) and Cu(II) coordination polymers (**CP1** and **CP2)** derived from 2,5–dihydroxyterephthalic acid and 2,2'–bipyridine ligands were synthesized and characterized by multispectroscopic (UV–vis, FTIR, EPR, sc–XRD) and analytical techniques. Single crystal X–ray diffraction studies revealed a monoclinic crystal system with I2/a and $P2_1/m$ space group for **CP1** and **CP2**, respectively. The DFT studies were performed to study the structural and electronic properties of **CP1** and **CP2** and the results revealed that HOMO electron density was localized around the central metal ions whereas, LUMO electron density is diffused throughout the polymeric structures and was mostly localized on 2,2'–bipyridine ligand**.** Additionally, the Hirshfeld studies analysis was carried out to study the various intra–/intermolecular interactions that stabilize the crystal structure and our results showed that **CP1** and **CP2** were majorly stabilized by H–H interactions. The chemotherapeutic efficacy of **CP1** and **CP2** were explored by studying the *in vitro* DNA binding interactions utilizing multispectroscopic techniques including UV–visible, fluorescence, circular dichroism and cyclic voltammetry. The synthesized coordination polymers were also evaluated for their biosensing activity and the finding revealed that **CP1** showed selective sensing for levofloxacin (LVF) whereas, **CP2** proved to be an efficient sensor for chloramphenicol (CLAM), LVF and nitrofurantoin (NFT). We have further evaluated the catechol oxidase activity of **CP1** and **CP2** was assessed by using 3,5–DTBC as a potential substrate. The chemotherapeutic potential of **CP1** and **CP2** was ascertained by carrying out *in vitro* cytotoxic activity against neuroblastoma (SH–SY5Y) cell line employing cisplatin as a reference and the results displayed better anticancer activity of **CP2** which was evident from their IC_{50} values.

sciforum-176556: Structure of a Cu(II) Complex Based on 1,10-Phenanthroline and Benzhydroxamic Acid Ligands

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Inorganic chemistry is rapidly producing novel molecules and useful materials. Mixed-ligand complexes of copper (II) ions with 1,10-phenanthroline (Phen) have been developed, and their optical and magnetic properties, stability, antibacterial activity, and crystal structures have all been comprehensively explored [1-2]. Based on these findings, Phen-containing mixed-ligand complexes were created. Their crystal structures, IR and UV-visible spectra, and how the copper ion coordinated and remained stable at high temperatures were next examined by the researchers [3].

This work synthesized a mixed-ligand complex, $[Cu(C_{12}H_8N_2)(C_6H_5CONHO)\cdot NO_3]\cdot H_2O$, from Phen and benzhydroxamic acid. The crystal structure and physicochemical characteristics were studied using UV-Vis and IR spectroscopy, thermogravimetric (TG) analysis, and Hirshfeld surface analysis.

A mixed-ligand complex was synthesized by dissolving 1 mmol of Phen 1 mmol of benzhydroxamic acid and 1 mmol of $Cu(NO_3)_2\cdot 5H_2O$ (0.20 g) in ethanol to obtain 0.05 M solutions. The $Cu(NO_3)_2$ and BA solutions were first mixed, followed by dropwise addition of the Phen solution under magnetic stirring. The mixture was heated at 50 °C for 20 min and then allowed to evaporate at room temperature. After 20 days, dark-green single crystals were obtained.

The Cu(II) complex was found to possess a square-pyramidal coordination geometry. The Cu(II) ion is coordinated in the equatorial plane by two nitrogen atoms from the Phen ligand (Cu1—N1 1.986(3) Å, Cu1—N2 1.986(3) Å) and two oxygen atoms from the benzhydroxamic acid ligand (Cu1—O1 1.919(2) Å, Cu1—O2 1.920(2) Å). In the axial position, an oxygen atom from the nitrate ion is coordinated (Cu1—O4 2.580(4) Å). According to the Hirshfeld surface analysis of the complex compound, the two-dimensional fingerprint plots indicate that H···H and O···H/H···O interactions make the major contributions to the intermolecular contacts. In the UV–visible spectrum, a low-intensity absorption band corresponding to d–d transitions was observed at 634 nm.

sciforum-176919: Studies of mixed lithium-sodium polymolybdates phase diagram

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Nowadays, in the rare events physics field, projects to study Neutrinoless Double Beta Decay ($0\nu\beta\beta$) are actively developing, as $0\nu\beta\beta$-decay registration will allow calculating the energy and mass of neutrinos. $0\nu\beta\beta$ process is theoretically possible in a number of nuclei, one of most promising is ^{100}Mo [1], thus, the compounds with maximal ratio of molybdenum are of interest.

The use of light alkali metals as cations helps to reduce the scintillator's radiation background and increase molybdenum content in the compound. In turn, an increased molybdenum content in the crystal increases the probability of $0\nu\beta\beta$-decay registration. In the course of this study, samples of the $(Na,Li)_6Mo_9O_{30}$ composition (x = 1-5 with a step of 1.0 were obtained by solid-phase synthesis. Solid-phase synthesis was carried out with a gradual increase in temperature until complete synthesis was determined in all samples. Completeness of the reaction, phase composition and unit cell parameters of the obtained samples were controlled using X-ray diffraction analysis.

Melting temperatures of the samples were determined by Differential Scanning Calorimetry (DSC). During the synthesis, it was found that the fractional composition sample had the lowest synthesis temperature (455℃) of all the studied compositions, which confirms the hypothesis that the compound of this composition belongs to the eutectic point.

Based on the data obtained, stable phases in the binary system $Na_6Mo_9O_{30}$-$Li_6Mo_9O_{30}$ were identified. Conditions for growing single crystals using the low-thermal-gradient Czochralski technique were proposed.

Acknowledgements

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sciforum-179458: Study of Structural Evolution and Dielectric Properties of Solid Solutions $A_2(Sm_{1-x}RE_x)Ti_2Nb_3O_{15}$ (A = Sr, Ba; RE = Nd, Sm, Gd, La)

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Tetragonal tungsten bronzes (TTB) represent an important class of functional ceramics, known for their high dielectric properties and thermal stability. Tailoring the properties of these materials through ionic substitution enables modulation of the crystal structure and, consequently, their electrical performance. In this context, the study of solid solutions $A_2(Sm_{1-x}RE_x)Ti_2Nb_3O_{15}$ (A = Sr, Ba; RE = Nd, Sm, Gd, La) provides an ideal framework to examine the influence of rare-earth ionic radii on the TTB structure and its dielectric properties, offering key insights for the development of high-performance ceramics.

The compounds $A_2(Sm_{1-x}RE_x)Ti_2Nb_3O_{15}$ (A = Sr, Ba; RE = Nd, Sm, Gd, La) were synthesized via solid-state reaction. The resulting ceramics were characterized using various techniques, including X-ray diffraction (XRD), scanning electron microscopy (SEM), and dielectric measurements. Substitution with different rare-earth elements in the TTB compounds leads to a gradual decrease in lattice parameters as the ionic radius decreases (from La to Gd), accompanied by a space group transition from P4bm for La, Sm, and Nd to P4/mbm for Gd. Dielectric properties show significant variation depending on the rare-earth element, with high dielectric constants and low losses, reflecting the influence of local polarization and structural distortions. SEM observations reveal changes in grain morphology and size consistent with the effects induced by ionic substitution. Overall, these results highlight a direct correlation between the RE ionic radius, lattice distortions, and dielectric properties, confirming the crucial role of substitution chemistry in tuning the properties of tetragonal tungsten bronzes.

sciforum-179451: Synergistic Effects of Medium Composition and Phenol Oxidase Induction on Fungal Nanoparticle Biosynthesis

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Introduction:

Green synthesis has emerged as an environmentally sustainable alternative to conventional chemical approaches for nanoparticle production. Fungal-mediated biosynthesis of silver nanoparticles (AgNPs) is particularly promising due to its efficiency in metal ion reduction and natural secretion of stabilizing biomolecules. This study examined whether stimulating phenol oxidase activity in culture media enhances the rate and yield of AgNP formation by the filamentous fungus *Aspergillus niger*.

Methods:

Six variants of Czapek–Dox medium were prepared using sucrose, starch, or glucose as carbon sources. Phenol oxidase stimulation was introduced into variants 2, 4, and 6 through copper(II) sulfate, oak sawdust, and hydrogen peroxide. *A. niger* was cultivated for 72 h in each medium, after which the biomass was transferred to ultrapure water for extracellular metabolite release. Following another 72 h, the biomass was removed, and a 1 mM silver nitrate solution was added to the filtrates. AgNP formation was monitored by UV–Vis spectroscopy over 120 h. Functional groups were identified by FTIR, and crystalline structure was confirmed using XRD.

Results:

A characteristic AgNP surface plasmon resonance peak at ~420 nm appeared in all variants. Media containing phenol oxidase stimulants showed notably higher absorbance and faster nanoparticle formation kinetics. FTIR spectra confirmed the presence of protein, enzyme, and carbohydrate functional groups involved in nanoparticle capping, while XRD verified the crystalline nature of the AgNPs across all samples.

Conclusions:

Phenol oxidase stimulation significantly enhanced the rate of AgNP biosynthesis without altering nanoparticle structure or capping composition. Medium optimization therefore represents a critical step toward scaling fungal-based AgNP production for industrial applications.

sciforum-176790: Synthesis and crystal structure of a polymeric Mn(II) coordination complex based on 3,4-pyridinecarboxylate

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In this study, a polymeric coordination compound with the composition $C_{10}H_{10}MnN_2O_5$ has been structurally characterised. The results indicate that the compound crystallises in the monoclinic crystal system with the space group $P2_1/c$. The unit cell parameters are a = 7.7002(6) Å, b = 10.2149(6) Å, c = 15.0286(12) Å, and β = 104.102(8)°, with a cell volume of 1146.48(15) Å^3.

The manganese(II) centre exhibits a coordination number of six, being surrounded by five oxygen atoms and one nitrogen atom, thereby forming a distorted octahedral geometry. The Mn–O bond lengths are in the range 2.154–2.176 Å, whereas the Mn–N bond length is 2.320 Å. These distances are consistent with those typically observed for Mn(II) coordination environments, confirming the expected bonding characteristics.

The organic ligand fragment contains an aromatic ring system that is essentially planar. The C–C bond lengths lie in the range 1.377(4)–1.400(4) Å, while the C–N bond lengths are 1.334(4)–1.345(4) Å, indicating the presence of a delocalised π-conjugated system. The carbonyl C–O bond distances, ranging from 1.226(5) to 1.254(4) Å, are in good agreement with expected values.

The crystal structure is primarily stabilised by metal–ligand coordination bonds together with weak supramolecular interactions, including C–H···O and C–H···π contacts. No significant solvent-accessible voids were observed within the lattice.

In the crystal packing, weak supramolecular interactions further contribute to stabilisation. In particular, weak C–H···π interactions are observed between aromatic rings, such as the C2A–H2AC···Cg1 contact with a distance of 2.839 Å. In addition, the centroid–centroid separation between adjacent aromatic rings is 5.456 Å, indicating weak π–π stacking interactions. Although no classical hydrogen bonds are present, weak C–H···O interactions also play a role in stabilising the crystal packing.

sciforum-179572: Synthesis, characterization, and physicochemical properties of copper halide-intercalated $RbLaTa_2O_7$ layered inorganic material

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Inorganic materials with layered architectures are made up of stacked atomic or molecular layers held together by weak van der Waals interactions. Examples of such materials include layered perovskites, clays, MXenes, transition metal dichalcogenides, layered double hydroxides, and carbon-based layered materials. The intercalation of various guest species (e.g., nanoparticles, molecules, polymer chains) into lamellar inorganic compounds is an effective strategy for creating multifunctional materials with enhanced physical and chemical properties relative to those of the parent compounds. Exfoliation of layered nanostructures into single nanosheets yields soft materials with distinct features. The intercalation process is affected by several critical factors, including interlayer distance, guest orientation in the interlayer space, and/or layer rigidity. Tailoring these factors enables the creation of high-performance intercalated materials with applications across energy storage, electronic devices, sensors, catalysis, and nanotechnology.

Herein, we report a soft chemical approach to intercalate copper species into the $RbLaTa_2O_7$ layered perovskite tantalate involving a copper halide precursor at a mild temperature. Both unmodified and $(CuCl)^+$- intercalated layered perovskite were characterized using multiple techniques to assess structural, optoelectronic, and morphological changes. The shifting of the (001) diffraction line confirmed the successful insertion of $(CuCl)^+$ species in between the perovskite layers. The FTIR technique validated structural modifications in the materials. UV-Vis spectroscopy demonstrated a decrease in the band gap of the $(CuCl)^+$- intercalated layered tantalate, thereby enabling visible-light absorption. Preliminary photocatalytic performance evaluations indicate that $(CuCl)^+$- based perovskite exhibits promising activity for phenol degradation, serving as an effective catalyst for environmental applications.

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sciforum-176848: Synthesis, Structure, and Luminescence Properties of a New Langbeinite-Type Phosphate $RbSrSc_2(PO_4)_3:Pr^{3+}$

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For multicomponent systems, maintaining precise stoichiometry during crystal growth remains a significant challenge. Langbeinite-type phosphates with the general formula $A^+B^{2+}B^{3+}_2(PO_4)_3$, where A^+ and B^{n+} represent different cations, often decompose into their constituent phosphates during growth, making single crystal synthesis particularly challenging. However, solid-phase synthesis can produce high-quality crystalline samples of these materials.

In this study, we successfully synthesized a langbeinite-type compound, $RbSrSc_2(PO_4)_3$, by a conventional solid-phase method and comprehensively characterized its structural and physical properties. Rietveld refinement of sample confirmed a langbeinite-type cubic structure (SG: $P2_13$), comprising corner-sharing $[ScO_6]$ octahedra and $[PO_4]$ tetrahedra, with [Sr,Rb] ions occupying distorted 9- and 12-coordinate cavities. The resulting samples doped with different amount of Pr^{3+} were examined for their luminescence behavior under UV and X-ray irradiation. The promising potential of the obtained langbeinite for modern photonic applications.

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sciforum-176958: Tunable Low Thermal Expansion in Calcite-Type $Febo_3$ and $Crbo_3$ Borates

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Transition-metal borates have attracted considerable interest due to their rich crystal chemistry and diverse functional properties (magnetic, electrochemical, optical and others). These materials exhibit rare phenomena such as high magnetic ordering temperatures, cascades of magnetic transitions, spin-liquid, glass and ice states. Owing to unique combination of properties, $FeBO_3$ has been developed as a commercial Mössbauer source for synchrotron facilities [1]. In $FeBO_3$, the magnetic ordering temperature is high ($T_N \approx 348$ K), whereas in $Fe_{1-x}Cr_xBO_3$ decreases with increasing Cr content [2].

In this work, $FeBO_3$ and $CrBO_3$ were investigated by *in situ* high-temperature powder X-ray diffraction (Rigaku Ultima IV, Cu $K\alpha$, 295–1173 K). Near T_N, $FeBO_3$ exhibits anomalous unit-cell behavior, whereas $CrBO_3$ shows no such anomalies. Both borates display positive uniaxial thermal expansion with low average coefficients: $\alpha = 8$ ($FeBO_3$) and $6 \times 10^{-6} K^{-1}$ ($CrBO_3$). The slight reduction in the expansion upon the Cr → Fe substitution arises from the smaller ionic radius of $^{VI}Cr^{3+}$ and shorter Cr–O bonds. $FeBO_3$ remains stable up to ~900 K, where a recrystallization to α-Fe_2O_3appears, while $CrBO_3$ is stable up to 1173 K. Thermal expansion is maximum along the *c* axis, i.e. perpendicularly to planes of the isolated BO_3 triangles, and minimum in the *ab* plane. These findings suggest that $Fe_{1-x}Cr_xBO_3$ borates are promising candidates for synchrotron, optical and magnetic applications requiring tunable low thermal expansion.

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Session 2. Liquid Crystals

sciforum-179293: Chiral Copper(I) N-Acylthiourea Complexes: From Synthesis to High Helical Twisting Power in Nematic Liquid Crystals

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This paper reports the synthesis and characterization of novel chiral copper(I) complexes, generated by the reaction of enantiopure N-acylthiourea ligands with copper(II) halides. Spectroscopic investigation (NMR, IR, UV-Vis) revealed the monodentate coordination of the ligands through the sulfur atom to the Cu(I) ion, confirming the formation of the mononuclear complexes.

The functional evaluation focused on applying these compounds as chiral dopants in the commercial nematic liquid crystal E7. Polarized optical microscopy (POM) and differential scanning calorimetry (DSC) confirmed the formation of a stable chiral nematic (N*) phase in all doped mixtures. The helical twisting power (HTP) was quantified using the Grandjean–Cano method. While the free ligand exhibited low HTP, the copper(I) complexes demonstrated substantial enhanced efficacy. This significant boost is attributed to the increased molecular weight and structural rigidity of the coordination complexes. The tight helical pitches induced by the complexes correspond to selective reflection in the near-infrared region (NIR), whereas the ligand induces a larger pitch. These results highlight the potential of these complexes for advanced photonic applications in the NIR and establish chiral copper(I) N-acylthiourea complexes as a promising new class of chiral dopants, with future prospects for achieving selective reflection in the visible region.

Building on our previous work [1], this study expands the ligand diversity and structural complexity of copper(I) complexes.

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sciforum-176690: Colossal Permittivity in Ferrogenic Nematic LCs

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Colossal Permittivity in Ferrogenic Nematic LCs.

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The long-awaited ferroelectric nematic LCs (NF) predicted more long time ago were finally discovered in 2017, independently in two different materials: RM 734 and DIO. However, the presence of spontaneous polarization did not offer any advantage for display technology. Recently we observed the colossal dielectric permittivity (CP) in non-ferroelectric materials with high dipole moment > 10 D [1]. Such permittivity exists not only in LC phases materials even in isotropic phase and was also observed in [2]. Therefore, the colossal permittivity is a property of extremely high dipole moment itself but not specific phase. Here we report the existence of such CP mode in ferroelectric materials; mixtures of WJ-16 (Hull, UK) with DIO and individual component SA-153 (Belfast, UK). Both materials show three relaxation processes, where lowest frequency process P0 is ionic mobility mode, the mid-frequency process P1 shows colossal permittivity (>= 10000) and exists in all phases including the isotropic and the last one P2 shows is typical para– ferroelectric transition. The relaxation process P1 was called as superparaelectric [1] but it exists in all phases/temperatures, so the better name is “hi-permittivity” or “hyper permittivity” mode [3]. This mode opens a new range of applications of ferrogenic liquid crystals as the working media for supercapacitors with the potential of using them in energy storage devices.

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sciforum-177207: Electric Permittivity Behavior in Highly Polar Liquid Crystals: From Paraelectricity through Ferroelectricity to Superparaelectricity

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The discovery of polar order in achiral liquid crystals has revolutionized the field of soft matter, offering properties comparable to solid-state ferroelectrics.

In this study, the dielectric response of several homologous series of rod-like compounds was analyzed, on how molecular architecture determines polar properties. By analyzing several homologous series of rod-like compounds, we investigate how specific structural modifications, such as terminal groups and core substitutions, influence mesophase stability and electrical response. The primary focus is placed on the role of terminal groups, including nitro, cyano, and fluorine fragments. Additionally, we examine how minimal structural changes, such as the addition of a single methylene unit, can radically shift a material from a paraelectric to a ferroelectric state.

The research shows that the emergence of the ferroelectric order is driven by a specific collective mode. In this state, molecules within different domains vibrate in or out of phase depending on their polarization direction. We also analyzed two achiral smectic phases. In the ferroelectric smectic A phase, we observed a soft mode (amplitude mode) where the dielectric strength increases and the relaxation frequency decreases as the temperature decreases. While, in the ferroelectric smectic C phase, a phason mode appears, similar to the Goldstone mode in chiral systems.

Furthermore, in a specially designed mixture, we observed a very high values of electric permittivity. These values are comparable to those found in ferroelectric fluids, even though the mixture itself does not have full ferroelectric properties. Instead, it can be described as superparaelectric. Understanding the specific dielectric modes and the phenomenon of superparaelectricity allows us to design stable, high-performance materials that respond quickly to electric field.

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sciforum-175964: Evaluation of applied methods for the determination of viscoelastic effects in chiral liquid crystals

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The material characteristics of liquid crystals play a crucial role in shaping the structure, order, and properties of a particular mesophase and its adjacent phases. This is vital for the development of high-performance optoelectronic devices such as liquid crystal displays, light modulators, apertures, and filters. While the elasticity and viscosity constants are seldom measured, they are essential for evaluating a material's applicability. Leveraging the ferroelectric and antiferroelectric properties of smectics enhances various parameters of information visualization devices, including grayscale, switching speed, contrast, and information content [1, 2].

The newly established method for calculating the absolute values of the coefficients related to the linear and quadratic electro-optical effects in low electric fields enables the assessment of elasticity constants (derived from the depth of light modulation) and rotational viscosity (based on frequency dependence), all while maintaining laminar flow and low strain conditions. Additionally, the type and characteristics of the phase transformations that occur in the material being examined can significantly impact both the magnitude of the determined coefficients and their dependence on temperature [3].

This study focuses on reviewing the methods employed to assess viscoelastic effects in ferroelectric and antiferroelectric chiral liquid crystals, their mixtures, composite materials, and even dielectric systems. The goal is to establish a universal method that permits the application of relatively low electric fields. For chiral liquid crystals with ferroelectric and antiferroelectric phases, as well as their subphases, the following principle holds: adherence to Hooke's law (for elastic coefficients) and maintenance of laminar flow (for viscosity coefficients) [4].

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sciforum-179532: Exploring Inter-Nanoparticle Repulsion Effects on Structural Phases and Diffusivity in Polymer Nanocomposites: A Langevin Dynamics Simulation Study

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Polymer nanocomposites (PNCs) combine polymer matrices with nanofillers to achieve exceptional mechanical, thermal, and functional properties. However, understanding how inter-nanoparticle (NP) repulsive interactions influence structural assembly and transport properties in confined domains remains under-researched. In this study, we employ GPU-accelerated Langevin dynamics simulations to systematically investigate how varying inter-NP repulsive strength drives phase behaviour in strongly confined PNC systems. Semi-flexible polymer chains and spherical NPs were simulated in extremely confined (quasi-2D) geometries with fixed monomer and NP volume fractions. Structural properties were studied via radial distribution function, cluster analyses, crystallinity and nematic order parameter calculations, while diffusivity was assessed through mean-square displacement analysis. Depending on the strength of repulsion the composite system self-assembles into distinct morphologies: i) a droplet phase, characterised by complete NP phase separation; ii) a slab phase featuring percolating networks and maximum nematic order iii) a broken-slab phase showing polymer infiltration and fragmented assemblies; and iv) a dispersed phase with ordered NP distribution, exhibiting increased smecticity at higher repulsion strengths and displaying crystalline spatial organisation as confirmed by RDF and crystallographic analysis. Diffusivity exhibits non-monotonic behaviour, with optimal nanoparticle mobility at intermediate repulsive strengths while polymer diffusivities show inverse trends indicating competing dynamics between the two components. These findings demonstrate that fine-tuning inter-nanoparticle repulsions provides precise control over structural phases and transport properties, offering design principles for PNCs with the required functionality.

sciforum-179951: Influence of Biologically Active Additives on the Viscosity of Lamellar Liquid Crystals

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Lamellar mesophases based on lecithin are of interest for the development of topical formulations due to their ability to accommodate components of different polarity and their structural similarity to stratum corneum lipids. Rheological behavior is a key parameter that affects both the application properties and the release profile of active ingredients.

In this work, we investigated how the addition of gelatin and several plant extracts (dioscorea, onion, red wine) modifies the viscous properties of lamellar liquid crystals formed in a quaternary system: lecithin – olive oil – tea tree oil – water. All samples were prepared using a previously developed procedure; the presence of a lamellar mesophase was confirmed by polarized light microscopy. Rheological tests were carried out on a Haake Viscotester IQ rotational viscometer at 25 °C. All compositions exhibited pseudoplastic behavior, i.e., the effective viscosity decreased with increasing shear rate.

Incorporating gelatin solutions at concentrations of 1, 2, 3, and 5 % into the liquid-crystalline matrix increased the viscosity in the shear rate range 0.01–1.0 s^{-1} by factors of 1.23, 1.49, 1.58, and 1.79, respectively, compared to the control sample. The most pronounced effect was observed at 5 % gelatin, which can be attributed to the formation of a three-dimensional gel network within the aqueous interlayers.

Plant extracts also significantly altered the rheological response. The dry extract of dioscorea raised the viscosity by a factor of 1.23 on average, whereas the alcoholic extract of dioscorea gave a 7.5- to 13.1-fold decrease depending on the shear rate. Onion alcoholic extract resulted in a 3.4- to 9.6-fold viscosity reduction. For red wine dry extract, a clear concentration dependence was found: at 1, 2, and 5 % the viscosity increased by factors of 1.40, 1.66, and 2.02, respectively. After two weeks of storage, all samples retained their liquid-crystalline structure, indicating good physical stability.

The results demonstrate that the rheological properties of lecithin-based lamellar phases are highly sensitive to the nature and concentration of incorporated additives. These findings provide a basis for tailoring the viscosity and release characteristics of lecithin liquid-crystalline formulations intended for dermatological and cosmetic use.

sciforum-177002: Observation of Fano Resonance in Self-Assembled Copper Nanoparticles-Blue phase liquid crystal Hybrid Metamaterial

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Blue Phase liquid crystals (BPLCs) offer a sophisticated 3D self-assembled scaffold for templating functional nanomaterials. This study investigates the optical coupling within BPLCs doped with Copper (Cu) nanoparticles (NPs), specifically focusing on the interference between localized plasmonic modes and the 3D photonic lattice. Using dark-field hyperspectral imaging (HSI), we resolve the far-field scattering of individual Cu NPs embedded within the BPLC matrix.

A central finding of this work is the experimental observation of Fano resonance, manifested as a distinct spectral asymmetry with a pronounced shoulder and dip—in the broad scattering profile of the Cu NPs. This spectral feature occurs precisely at the wavelength range corresponding to the narrow selective reflection peak of the BPLC lattice. We attribute this to the interference between the broad plasmonic continuum of the Cu NPs and the discrete Bragg modes of the BPLC scaffold. These results are supported by polarized optical microscopy (POM) and temperature-dependent reflection measurements, which confirm the spatial and spectral correlation between NP scattering and the BPLC's 3D photonic bandgap. These observations are validated through a finite-element method (FEM) framework, using COMSOL Multiphysics to simulate the reflection and scattering spectra. This multimodal approach demonstrates that Cu-BPLC architectures function as tunable, hybrid metamaterials, offering a pathway for designing responsive chiro-optical devices through precision spectral engineering.

sciforum-179663: Role of elastic constants in the textures of the 8CB-CB7CB mixtures

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Nematic liquid crystals possess long-range orientational order described by a director field whose distortions are mainly determined by the Frank elastic constants for splay (K_{11}), twist (K_{22}), and bend (K_{33})[1]. In bent-shaped dimers such as CB7CB, the bend elastic constant K_{33} becomes anomalously low near the nematic twist-bend phase[2], strongly influencing director configurations and electro-optic textures. When CB7CB is mixed with the rod-like compound 8CB, the resulting nematic phase maintains the usual orientational order while inheriting a very low[3] K_{33} value, making the system ideal for studying elasticity-affected textures.

This work demonstrates how such variations in elastic constants[1] shape the texture of a chiralized nematic. Usually adding a small amount of a chiral dopant to a nematic phase only induces a spontaneous twist and results in homogeneous textures. We show this is no more the case with reduced bend constant. Mixtures of 8CB and CB7CB were prepared and filled into planar and twisted-nematic cells. Elastic constants K_{11}, K_{22}, and K_{33} were then measured as with changing temperature and composition using impedance spectroscopy and electro-optic response analysis. Texture evolution of these mixtures doped with the chiral compound S811 was observed using polarized optical microscopy. Mixtures with higher CB7CB content show a significant reduction in K_{33}, while K_{11} and K_{22} vary more moderately. This low- K_{33} regime leads to voltage-induced striped and heliconical-like textures, with periodicity varying with the temperature. Elastic anisotropy—particularly when K_{33} becomes very small—plays a central role in forming and stabilizing non-uniform nematic textures.

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sciforum-179179: SELECTIVE REFLECTION ZONES IN MODULATED FLEXOELECTRIC STRUCTURES INDUCED BY A PLANAR ELECTRIC FIELD

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Liquid crystals (LCs) exhibit anisotropic optical and dielectric properties, allowing them to effectively manipulate light by changing the orientation of the long axes of the molecules (the n-director) under the influence of an electric field. This makes LCs unique materials for photonics.

Along with the traditional switching of LC states, in which the director reorientation occurs due to the dielectric effect, there is a variant of the electric field interaction with flexoelectric polarization. The flexoelectric effect (FE) in liquid crystals, first theoretically predicted in 1969 by Meyer [1], arises in LCs as a result of splay and bend deformations. At low values of dielectric anisotropy, the FE becomes predominant in electrically induced orientational transitions and can manifest itself as a periodic supramolecular structure or flexolattice [2, 3].

In this research for the first time periodic flexostructures are investigated using planar interdigital electrodes. A nonuniform electric field generated by a such electrode system leads to the formation of modulated flexoelectric structures in the above-electrode and interelectrode regions, with wave vectors directed perpendicular and parallel to the LC layer normal, respectively. The cycloidal director distribution arising in the interelectrode region with refractive index modulation along the normal to the LC layer leads to the appearance in the transmission spectrum of a selective reflection band. The spectral position of the band depends on the amplitude of the applied voltage and on the light incidence angle relative to LC layer normal. Numerical modeling methods were used to study in detail the LC director distributions and the spectral features of the field-induced transition.

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sciforum-163529: Separation of Lithium Isotopes: Electromigration Coupling with Crystallization Li^6

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This work reports the design, development, and validation of an integrated system that couples electromigration-based lithium isotope separation with controlled crystallization of lithium carbonate enriched in lithium-6 (^{6}Li). The research aims to provide a sustainable and scalable technological alternative for isotope enrichment processes, with direct relevance to nuclear materials and next-generation battery applications.

The experimental setup combines a dual-module electromigration cascade with a thermostated crystallization unit, interconnected through a fully automated robotic and fluidic transfer system. This configuration enables continuous operation, real-time process control, and zero-loss transfer of the Li^6-enriched cathodic solution. Four types of ion-conducting membranes were investigated: Nafion 212, Nafion 117, Celgard 2325, and a novel PEG-crosslinked PS-9 prototype developed at ICSI ENERGY. All membranes were tested under constant potential (5 V) for 120 h, ensuring comparable electrochemical conditions.

Following separation, the Li^6-enriched cathodic solution underwent a crystallization protocol optimized for pH (7.2–7.5), concentration, and temperature (4 °C). Ammonium carbonate ($(NH_4)_2CO_3$) was used as a controlled nucleating agent, promoting selective precipitation of Li_2CO_3 (^{6}Li). FTIR analysis confirmed the presence of Li–O and CO_3^{2-} vibrational bands, indicating pure lithium carbonate formation. SEM characterization revealed uniform prismatic microcrystals (1–3 μm), with morphology dependent on membrane architecture — well-faceted for Nafion, compact for PS-9, and large aggregates for Celgard.

Crystallization kinetics were evaluated using the Avrami model, yielding $n \approx 2.8$ and $k = 0.3\ h^{-n}$, consistent with instantaneous nucleation followed by three-dimensional diffusion-controlled growth. The entire process achieved a Li^6 recovery of 95.7 ± 0.3% and >98% crystalline purity.

The results confirm the system's efficiency, reproducibility, and full automation, demonstrating a novel technological pathway for lithium isotope enrichment through synchronized electromigration–crystallization coupling.

sciforum-178903: The effect of the presence of 5CB liquid crystal molecules in the electrolyte on the current-voltage parameters of the DSSC cell

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The work experimentally compare the operating characteristics of dye-sensitized solar cells (DSSCs) with cis-bis(isothiocyanato)bis(2,2′-bipyridyl-4,4′-dicarboxylato)ruthenium(II) (N3) dye for two iodide/tri-iodide liquid electrolyte (AN-50) variants: (a) classic AN-50 iodide electrolyte, (b) AN-50 modified with 4-*n*-pentyl-4'-cyanobiphenyl (5CB) liquid crystal (LC) additive (10%) at an operating temperature of 300–303 K. The aim was to determine the effect of the 5CB additive on the open circuit voltage (Voc), short circuit current (Isc), fill factor (FF), power of the real cell (Pmax) parameters and resistive loss indices (Rs - Joule effect losses, Rsh - shunt resistance) and to formulate mechanistic conclusions (ion transport vs. recombination/interface). For each sample, a quasi-static measurement run was performed under constant illumination (116 klx) and controlled sample temperature. Load conditions were varied over time (sweep), while the sample voltage V(t) and current I(t) were recorded. The current–voltage (I–V) and power–voltage (P–V) characteristics were determined from the (V, I) pairs after their time synchronization. The introduction of 5CB into the AN-50 electrolyte affects the balance between ion transport/diffusion of redox couples I^-/I_3^- and recombination losses at the photoanode-electrolyte interface. Literature shows that LC used as electrolyte additives can increase the "transmission paths" of redox couples, which favors an increase in Isc; however, the effect is concentration-dependent and can be reversed if the additive content is too high. In the tested samples, higher Voc and Isc were observed on average compared to the single control, with a simultaneous lower FF. This combination is consistent with the hypothesis of: (a) partial improvement in generation/transport (Isc), but (b) increased resistive-transport losses or changes in electrode kinetics that reduce FF. Due to the single control and different measurement dates, this conclusion should be considered preliminary and requires confirmation by measurements under identical conditions.

Session 3. Organic Crystalline Materials

sciforum-169949: Synthesis and biological activity of a styrylquinolinium derivative

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The application of styrylium dyes as organic nonlinear optical materials in several photonics fields has been studied for many years. Recently, the biological activity of styrylium dyes has also been examined, namely their antibacterial effects. Therefore, our primary objective was to synthesize a styrylium compound with an antibacterial effect. Knoevenagel condensation was used to obtain a new styrylquinolinium derivative. To verify its structure, spectroscopic methods such as IR, NMR (^{1}H, ^{13}C, COSY, HSQC, and HMBC), HRMS spectra, and X-ray studies were employed.

The compound's antibacterial and anti-inflammatory properties were also evaluated. It was found that the stytylium derivative had excellent antibacterial action against fungi, three Gram-negative strains, and five Gram-positive strains. The compound's most noticeable effects were against *Pseudomonas aeruginosa* and *Escherichia coli*. In addition, ex vivo immunohistochemistry was used to assess the compound's anti-inflammatory properties. The substance showed promising immunomodulatory and antimicrobial properties. It can be regarded as a regulated modification of the immune response, particularly in situations requiring local immunological activation, because of its capacity to both stimulate IL-1β and moderately decrease NOS3.

Furthermore, the biological activity was verified using molecular docking modeling. The compound's successful binding to the bacterial protein's active site was demonstrated by docking simulation, which corroborated the compound's antibacterial activity as reported in experiments.

sciforum-176965: Synthesis, Crystal Structure and Hirshfeld Surface Analysis of 3-butylquinazolin-4(3H)-one Hydrochloride

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Introduction.

One of the key tasks of modern chemistry is the targeted synthesis of new highly efficient biologically active compounds and their use in agriculture and medicine to combat diseases. In recent years, biologically active substances have been identified among substituted derivatives of quinazolin-4(3H)-one. Therefore, developing effective and environmentally safe preparations based on inexpensive raw materials and improving their physicochemical and biological properties remains an important scientific direction.

Experimental.

3-Butylquinazolin-4(3H)-one was dissolved in acetone with thorough stirring using a magnetic stirrer. When hydrogen chloride (HCl) gas was introduced into the solution through a tube, a white precipitate formed. The resulting solid was filtered, and the filtrate was washed 2–3 times with acetone. As a result, pure 3-butylquinazolin-4(3H)-one hydrochloride was obtained with an 88% yield. R_f = 0.66 (system: water : methanol, 1:1); melting point 179–181 °C.

Results

The crystal structure crystallized in the monoclinic system with the *P-1* space group. The asymmetric unit contains one molecule. The crystal structure exhibits three types of intermolecular hydrogen bonds: Cl–H···N, N–H···Cl, and C–H···N. The N–H···Cl hydrogen bonds connect the molecules in the crystal and form a chain-like network along the [110] direction. This indicates that the chlorine atom of the molecule and the inversion center link the quinazoline molecules together. In addition, π···π interactions between the molecules contribute to the formation of a three-dimensional structure. The crystal structure was further analyzed using Hirshfeld surface analysis.

Conclusion

In this study, we examined not only the synthesis and structure of 3-Butylquinazolin-4(3H)-one hydrochloride, but also its Hirshfeld surface analysis. Biological tests of the synthesized 3-Butylquinazolin-4(3H)-one hydrochloride confirmed its insecticidal activity.

sciforum-177911: Bulk Crystallization as a High-Potential Purification Strategy for C-Phycocyanin

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In the history of protein crystallization, one of the earliest purposes of crystallization was separation and purification of proteins from mixtures. Nowadays, the rising demand for pure proteins in biomedicine, biochemical research, and the food industry highlights the need for cost-effective purification methods. Although chromatography dominates large-scale processes, crystallization offers a low-cost alternative for obtaining highly purified products, though its industrial implementation remains challenging.[1] In this context, crystallization is re-emerging as a promising strategy due to its inherent selectivity and potential for cost-effective scalability.

Phycobiliproteins (PBPs) are water-soluble light-harvesting pigment-proteins from cyanobacteria and red algae.[2] In addition to their role in photosynthetic energy capture, they exhibit diverse biological activities, including antioxidant, antibacterial, and anticancer effects, which make them promising candidates for biotechnological applications in fields such as biomedicine, bioenergy, and scientific research.[3] Among PBPs, C-phycocyanin (C-PC) is a high-value pigment widely used in health, food, and analytical applications. Current downstream processes, however, rely mostly on multistep chromatographic workflows that increase production costs and complexity.[4]

Through this work, we are exploring protein crystallization as an alternative route for C-PC purification from raw materials, aiming to establish its feasibility as a scalable method that integrates high product quality with improved process sustainability. Preliminary results support the potential of crystallization to enhance recovery of C-PC, thereby contributing to more efficient bioprocessing.

sciforum-179601: Comparative study of fluid inclusions in Dicumyl and Benzoyl Peroxides

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The formation of fluid inclusions is often an anathema for many applications of crystallized phases. For instance: Active Pharmaceutical Ingredients (solvent content above ICH guidelines), second harmonic generation (yield in the intensity of the secondary beam and chemical degradation of the SHG material), energetic material (shock sensitivity), solid oxidizers (loss of the rocket booster power) [1-2], etc...

This study focuses on two organic compounds: dicumyl peroxide [3-4] and benzoyl peroxide. Besides the obvious similarity in their formulas and the propensity of dissolved CO_2 to induce the formation of fluid Inclusions [5], these fluid inclusions present different: thermal behaviors, shapes and frequencies which will be detailed. They reveal different formation and relaxation mechanisms. Further extension of these findings to other peroxides are currently under investigations.

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sciforum-179658: Complete the circle: cocrystal formation thermodynamics derived from congruent sublimation and solution cycles

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High potential of cocrystals in drug delivery[1] and functional materials[2] draws attention to the problems of rational design of cocrystals with desired properties. These properties including stability and solubility are determined by the difference in lattice free energy of a cocrystal and its constituents . Sublimation is used as a green and effective cocrystallization method [3, 4]; however, the only reports of cocrystal sublimation thermodynamics consider the systems where only one component is volatile. [5, 6]

We introduce the term 'congruent sublimation' for equilibrium of the solid cocrystal with the molecular vapor of its components of the same ratio. In the transpiration experiment, the [caffeine + 3-hydroxybenzoic acid] cocrystal vapor was carried by slow stream of nitrogen through a tube furnace and condensed downstream. The sublimate was identified as pure cocrystal by DSC, PXRD and FTIR spectroscopy. Vapor pressures of both components were determined to be close to equal according to HPLC analysis. Sublimation thermodynamic functions were derived according to Clausius-Clapeyron equation and corrected to 298.15 K using experimental solid molar heat capacities and theoretical gas-phase heat capacities. From the experimental sublimation functions of the cocrystal and literature data for pure components, cocrystallization thermodynamic functions were determined. Alternatively, the cocrystallization enthalpy and Gibbs energy were derived from solubility data of the cocrystal and pure components in acetonitrile at five different temperatures between 293 and 313 K.

The equality of vapor pressures of caffeine and hydroxybenzoic acid confirms the congruent sublimation across the experimental temperature range. No gas-phase complexes were observed in the synchronous DSC/TG/MS experiment. The cocrystal formation process was found to be enthalpy-determined. The cocrystallization enthalpy and Gibbs energy values derived from the sublimation and solubility cycles were found to be within 2 kJ/mol, which supports the proposed sublimation mechanism.

sciforum-170550: Crystal structure of novel 22- and 23-membered acylhydrazone-based macrocycles

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Macrocyclic compounds are a versatile group of ligands that can be used for selective complexation of cationic, anionic, and neutral chemical species. Macrocyclic compounds containing an acylhydrazone functional group can be prepared by the reaction of polyhydrazine and polyaldehyde precursors. To investigate the structural features of acylhydrazone macrocycles, we have prepared and crystallized two novel macrocyclic compounds (**achyM5** and **achyM6**). The prepared compounds are ring analogs containing 22 (**achyM5**) and 23 (**achyM6**) atoms in the inner macrocyclic ring. Both compounds are N_5O_4-donor macrocycles composed of a pyridine and dibenzaldehyde moieties connected by acylhydrazone groups. Although rather similar, the compounds differ in the subtle geometrical parameters such as dihedral angles, puckering amplitude, and inner macrocyclic hole size. These parameters show that the larger macrocycle (**achyM6**) is more deformed (puckering amplitude of 2.721(3)). In the crystal structure of **achyM5** the adjacent macrocycles are connected *via* N-H···O hydrogen bonds between NH groups and carbonyl oxygen along the *a*-axis. Interestingly, there is a short contact between the imine and pyridine N atoms (3.045 Å) of adjacent macrocycles that can be regarded as a weak N···N pnictogen bond. The final 3D arrangement is achieved *via* weak C-H···C and π···π interactions. The **achyM6** crystallizes as a water solvate, with 2 symmetry-independent molecules in the asymmetric unit. The water molecule is located approximately in the center of the macrocyclic ring and connected *via* N-H···O hydrogen bonds. In the crystal, the adjacent macrocyclic molecules are primarily connected through O-H···O hydrogen bonds that involve a water molecule and carbonyl oxygen, and N-H···O hydrogen bonds between NH groups and carbonyl oxygen. A short N···N contact between the imine and pyridine N atoms (3.007 Å) of adjacent macrocycles is also present, implying the importance of these interactions in the overall crystal stability of these systems.

sciforum-176858: Crystal Structure, Supramolecular Assembly, and Molecular Arrangement of Mansorin A: A Bioactive Natural Product from *Mansonia gagei*

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This paper presents a comprehensive review of the current state of knowledge regarding the crystalline architecture and solid-state behavior of Mansorin A, a key bioactive secondary metabolite isolated from the heartwood of *Mansonia gagei*. Despite its recognized pharmacological potential, including its antifungal and cytotoxic effects, the physical chemistry of its crystalline form is often overlooked. This paper systematically categorizes existing crystallographic data to provide a holistic understanding of how molecular structure dictates the material properties of this natural product. The analysis focuses on the supramolecular assembly of Mansorin A, highlighting the role of the planar naphtofurane-type skeleton in promoting specific molecular arrangements. The reported unit cell parameters and the hierarchy of non-covalent interactions are examined, specifically emphasizing the π- π stacking motifs and the complex networks of C-H···O hydrogen bonds that stabilize the lattice. Furthermore, this review evaluates the impact of polymorphism and solvate formation on the solubility and thermodynamic stability of the compound. By synthesizing data from chemical, structural, and pharmacological studies, this review identifies critical gaps in the current research, particularly concerning the structure-property relationships that affect the bioavailability of Mansorin A. It is concluded that a deeper understanding of its crystal engineering aspects is essential for developing effective delivery systems. This work serves as a foundational resource for researchers aiming to optimize the formulation of Mansorin-based compounds for future therapeutic applications.

sciforum-176759: Deciphering Intermolecular Interactions in Molecular Crystals through Quantum Crystallography and Non-Covalent Interaction Analysis

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Understanding intermolecular interactions in molecular crystals is fundamental for interpreting crystal packing, supramolecular organization, and the resulting physical or chemical properties of materials. Quantum crystallography provides a powerful tools for investigating these interactions directly from experimentally derived electron density distributions. In this presentation, I will discuss a series of studies on organic and metal–organic molecular crystals where experimental crystallography is integrated with electron-density–based analysis to obtain a deeper understanding of intermolecular interactions in the solid state.

Single-crystal X-ray diffraction experiments were used to determine accurate molecular geometries and crystal structures. To improve the description of hydrogen atoms and the underlying electron density distribution, Hirshfeld Atom Refinement (HAR) was employed, allowing the incorporation of quantum mechanical information into the crystallographic refinement process. The resulting electron density models were analyzed using the Quantum Theory of Atoms in Molecules (QTAIM), which provides a detailed topological framework for identifying bond critical points and characterizing the nature and strength of both covalent and non-covalent interactions.

To complement this analysis, non-covalent interaction (NCI) analysis and Hirshfeld surface approaches were used to visualize and quantify weak intermolecular contacts within the crystal lattice. These methods enable the identification of hydrogen bonding, π–π interactions, and dispersive contacts that collectively govern crystal packing and structural stability. By combining HAR refinement with QTAIM topology and NCI visualization, a consistent picture of intermolecular interactions emerges at both the electronic and structural levels.

Overall, this integrated crystallographic strategy demonstrates how modern electron-density analysis can provide detailed insight into supramolecular organization and structure–property relationships in molecular crystals, highlighting the growing role of quantum crystallography in contemporary structural chemistry.

sciforum-179521: Isolation, crystal structure, Hirshfeld surface analysis of artapshin

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Sesquiterpenes are widely regarded as key and often defining compounds within the *Artemisia* genus. This group of natural products is highly diverse, with more than 5,000 identified molecules to date. They have attracted significant interest due to their broad spectrum of biological activities, including antitumor, antimicrobial, anti-inflammatory, antioxidant, antidiabetic, anti-vitiligo, cytotoxic, and neuroprotective effects [1]. However, despite these beneficial properties, terpenoids may also produce adverse effects such as respiratory distress, central nervous system disturbances, nausea, and vomiting [2]. During the investigation of the chemical composition of *Artemisia scotina*, the compound artapshin, previously known but lacking a characterized crystal structure, was successfully isolated. Analysis of the spectral data (UV, IR, and NMR), together with comparison to published literature and an authentic reference sample, confirmed that the isolated compound is artapshin [3]. As part of our continued work, both the isolation and crystal structure of artapshin **(1)** were further examined. According to the X-ray analysis results, the asymmetric unit in the crystal consists of four molecules of the compound. Compound 1 was found to crystallize in the orthorhombic system ($P2_1$, Z=4). In the crystal, O—H···O and C—H···O hydrogen bonds link the molecules into infinite chains with a $C_{15}H_{24}O_5$ chain motif along the c-axis direction. Hirshfeld surface analysis showed that the structures are dominated by H···H, H···C/C···H and H···O/O···H contacts, these interactions present in the determined molecular structure were characterized as stabilizing factors in the unit cell.

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sciforum-166194: Novel 1,2-Binaphthyl-tethered *closo*-Rhodacarborane: Synthesis, Structure and Catalytic Applications

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Carboranes are noted for their three-dimensional aromaticity and exceptional stability. Their partially deboronated derivative, the nido-dicarbollide anion, serves as an analog of the cyclopentadienyl ligand, forming metallacarboranes with potential in catalysis and materials science. However, the application of such complexes in homogeneous catalysis remains largely underexplored. This work reports the synthesis and crystal structure of a novel binaphthylene-bridged closo-rhodacarborane complex, μ-1,2-[$(CH_2)_2C_{20}H_{12}$]-3-(η^3-C_8H_{13})-3,1,2-closo-$RhC_2B_9H_9$ (6), and its ligand precursor μ-1,2-$C_{20}H_{12}(CH_2)_2$-1,2-closo-$C_2B_{10}H_{10}$ (4). The structures of compounds 4 and 6 were fully characterized by single-crystal X-ray diffraction, high-resolution mass spectrometry, infrared spectroscopy, and NMR. Crystallographic analysis of 6 reveals a unique exo-polyhedral agostic C–H···Rh interaction, along with a network of intra- and intermolecular noncovalent interactions, including intramolecular C–H···π, and intermolecular C–Cl···π, C–H···π, C–H···H–B, and C–H···H–C contacts. In the crystal lattice of compound 4, significant intermolecular B–H···π and C–H···H–B interactions are observed. These weak interactions are crucial for understanding the solid-state packing and stability of these molecules. Preliminary catalytic studies demonstrate that complex 6 acts as a well-defined Rh(III) catalyst. It exhibits high activity at low loadings in selective cyclopropanation, epoxidation, C–H insertion, and Curtius-type rearrangement reactions under mild conditions. This work provides a new molecular prototype for crystal engineering and the design of catalytic materials based on metallacarboranes.

sciforum-152894: Novel Sulfanilamide-Derived Schiff Base: Synthesis, FT-IR spectroscopy, Crystal Structure, Hirshfeld Surface Analysis, and in silico ADME investigation

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Introduction

–Schiff bases are of significant importance in pharmaceutical chemistry due to their simple synthesis, structural flexibility, and broad biological activities. Sulfanilamide-derived Schiff bases are particularly advantageous, as they combine the bioactive sulfonamide moiety with the azomethine linkage, often resulting in enhanced antibacterial, anticancer, and enzyme-inhibitory properties. Their ability to form strong hydrogen bonds and π–π interactions further enhances their potential as therapeutic agents. In this work, we report the microwave assisted synthesis, FT-IR characterization, crystal structure, Hirshfeld surface analysis, and ADME prediction of a new sulfanilamide derived Schiff base, namely. (Z)-4-(((4,5-dihydroxy-6-oxocyclohexa-2,4-dien-1-ylidene)methyl)-amino)benzenesulfonamide (I).

Experimental

–Compound (I) was synthesized using microwave irradiation. The FT-IR spectra were recorded on Diamond ATR spectrometer in the 4000–400 cm^{-1}range. Single crystal X-ray data were collected at 296,15 K on a STOE IPDSIIdiffractometer, using Mo-Ka radiation and processed using the programs available in Olex2 [5]. Hirshfeld surface analysis was performed using CrystalExplorer21. ADME parameters were estimated using SwissADME(https://www.swissadme.ch).

Results and Discussion

–The FT-IR spectra indicated the keto-enamine tautomeric form, displaying characteristic bands at 2900 and at 1610 cm^{-1} corresponding to enamine and ketostretching modes, respectively. Single crystal X-ray diffraction revealed that compound (I) crystallizes in the P -1 space group as keto-enamine tautomer, with two crystallographically independent molecules in the asymmetric unit. The crystal features N–H···O, O–H···O and C–H···O hydrogen bonds, and ··· Additionally, Hirshfeld surface analysis revealed that O···H/H···O (39.0%), H···H (25.3%), and C···H/H···C (17.2%) contacts dominate the crystal packing, followed by C···C (8.5%). Finally, in silico ADME analysis suggested that (I) exhibited favorable physicochemical properties and good oral absorption, highlighting its potential as a viable pharmacological scaffold.

Conclusions

-A new sulfanilamide-derived Schiff base was successfully synthesized and characterized. In silico SwissADME analysis revealed favorable physicochemical properties and good oral absorption, highlighting its potential as a promising pharmacological scaffold.

sciforum-178599: Preliminary Characterization of Cross-Linked Amidase Crystals

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Cross-linked enzyme crystals (CLECs) are highly purified and stabilized biocatalysts produced through enzyme crystallization followed by chemical cross-linking, which locks the enzymes into an insoluble crystalline matrix. This self-immobilization approach exhibits high stability, controllable size, and easy reuse, turning them into particularly attractive and efficient biocatalysts for a variety of applications. Furthermore, CLECs have been explored as microporous platforms for the controlled and sustained release of protein and peptide therapeutics, as integral components of CLECs-based biosensors, and for several promising medical and biotechnological applications [2, 3]. However, their principal limitation is the strict requirement for enzyme crystallization, an expensive, time-consuming, and labor-intensive process that necessitates highly purified enzymes and carefully optimized crystallization conditions [1].

By optimizing crystal morphology and crystallization conditions, CLECs can preserve catalytic activity and selectivity similar to those of soluble enzymes in aqueous media, while also maintaining functional behavior comparable to crude enzymes in organic solvents [3]. In this work, we have purified, crystallized, and produced CLECs of a new penicillin-binding protein showing D-amidase activity from *Rhizobium* species (RhiDamid). After enzyme characterization in solution, its crystallization conditions were systematically optimized in order to obtain well-formed and stable crystals suitable for further processing. The resulting crystals were then successfully cross-linked with glutaraldehyde to obtain Cross-Linked Amidase Crystals (CLACs), retaining D-amidase catalytic activity after the cross-linking step. Preliminary data regarding the physicochemical and catalytic characterization of these CLACs is presented, highlighting their potential stability and applicability as reusable biocatalysts in future biotechnological developments.

sciforum-179675: Quantitative Raman Spectroscopic Analysis of Crystallographic and Molecular Orientation in Rubrene Films

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Understanding and controlling the structure of molecular crystals is essential for advancing high-performance molecular electronics and biocompatible devices. Among organic semiconductors, rubrene, a tetraphenyl derivative of tetracene, stands out due to its exceptional charge carrier mobility in single-crystal form. In this work, we investigate the crystallographic and molecular orientation of rubrene thin films grown by hot-wall epitaxy on mica substrates using ex-situ polarized Raman spectroscopy.

Polarized Raman spectroscopy provides a powerful, non-destructive approach to probe both molecular anisotropy and chemical identity. By exploiting the symmetry properties of Raman tensors and the polarization dependence of scattered light, we determine the orientation of rubrene molecules within crystalline films. Measurements were performed using a 784 nm polarized laser in a backscattering configuration, with systematic in-plane rotation of the sample to resolve angular-dependent Raman responses.

Rubrene films exhibit a characteristic evolution from an amorphous phase to spherulitic structures and finally to a coalesced crystalline film. Across all growth stages, the Raman breathing mode at 1003 cm^{-1} remains invariant, serving as a robust spectral fingerprint. To extract molecular orientation, additional internal vibrational modes associated with phenyl groups were analyzed under different polarization conditions. The resulting dataset enabled the construction and iterative solution of Raman tensor elements through a back-and-forth computational approach.

The analysis reveals clear anisotropic behavior and provides quantitative insight into molecular alignment and dipole–dipole interactions within the films. These results demonstrate the capability of polarized Raman spectroscopy to resolve crystallographic properties of organic molecular solids using relatively low-energy excitation, offering a versatile tool for the structural characterization of functional molecular materials.

sciforum-179671: Synthesis and crystal structure of 3-((1-(p-tolyl)-1H-1,2,3-triazol-4-yl)methyl)thieno[3,2-d]pyrimidin-4(3H)-one

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These five-membered heterocyclic compounds with a heteroatom of the sequence N-N-N are copper(1)-catalysed azide-alkyne cycloaddition reactions. In the case of Anticancer drugs, there are several specific requirements: stable, non-differentiating between cancer and non-cancerous cells, minimal toxicity and lack of side effects, requiring different mechanisms for successful treatment. In recent years, 1,2,3-triazoles has become one of the attractive research objects to heterocyclic chemistry **[1]**. 1*H*-1,2,3-Triazoles are used in pharmaceuticals as anti-inflammatory, as herbicides in agriculture. In addition, 1,2,3-triazoles have antimicrobial, anti-inflammatory, anti-leishmania, and antidiabetic activity **[2].** In the present study, we provide a detailed structural analysis of 3-((1-(p-tolyl)-1H-1,2,3-triazol-4-yl)methyl)thieno[3,2-d]pyrimidin-4(3H)-one (**1**) based on experimental X-ray diffraction. We conducted a 1,3-bipolar cycloaddition reaction of synthesised propargyl ethers with para-azidobenzoic acid ethyl ether. The progress of the reaction was monitored by thin layer chromatography. The precipitate was filtered off, dried and recrystallized through methanol; the product was obtained in 84% yield. Compounds **1** crystallize in the orthorhombic space group $Pna2_1$. The asymmetric unit for title compound consists of one molecule. Energy framework analysis is the important quantitative analysis of interaction energies architecture of molecules in the single crystal. It can give information on the interaction energy of new triazole organic compounds, for example, and can detect interactions such as C–H··· π, C–O··· π, C–N··· π**,** also, Hirshfeld surface analysis gives to us information about interaction between close contacts of hydrogen and another molecule in the triazole compounds**.** In 1 crystal the central 1,2,3-triazole and benzene rings are almost plane. In the crystal structure of title compound, the molecules are linked by intermolecular C—H···O, C—H···S, C—H···N hydrogen bonds. These interactions in combination with C—H···*Cg* contact form a three-dimensional framework.

sciforum-176966: Synthesis, Crystal Structure and Hirshfeld Surface Analysis of 3-Ethylquinazolin-4(3H)-one Hydrochloride

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Introduction. Quinazolines belong to the class of synthetic organic compounds exhibiting remarkably high pharmaceutical activity. Quinazoline and its derivatives are generally soluble in alcohols or organic solvents; however, this property limits their administration into the body. In contrast, the compounds formed with the chloride anion demonstrate solubility in water and isotonic solutions, which makes them suitable for parenteral (injectable) administration.

Experimental. 3-Ethylquinazolin-4(3H)-one was dissolved in acetone, and hydrogen chloride gas was passed through the solution, resulting in the formation of 3-ethylquinazolin-4(3H)-one hydrochloride. Rf = 0.67 (system: water : methanol, 1:1), melting point 175–177 °C.

Results and Discussion. The crystal belongs to the triclinic crystal system and crystallizes in the P-1 (No. 2) space group. The crystal lattice is of the primitive type. An inversion center is present in the structure, with the number of formula units per unit cell Z = 2. ADDSYM analysis revealed the presence of pseudotranslational symmetry (1/2, 0, 0).

In the compound, intermolecular N–H···Cl and C–H···Cl hydrogen bonds were identified. In addition, intramolecular N···C and C···Cl interactions were observed. Furthermore, Hirshfeld surface analysis and fingerprint plot analysis were performed, showing that the largest contribution arises from H···H/H···H contacts.

Conclusion. In this study, we reported the synthesis, structural characterization, and Hirshfeld surface analysis of a new quinazoline-based compound, (compound name). Based on the obtained results, the newly synthesized compound was found to exhibit confirmed biological activity.

Session 4. Hybrid and Composite Materials

sciforum-178944: Additive effect of ytterbium and neodymium for efficient and stable $CH_3NH_3PbI_3$ perovskite solar cells

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Co-additive effects of ytterbium (Yb) and neodymium (Nd) for efficient and stable $CH_3NH_3PbI_3$ ($MAPbI_3$) perovskite solar cells were investigated. Compared to single-addition, co-addition of 0.5 at% Yb and Nd supported to improve the photovoltaic characteristics, resulting in increase of open-circuit voltage (V_{oc}), short-circuit current density (J_{sc}), conversion efficiency (η) and stability. Morphological observation and crystal structure analysis showed that the grain boundaries within the perovskite layer were reduced, and stable, dense films were formed through crystal growth and orientation. Surface observation and composition analysis using energy dispersive X-ray spectroscopy confirmed the presence of Pb, I, Yb and Nd elements in the perovskite crystal grain. The band structure and density of state predicted the state of carrier mobility near valence and conduction band states. The electron density distribution of 4f and 5d orbitals of Yb and Nd ions and 5p orbital of I ion expected to promote the charge transfer related to the semi-conductive properties. The optical properties from ultraviolet to near-infrared regions based on the excitation process between the 4f and 5d orbitals of Yb and Nd ions in the crystal. The co-doped system had stabilization while suppressing distortion in the coordination structure. The photovoltaic characteristics were discussed by comparing experimental and calculated results in *J-V* curves of the solar cell using SCAPS-1D simulation. The photovoltaic characteristics originate from state of carrier diffusion while suppressing carrier recombination near the grain boundaries and interface between perovskite film and hole-transporting layer. In the co-addition system, passivation occurred more effectively than in the single-addition system, resulting in the photovoltaic characteristics with increase of J_{sc}, V_{oc}, η and stability.

sciforum-179634: An Ultramicroporous Fe(II)-Anilato MOF for CO_2 Capture and Environmental Applications

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The development of sustainable porous materials for gas capture and environmental remediation is a central challenge in materials chemistry. Herein, we report the green, scalable synthesis and multifunctional integration of a novel Fe(II)-based metal–organic framework, $Fe(trz_2An)\cdot 3H_2O$ (trz_2An = 3,6-N-ditriazolyl-2,5-dihydroxy-1,4-benzoquinone), designed for CO_2 capture and pollutant removal. The material is obtained via an optimized aqueous synthetic route under mild conditions achieving high crystallinity and yields up to 85%. The use of NH_3 as a weak base significantly enhances sustainability metrics, leading to a space–time yield of ~10,000 kg m^{-3} day^{-1}, among the highest reported for green MOF syntheses.

Single-crystal X-ray diffraction reveals a 3D neutral framework with ultramicroporous channels (~3.8 Å), closely matching the kinetic diameter of CO_2. The structure exhibits high porosity (28.8% void volume), excellent thermal stability up to 300 °C, and remarkable stability in aqueous environments across a pH range of 3-8.

CO_2 adsorption studies show an uptake of ~2500 μmol g^{-1} at 30 °C, with low differential heats of adsorption indicative of physisorption and facile regeneration. Beyond gas capture, the material demonstrates promising ion-exchange capabilities toward toxic heavy metals, such as Cd^{2+} and Pb^{2+}, with uptake capacities up to 300-500 mg g^{-1}, highlighting its potential for water remediation.

Furthermore, the MOF has been successfully incorporated into biopolymer-based matrices, specifically carboxymethylcellulose (CMC), to form composite membranes. Ongoing studies indicate good reproducibility and promising separation performance, supporting the development of hybrid materials for practical applications.

These results establish $Fe(trz_2An)\cdot 3H_2O$ as a versatile and scalable platform for integrated gas capture and environmental remediation technologies.

sciforum-176445: Antimicrobial activity of Iron oxide nanoparticles (IONPs) functionalized with anthocyanin extracted from blackcurrants (*Ribes nigrum*)

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Iron oxide nanoparticles (IONPs) have attracted significant attention in recent years due to their versatility and facile synthesis. They are considered a promising platform for the development of novel antimicrobial delivery systems, particularly in the context of the emerging antibiotic resistant pathogens that continue to pose a global threat. This study aims to investigate the potential antimicrobial efficacy of IONPs, synthesized using the co-precipitation method, and functionalized with anthocyanins, which act as bioactive agents that have been extracted from blackcurrants (*Ribes nigrum*), forming a core-shell architecture. Anthocyanins are pH-dependent phenolic pigments, naturally occurring in various berries and fruits, that exhibit a strong antioxidant activity, strongly associated with antimicrobial and anti-cancer properties. The resulting bio-composite was characterized by Scanning electron microscopy (SEM) and Transmission electron microscopy (TEM), which confirmed it's spherical morphology, with an average particle size of approximately 10 nm, while Fourier-transform infrared spectroscopy (FTIR) demonstrated the successful organic coating of the nanoparticles. Furthermore, the antimicrobial activity of the functionalized IONPs was assessed against both Gram-positive and Gram-negative bacteria using the disk-diffusion method and broth microdilution assays in 96 microtiter plates. The obtained results highlight the potential of anthocyanin-functionalized IONPs as sustainable, plant-derived antimicrobial agents.
By combining natural bioactive compounds with biocompatible nano-delivery systems, this approach offers a promising strategy for developing alternative antimicrobial therapies capable of overcoming resistance mechanisms.

sciforum-176784: Biogenic shell-derived particles as functional additives in metakaolin geopolymers

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The valorization of marine biogenic waste represents an important direction in the development of sustainable functional materials. In this study, geopolymer composites incorporating biogenic particles derived from marine shell waste were synthesized and structurally characterized. The biogenic particles consist of calcium-rich crystalline powders (primarily $CaCO_3$ and CaO phases) obtained through cleaning, thermal treatment, and mechanical size reduction of shell materials. These particles were introduced as functional additives into metakaolin-based geopolymers synthesized from calcined kaolinite ($Al_2Si_2O_5(OH)_4$) and activated using alkaline solutions (NaOH, KOH and Na_2SiO_3), leading to the formation of a three-dimensional aluminosilicate network. The geopolymerization process resulted in hybrid inorganic composites in which the biogenic calcium-based particles are dispersed within an amorphous aluminosilicate matrix. Structural and morphological investigations were performed using X-ray diffraction (XRD) and scanning electron microscopy (SEM) to evaluate phase composition, crystallinity and particle dispersion. The results indicate that the incorporation of shell-derived particles influences the microstructure of the geopolymer matrix and contributes to the development of hybrid inorganic composites combining amorphous geopolymeric phases with crystalline calcium-based particles. The results demonstrate that marine shell waste can be successfully transformed into functional additives for geopolymer materials. This approach contributes to waste valorization while enabling the development of sustainable geopolymer composites with potential applications in environmentally friendly construction materials and environmental remediation technologies.

sciforum-179541: Chiral Redox-Active Metal–Organic Frameworks Based on Benzoquinone-Derived Linkers

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Metal-organic frameworks (MOFs) are porous materials formed by the self-assembly of metal nodes and organic linkers. MOFs based on redox-active ligands represent versatile platforms for the design of functional materials, while the inclusion of chiral moieties introduces additional stereochemical complexity. Therefore, the combined influence of chirality and redox activity on framework formation and resulting properties has not yet been comprehensively investigate.

Here, we report the design and synthesis of novel redox-active linkers benzoquinone derivatives functionalized at the 2,5-positions with chiral amino acid moieties, with the goal of introducing chirality into the ligand framework. These chiral linkers were employed in the assembly of MOFs with both transition metal and lanthanide ions under solvothermal conditions. Synthetic parameters, *i.e. i)* solvent choice, *ii)* temperature, *iii)* reaction time, and *iv)* precursor ratios, were systematically varied to investigate their influence on framework formation, crystallinity and linker incorporation.

The synthesized MOFs were fully characterized by Single-crystal and powder X-ray diffraction spectroscopic and elemental analyses, to assess their structural framework and chemical composition.

The obtained results show that both the chirality of the linkers and the choice of metal ion play an important role in the assembly of the frameworks, influencing structural characteristics and coordination environment. The comparison with non-chiral analogues emphasizes the effect of amino acid-derived chirality. These observations outline consistent trends that can support the further design of chiral redox-active MOFs.

sciforum-179659: Crystallography-inspired Hierarchical Multiscale Mechanical Metamaterials

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Architected metamaterials derive their exceptional mechanical performance from precisely tailored topologies, enabling access to regions of materials selection charts unattainable by conventional materials. While substantial advances have been achieved at micro-, meso-, and macroscales, further improvements are increasingly constrained, motivating exploration of nanoscale architected materials, where surface and size effects dominate. Here, we resort to molecular dynamics simulations to systematically explore the mechanical response of nickel-based nano-architected metamaterials. By varying topology, relative density, crystallinity, and grain size, we demonstrate the broad tunability of elastic moduli, strength, and Poisson's ratio enabled by the rational design of underlying nano-architecture. Notably, the proposed nano-architected metamaterials outperform most previously reported architected materials at comparable densities, highlighting the effectiveness of nanoscale topology-driven design. Atomistic analyses reveal that nanoscale free surfaces promote dislocation nucleation while inhibiting dislocation propagation, leading to flow stresses exceeding those of bulk counterparts. To bridge length scales and draw inspiration from crystallography, we further design and 3D print hierarchical polymeric metamaterials and experimentally characterize their mechanical behavior. Despite being fabricated from an intrinsically brittle polymer, these structures exhibit topology-dependent stiffness and strength, alongside ductile plastic deformation and enhanced toughness, attributable to their hierarchical architectures. Together, this work establishes a crystallography-inspired architectural design paradigm for mechanical metamaterials and imparts scalable design guidelines for achieving lightweight, mechanically efficient structures across multiple length scales.

sciforum-176435: Electrical and Structural Characterization of Graphene–Polypyrrole Composite Thin Films for Flexible Wearable Electrodes

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This study investigates the electrical behavior of conductive polypyrrole (PPy) thin films designed for flexible electrode applications in wearable sensing systems. A reference p-toluenesulfonic acid doped PPy (PPy-TSA) film was compared with graphene-modified PPy composites developed to enhance mechanical robustness and electrical stability under deformation.

Morphological analysis (SEM) shows that the reference PPy–TSA exhibits a typical cauliflower-like structure, while graphene incorporation induces elongated, layered features associated with well-dispersed nanosheets, without disrupting the polymer matrix integrity. XPS confirms that the chemical structure and doping state of PPy are preserved after graphene incorporation. Mechanical characterization reveals that the reference PPy-TSA film exhibits a low Young's modulus (~0.008 GPa), while graphene increases stiffness (~0.016 GPa) and improves mechanical robustness. In contrast, the PPy-PEG graphene system maintains a low elastic modulus (~0.009 GPa), indicating an optimal balance between flexibility and reinforcement.

Electrical measurements show that PPy-TSA exhibits a conductivity of ~208 S/cm, while graphene-modified films show reduced conductivity (~62 S/cm) due to incomplete percolation. However, these films retain conductivity within the range required for electrocardiographic (ECG) sensing, while temperature-dependent measurements (25-85 °C) confirm stable semiconducting behavior. Optical analysis reveals a redshift of the π–π* transition and enhanced VIS–NIR absorption, indicating modified electronic structure without proportional improvement in macroscopic conductivity.

Overall, graphene incorporation improves mechanical robustness and signal stability while maintaining adequate conductivity for ECG applications. The PPy-PEG-graphene composite shows the best balance between flexibility, conductivity, and signal quality, making it a promising candidate for flexible, gel-free wearable electrodes.

sciforum-176409: Flexible Polypyrrole Composite Films with Organic and Inorganic Fillers for Electrocardiographic Sensing Applications

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Conductive polymers have emerged as promising materials for flexible electrodes in wearable biomedical devices. Among them, polypyrrole (PPy) is particularly attractive due to its intrinsic electrical conductivity, chemical stability, and compatibility with soft substrates. However, pure PPy films may exhibit limited mechanical robustness and reduced stability under repeated deformation. To address these limitations, the incorporation of functional fillers represents an effective strategy to tailor the structural, electrical, and mechanical properties of the polymer matrix.

In this study, composite thin films based on p-toluenesulfonic acid doped polypyrrole (PPy-TSA) incorporating both organic and inorganic fillers, such as polyethylene glycol (PEG), poly(vinyl alcohol) (PVA), graphene (GR), carbon nanotubes (CNT), and zeolite (ZE), were developed and investigated. The films were obtained by electrochemical polymerization using a galvanostatic method, where pyrrole was polymerized in the presence of fillers dispersed in the electrolyte. The fillers were commercially available, while the PPy matrix was synthesized in situ.

The morphology and structural organization of the films were analyzed by scanning electron microscopy (SEM), while Fourier-transform infrared (FTIR) and ultraviolet–visible (UV–Vis) spectroscopy were used to investigate the chemical structure and interactions within the composites. Electrical properties were evaluated through conductivity and sheet resistance measurements, including temperature-dependent analysis and bending tests to assess stability under deformation.

The results show that the combined incorporation of organic and inorganic fillers enables tuning of both electrical response and mechanical integrity. These properties are relevant for the development of flexible electrodes capable of detecting low-amplitude bioelectrical signals. The investigated PPy composite films demonstrate promising potential for electrocardiographic (ECG) sensing in wearable health monitoring systems.

sciforum-176596: Formation and Crystallization Behavior of a New Organic–Inorganic Hybrid Crystalline Compound in the $Ca(ClO_3)_2 \cdot 2CO(NH_2)_2$ – $CH_2ClCOOH \cdot (C_2H_4OH)_3N$ – H_2O System

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The formation of hybrid crystalline materials based on organic and inorganic components is of considerable interest due to their structural diversity and potential applications in agrochemical and functional materials. In this work, the physicochemical interactions and phase equilibria in the ternary aqueous system $Ca(ClO_3)_2 \cdot 2CO(NH_2)_2$ – $CH_2ClCOOH \cdot (C_2H_4OH)_3N$ – H_2O were systematically investigated over a temperature range from –24 to 60 °C. The study was carried out using the visual-polythermal method, which allowed the determination of solubility relationships and the construction of a complete polythermal phase diagram of the system. Analysis of the phase diagram revealed several crystallization regions corresponding to ice, $Ca(ClO_3)_2 \cdot 2CO(NH_2)_2 \cdot 2H_2O$, $CH_2ClCOOH \cdot (C_2H_4OH)_3N$, and a newly formed crystalline phase with the composition $CH_2ClCOOH \cdot Ca(ClO_3)_2 \cdot (C_2H_4OH)_3N$. The presence of a distinct crystallization field for this compound indicates the formation of a stable individual hybrid crystalline material in the studied system. The compound was isolated from solutions corresponding to its crystallization domain and subjected to chemical and physicochemical characterization. Elemental analysis results showed good agreement between experimental and calculated values for calcium, chlorate ions, and nitrogen, confirming the proposed stoichiometric composition. Infrared spectroscopy further supported the formation of the new hybrid compound. The spectra revealed characteristic vibrational bands associated with chlorate ions and carboxylate groups, as well as changes in the hydroxyl and amino group vibrations, indicating structural reorganization during complex formation. The obtained results demonstrate that the investigated system forms a stable organic–inorganic hybrid crystalline compound under specific temperature and concentration conditions. The constructed phase diagram provides valuable information on crystallization boundaries and phase stability. These findings contribute to a deeper understanding of intermolecular interactions and phase behavior in multicomponent aqueous systems and may serve as a physicochemical basis for the development of new complex-action defoliants and functional crystalline materials.

sciforum-179650: Grain Boundary Modification in Aluminum Hybrid Nanocomposites (Al6061-TiC) Using Brophene Material.

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Purpose

This study aims to explore the crystallographic properties and microstructural development of Al6061-TiC-Borophene hybrid composite materials and their impact on the mechanical and tribological properties. Crystal engineering in aluminum-based composite materials is a crucial step toward enhancing the mechanical properties, hardness, and wear resistance. The addition of titanium carbide particles as a reinforcing agent in the Al6061-TiC-Borophene composite material provides a hybrid strengthening mechanism. The crystal engineering in Al6061-TiC-Borophene composite materials aims to explore the crystal structure formation and the interaction between the phases, which enhance the structural and functional properties.

Approach

The crystallographic characteristics of Al6061-TiC-Borophene hybrid composite materials are studied using microstructural characterization and phase characterization methods. In the composite synthesis process, heterogeneous nucleation is carried out using TiC particles, which refine the aluminum crystal structure. Borophene help in the nanoscale reinforcement and interfacial bonding. X-ray diffraction, scanning electron microscopy, and electron backscatter diffraction methods are used to study the crystallographic characteristics.

Findings

The reinforcement of TiC and borophene contributes to better crystallographic stability and enhanced mechanical properties of Al6061. The development of refined equiaxed grains and stable interfacial compounds improves hardness and wear properties. In addition, it improves load-carrying properties. The reinforcement of TiC improves stiffness and acts as barriers to dislocations. Borophene contributes to strengthening and stress transfer. The crystal structure refinement contributes to reducing microstructural defects and improving uniformity in the composite matrix. This improves microstructural properties compared to conventional aluminum alloys.

Practical Implication

The optimized crystal structure of Al6061-TiC-Borophene composites provides a strong potential for lightweight structural components used in the aerospace, automotive, and advanced manufacturing industries. Enhanced wear resistance, strength-to-weight ratio, and thermal stability of the composites make them appropriate for the development of advanced engineering systems.

sciforum-176957: Improving the early reactivity of activated coal gangue by vibratory ball mill- The influence of particle fineness and specific grinding energy toward geopolymerization

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This study investigates the mechanical activation of coal gangue via vibratory ball milling for durations ranging from 1 to 120 minutes and its subsequent application as a geopolymer precursor. Coal gangue, a significant industrial byproduct, requires precise structural modification to overcome its inherent chemical inertness. The evolution of the mechanically activated coal gangue's physical properties including particle size distribution (PSD), specific surface area (SSA), and surface morphology was systematically characterized using Laser Diffraction and Scanning Electron Microscopy (SEM).

The influence of specific grinding energy on chemical reactivity and the resulting geopolymerization process was further evaluated through Fourier-transform infrared spectroscopy (FT-IR) and uniaxial compressive strength. A quantitative correlation was established between the specific grinding energy and characteristics of the activated coal gangue, and the final mechanical performance of the resulting geopolymer binders.

The experimental results demonstrate that while initial grinding significantly enhances reactivity by increasing the specific surface area , prolonged grinding beyond an optimal kinetic limit induces undesirable particle agglomeration. This over-grinding phenomenon leads to a reduction in effective surface area, which negatively impacts the dissolution rate and subsequent geopolymer strength. These findings provide a critical quantitative basis for optimizing grinding conditions, balancing energy consumption against material performance. Ultimately, this research offers a pathway for the enhanced value-added utilization of coal gangue in the production of sustainable, low-carbon geopolymer materials

sciforum-176430: Influence of Inorganic Fillers on the Mechanical Properties of Polypyrrole Composite Thin Films

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Conductive polymers such as polypyrrole (PPy) have attracted significant interest for flexible electronic applications due to their electrical conductivity, chemical stability, and ease of synthesis. However, pure PPy films often exhibit limited mechanical robustness, which can restrict their long-term performance in flexible devices. Incorporating inorganic fillers into the polymer matrix represents a promising strategy to improve the mechanical stability of conductive polymer films while maintaining their functional properties.

In this work, composite thin films based on p-toluenesulfonic acid-doped polypyrrole (PPy-TSA) incorporating inorganic fillers such as graphene (GR), carbon nanotubes (CNT), and zeolite (ZE) were investigated. The composite films were obtained by electrochemical polymerization using a galvanostatic method, in which pyrrole was polymerized in the presence of the inorganic components dispersed in the electrolyte solution. The inorganic fillers were used as commercially available materials, while the PPy matrix was synthesized in situ during the electrochemical process.

The morphology of the films was analyzed by scanning electron microscopy (SEM), highlighting the dispersion of the inorganic components within the polymer matrix and their effect on the structural organization of the films. Mechanical performance was evaluated through flexibility and repeated bending tests in order to assess the structural integrity of the composite films under deformation.

The results indicate that the incorporation of inorganic fillers contributes to improved mechanical stability and resistance to structural damage during bending, suggesting a reinforcing effect within the PPy matrix. These findings highlight the potential of inorganic filler-reinforced polypyrrole films for flexible electronic applications where both electrical functionality and mechanical durability are required.

sciforum-179669: MOF-Based Composites for Sustainable Processes

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The development of energy-efficient solutions for indoor air control systems is a key challenge in sustainable processes. Metal-Organic Frameworks (MOFs) offer great potential for this purpose; however, their practical implementation in HVAC (Heating, Ventilation, Air Conditioning) is often hindered by difficulties in material handling and effective confinement within operating devices, mainly due to their powdered form.

This study addresses these limitations by developing MOF-based composites, hybrid materials obtained by embedding Al-fumarate MOF particles into a poly(vinylidene fluoride-co-hexafluoropropylene) (PVDF-HFP) matrix. The obtained samples successfully combine the water adsorption properties of the dispersed crystalline phase with the mechanical robustness and flexibility of the polymer. Two easily scalable fabrication strategies were used: Mixed-Matrix Membranes (MMMs) via solvent casting and non-woven fabrics via electrospinning.

The MMMs retain approximately 90% of the pristine MOF surface area and water vapor adsorption capacity, with minimal loss of active sites. The membranes exhibit remarkable water vapor adsorption characteristics, including fast kinetics and negligible hysteresis, key parameters for efficient dehumidification and passive cooling cycles, contributing to reduced energy consumption. Notably, these hybrid systems outperform traditional desiccants in both adsorption capacity and reversibility, highlighting their potential for sustainable HVAC applications. The non-woven architecture is particularly promising for maximizing MOF particle accessibility, thanks to its typical texture.

Developed composites offer also solutions in different fields, such as anti-fogging systems in packaging and humidity sensing. Work is currently underway to assess the performance of the developed composite systems in prototypal devices.

sciforum-179536: Multivariate Anilate-Based Metal-Organic Frameworks: Exploring Assembly and Linker Exchange Pathways

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The diverse optical, magnetic, and electronic behaviors of crystalline materials arise from their structure and the nature of their coordination environment. Metal-organic frameworks (MOFs) based on anilate linkers possess rich composition tunability with complex multidimensional architectures, yet multivariate architectures incorporating secondary ligands remain comparatively underinvestigated. Here, we report a comprehensive investigation of the synthetic conditions governing the assembly of multivariate MOFs constructed from anilate and secondary linkers, enabling precise control over their composition and peripheral functionalities. Controlled assembly was achieved by systematically varying synthetic parameters (solvothermal, hydrothermal, and reflux conditions), with particular attention to mild reaction regimes and reaction times to assess their effect on linker incorporation. In addition, post-synthetic linker exchange was explored as a complementary approach to assess the effective tunability of the framework functional properties and to gain insight into coordination dynamics, particularly how effect such as electron-withdrawing substituents modulate exchange efficiency and incorporation patterns. The resulting materials were characterized by single-crystal and powder X-ray diffraction, spectroscopy, and elemental analysis to confirm framework structures, ligand incorporation, and functional integrity. Our findings reveal that careful control of synthetic conditions and post-synthetic linker exchange enables frameworks with predictable multivariate ligand distributions, tunable photophysical properties, and defined coordination dynamics, highlighting design principles for multifunctional MOFs with enhanced compositional and functional control.

sciforum-176997: Novel Hybrid MS/RF PECVD Approach for the Formation of Titanium-Based 2D Structures in Layered Ti/C Coatings

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Introduction:

Titanium-based nanostructures are attracting interest due to their significant application potential in medicine, electronics, electrical engineering and energy storage systems. They are most often obtained by top-down methods, which require the use of toxic reagents and multi-stage etching processes. In this work, titanium and carbon-based coatings were developed using an innovative hybrid method combining magnetron sputtering (MS) with radio frequency plasma-enhanced chemical vapour deposition (RF-PECVD).

Methods:

Nanolayered Ti/C coatings were fabricated on silicon substrates using a hybrid method. Titanium layers were deposited by magnetron sputtering at a constant target power of 0.23 kW, while carbon layers were deposited by RF-PECVD at a constant negative self-bias potential of −400 V. The individual sample series differed in the deposition time of the layers, enabling control of their thickness. Selected samples were subsequently annealed in a vacuum furnace at 500 °C for 1 h. Both the as-deposited and annealed samples were characterized using Raman spectroscopy, X-ray diffraction (XRD), and scanning electron microscopy (SEM) coupled with energy-dispersive X-ray spectroscopy (EDS).

Results:

Optical profilometry measurements confirmed the formation of coatings with thickness in the nanometer range. The obtained results indicate that the hybrid MS/RF-PECVD method enables the fabrication of nanolayered Ti/C systems with controlled layer thickness and uniform morphology. Raman spectra revealed bands characteristic of carbon structures in the 1300–1500 cm^{-1} range (D and G bands). Signals in the region of ~300 cm^{-1} were also detected, which may be associated with the presence of titanium compounds.

Conclusions:

Results confirm that the hybrid MS/RF-PECVD method represents a promising approach for the fabrication of controlled nanolayered Ti/C systems, which may serve as a platform for the synthesis of new two-dimensional materials.

sciforum-176421: POLYPYRROLE-FUNCTIONALIZED MAGNETIC ZEOLITE FOR EFFICIENT RECOVERY OF WASTE OIL FROM WATER SURFACES

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In this study, a magnetic composite based on zeolite, functionalized with magnetite (Fe_3O_4) and polypyrrole (PPy), was developed to obtain a material combining magnetic properties with hydrophobic–oleophilic characteristics. Zeolite was used as a support material due to its porous structure and high specific surface area, which facilitates the uniform dispersion of Fe_3O_4 nanoparticles. These nanoparticles are responsible for the magnetization of the composites and enable rapid and efficient separation under an external magnetic field. Functionalization with polypyrrole modified the surface properties, providing hydrophobicity and enhanced affinity for nonpolar organic compounds and petroleum products.

The obtained composite was evaluated for the recovery of used motor oil from the water surface, showing an absorption efficiency of 90–95%. These results demonstrate the high potential of the developed magnetic composite material for applications in oil spill remediation and aquatic environmental depollution. In addition, the magnetic nature of the material allows its easy collection after the adsorption process, reducing secondary contamination and facilitating possible reuse of the composite.

The combination of zeolite's porous framework with the magnetic response of Fe_3O_4 and the conductive polymer coating provided by polypyrrole contributes to improved stability and adsorption performance. Furthermore, the material exhibits good structural stability and maintains its functional properties during repeated contact with oil–water mixtures. Such characteristics highlight the potential of this composite as an efficient, low-cost, and environmentally friendly solution for the treatment of contaminated water surfaces and the mitigation of pollution caused by petroleum-based products.

sciforum-176906: Scaling of HKUST-1 metal-organic framework polymer with catalytic and adsorption properties

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Metal-organic frameworks of HKUST-1 $\{[Cu^{2+}_2(BTC)^{3-}_2)(Solv)_x]\times G_y\}_n$ (CuBTC; *Solv.*-solvent in framework; G-guest in voids) are composed of Cu^{2+} dimers linked by benzene-1,3,5-tricarboxylate (BTC). CuBTC exhibits cubic symmetry (sp.gr.*Fm*3*m*,*Z*=16), an ordered 3*D* pore structure, high specific surface area, thermal stability, adsorption capacity, and selectivity. The use of CuBTC is related to technological feasibility: CuBTC can be produced in required quantities with reduced cost and high performance characteristics, which became the motivation for study.

Synthesis (reagents: $Cu(NO_3)_2\times 3H_2O$, H_3BTC; solvents: water, ethanol, DMF) was carried out by solvothermal method (SA; *t*=130°C,t=8 h;*n*=1 gram-product weight) and express method in a water bath (WB/*n*;*t*=84°C,t=3 h;*n*=4 and 10grams) with the thermal treatment (*t*=200°C, t=5 h) of WB/10 to open the active centers in the structure of dehydrated/desolvated WB/10D.

XRD, IR spectroscopy, SEM/EDX, BET shows change in microstructure and morphology/habitus from a large number of octahedra (10–20 mm) and a small number of shapeless crystals in WB/4 to octahedra, intergrowths and twins (from 10 to 60 mm) in WB/10. Decrease in specific mesoporous surface area from 893m^2/g in SA to 810m^2/g in WB/10 was revealed. A significantly smaller amount or even absence of *G* in WB/10D compared to WB/10 was found, and the compositions of WB/4 and WB/10 are similar.

Low-temperature adsorption activity for N_2 is higher for SA (~272cm^3/g) compared to WB/10 (~258cm^3/g); the conversion of allyl alcohol and hydrogen peroxide to glycidol is higher for WB/10D than for WB/10, but the selectivity of GD for HP is significantly higher for WB/10. This indicates different mechanisms of catalytic process due to changes in the nature of active centers.

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sciforum-162413: Structural, Optical, and Dielectric Properties of $BaTiO_3$/Graphene/PVA Hybrid Composite Films

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$BaTiO_3$/graphene/PVA hybrid composite films were fabricated by a solution-casting approach and systematically investigated to establish crystal–polymer interface effects on their structural and functional behavior. X-ray diffraction confirmed the presence of tetragonal $BaTiO_3$ (P4mm) nanocrystallites with sizes of 13.4–17.0 nm and microstrain $\varepsilon \approx 0.114\%$, embedded within an amorphous PVA matrix and accompanied by a weak graphene (002) reflection. Semi-quantitative RIR evaluation revealed a three-phase composition of $BaTiO_3 \approx 20.7$ wt%, graphene ≈ 17.5 wt%, and PVA ≈ 61.8 wt%. SEM imaging showed a heterogeneous layered morphology with platelet-like regions (23–42 μm) and localized agglomerates, indicating non-uniform filler dispersion and high interfacial area density. FTIR and Raman spectra confirmed the coexistence of PVA vibrational modes, graphene domains, and $BaTiO_3$ lattice vibrations, evidencing strong interactions at phase boundaries.

Optical measurements demonstrated wide band-gap behavior with direct and indirect transitions at 6.38 eV and 6.06 eV, respectively, and ~50% visible-range transparency. Dielectric spectroscopy revealed pronounced Maxwell–Wagner–Sillars interfacial polarization at low frequencies, decreasing dielectric losses with increasing frequency, and AC conductivity transitioning from quasi-DC behavior to dispersive hopping at high frequencies. Temperature-dependent permittivity and conductivity further confirmed thermally activated interfacial and carrier-transport processes.

These results show that crystallite size, phase distribution, and interfacial heterogeneity dominate the functional response of the $BaTiO_3$/graphene/PVA hybrid, demonstrating its potential for transparent dielectric layers and UV-optoelectronic components within advanced composite crystalline material platforms.

sciforum-179609: Thermal Behavior, Crystallization Kinetics, and Morphology of PBT/MWCNT Composites: A Combined DSC and Hot-Stage POM Study

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Poly(butylene terephthalate) (PBT)/multiwalled carbon nanotube (MWCNT) composites were prepared using a simple and reliable melt mixing technique to understand how the addition of nanotubes affects the crystallization behavior and thermal properties of PBT. The non-isothermal crystallization process was studied using differential scanning calorimetry (DSC), while hot-stage polarized optical microscopy (HSPOM) was used to observe changes in microstructure at different cooling rates.

From a practical point of view, adding MWCNTs changes how PBT crystallizes. As the nanotube content increases, the viscosity of the system also increases, which restricts the movement of PBT chains and makes crystallization more difficult. Kinetic analysis shows that the basic crystallization mechanism remains similar, but the rate is influenced by the presence of MWCNTs. For pure PBT, the modified Avrami exponent (n) is 3.0 at a cooling rate of 15 °C min^{-1} and increases to 3.7 at 30 °C min^{-1}. When 1 wt% MWCNT is added, the values slightly decrease to 2.9 and 3.1 at 15 °C min^{-1} and 30 °C min^{-1}, respectively, indicating heterogeneous nucleation with minor changes in growth behavior. Kissinger analysis also suggests that higher energy is required for crystallization after adding MWCNTs.

Another important observation is the reduction in the crystal growth parameter after adding MWCNTs. It decreases from 6.1× 10^4 for pure PBT to 3. × 10^4 for the 1 % MWCNT into PBT. This shows that although MWCNTs help in nucleation, they also act as barriers that slow down the growth of crystals.

X-ray diffraction (XRD) results confirm that the crystal structure of PBT does not change with the addition of MWCNTs, as no new peaks are observed. However, a slight increase in crystallinity is seen due to the nucleating effect of the nanotubes.

Overall, MWCNTs play a dual role in the PBT matrix: they promote nucleation while also restricting chain movement and crystal growth. This balance leads to a more controlled crystallization process, which can be useful for improving material performance in practical applications.

Session 5. Materials For Energy Applications

sciforum-180044: Effect of crystal structure on the electrochemical performance of LLTO perovskite-type solid electrolytes for lithium-ion batteries

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The demand for batteries for energy storage for mobility and stationary energy storage system has increased significantly in recent years and sustained growth is expected due to the insertion of renewable energies, the increase in electric vehicles and energy efficiency. Lithium-ion batteries have high gravimetric and volumetric energy density. However, organic liquid electrolytes may react exothermically and raise safety and environmental concerns. Solid-state batteries have emerged as an alternative to conventional lithium-ion batteries, due to their greater thermal stability, which can provide them with high safety and service life. However, there are still major challenges to overcome, such as low conductivity of lithium ions in solid electrolytes, scalable synthesis methods, and wide windows of electrochemical stability.

Among the different families of solid electrolytes, perovskite ceramic oxides such as Li3xLa2/3-xTiO_3 (LLTO) exhibit high grain ionic conductivities (> 1 mS/cm), but their total conductivities are two orders of magnitude lower. This work seeks to increase the total ionic conductivity by adding dopants such as Zr4+, Ta5+ and V5+ in the structure synthesized by the sol-gel method. The materials were characterized by X-ray diffraction, Raman spectroscopy, Fourier transform infrared spectroscopy, scanning electron microscopy, X-ray photoelectron spectroscopy, electrochemical impedance, and galvanostatic charge-discharge curves.

All materials have a perovskite phase with a crystalline structure and space group P4/mm, and the dopants modify the TiO6 octahedral geometry, leading to changes in Ti–O bond distances and local structural distortion. Furthermore, the materials have vibrational modes typical of the ABO3 perovskite phase, low porosity, and relative densities greater than 95%, the 1% Zr-doped sample exhibited the highest total ionic conductivity (0.1 mS/cm), which can be associated with the more pronounced TiO6 octahedral distortion observed from the Ti–O bond lengths, and in the discharge-charge curves, the cells exhibited a coulombic efficiency of 90% after 10 cycles in lithium-ion batteries.

sciforum-177000: Monte Carlo simulation of the hysteresis behavior in a mixed-spin graphene bilayer

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In this work, we investigate the hysteresis behavior of a bilayer graphene system composed of mixed spins S = 7/2 and σ = 1/2 interacting through ferrimagnetic coupling. The system is described by a modified Blume–Capel Hamiltonian that incorporates both intra-layer and inter-layer exchange interactions (J1, J2, J3), as well as a uniaxial crystal field D and an external magnetic field. To analyze the magnetic properties, we employ Monte Carlo simulations based on the Metropolis algorithm, which allows us to explore the thermal and magnetic responses of the system in detail.

Particular attention is given to the effects of key physical parameters, including exchange interactions, crystal field, and temperature, on the hysteresis behavior. The obtained results reveal that the shape, size, and nature of the hysteresis loops are strongly dependent on these parameters. In particular, increasing temperature leads to enhanced thermal fluctuations, resulting in a gradual reduction of the hysteresis loop area. Above a certain critical temperature, the loops completely disappear, indicating a transition from a ferrimagnetic ordered phase to a paramagnetic state.

Moreover, variations in exchange interactions and crystal field significantly influence important magnetic characteristics such as coercivity, remanent magnetization, and loop symmetry. These findings are in good agreement with previous studies on multilayer magnetic systems and demonstrate the crucial role of competing interactions in determining the magnetic behavior.

Overall, this study provides valuable insights into the tunability of hysteresis properties in bilayer graphene systems, which could be useful for future applications in spintronics, particularly in the design of multistate magnetic memory devices.

sciforum-176162: Optoelectronic and Photovoltaic Properties of Lead-Free $Sn_2SbS_2I_3$: A DFT Study

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Lead-free absorber materials with strong light harvesting and suitable electronic structures are promising alternatives to Pb-based perovskites for sustainable photovoltaic technologies. In this work, density functional theory (DFT) calculations are performed using the CASTEP code and the meta-GGA R2SCAN functional to provide a comprehensive assessment of the structural, electronic, optical, and photovoltaic-related properties of $Sn_2SbS_2I_3$. Structural relaxation confirms a stable equilibrium configuration, indicating that the compound can maintain a well-defined crystalline arrangement after optimization. The computed electronic band structure shows that $Sn_2SbS_2I_3$ is a direct-band-gap semiconductor, with both the valence-band maximum (VBM) and conduction-band minimum (CBM) located at the Y point of the Brillouin zone. The resulting band gap is 0.91 eV, placing the material within a technologically relevant range for infrared-to-visible solar energy conversion.

To clarify the orbital origin of the band edges, total and partial densities of states (TDOS/PDOS) are analyzed. The results indicate that the upper valence region is predominantly governed by anion contributions, mainly S and I states, whereas the bottom of the conduction band is dominated by cation-derived states, primarily associated with Sb and Sn orbitals. Optical calculations reveal a strong light-harvesting capability, with absorption coefficients approaching 10^5 cm^{-1} above the absorption onset, together with moderate reflectivity remaining below 0.45, which is favorable for minimizing optical losses.

Photovoltaic descriptors extracted from the optical response further suggest efficient photogeneration. For an absorber thickness of t = 600 nm, the estimated short-circuit current density reaches Jsc = 20.00 mA cm^{-2}. The ideal radiative open-circuit voltage is approximated using Voc ≈ Eg/q, giving Voc ≈ 0.91 V. Overall, the combined electronic and optical characteristics support $Sn_2SbS_2I_3$ as a competitive lead-free absorber candidate for next-generation optoelectronic and photovoltaic applications.

sciforum-179717: Thickness-Driven Crystallization and Structural Evolution of Ultra-Thin p^+ Poly-Si Passivated Contacts

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High-efficiency and cost-effective photovoltaic technologies have driven a great interest in advanced ultrathin contact structures and their increasing demands, such as in TOPCon solar cells. The present work aims to develop ultra-thin boron-doped polysilicon (p^+ poly-Si) passivated contacts to minimize the optical losses while maintaining superb electrical performance. Ultra-thin poly-Si layers (40 nm) were prepared by LPCVD, and a systematic study was conducted to optimize key parameters such as boron diffusion temperature and forming gas annealing profile etc. Comprehensive structural and optical characterization revealed a pronounced thickness-dependent behaviour in p^+ poly-Si layers. Thinner p^+ poly-Si layers (10 nm) remains quasi amorphous and substrate-dominated, intermediate layers (20 nm) show partial crystallization, while thicker layers (~25 to 40 nm) exhibit well-developed polycrystalline structure with excellent passivation ($J_0 \approx 1.3$ to 2 fA/cm^2), high carrier lifetime (>2000 µs), and low contact resistivity (~ 1 to 1.5 mΩ.cm^2). Results of this work outperform or match the literature despite pushing the p^+ poly-Si to its thinnest level and provide a path to developing advanced TOPCon solar cells with higher efficiency. However, this will not be easy, as we have to consider optical perspective as well as overall stability, whether UV or thermal, for these ultra-thin p^+ poly-Si passivated contacts to integrate into prototype TOPCon solar cells.

sciforum-176826: Magnetic Doping–Induced Half-Metallicity and Large Anomalous Hall Effect in the Half-Heusler Alloy HfPtSi

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In recent years, doped half-Heusler compounds have attracted significant attention due to their tunable electronic, magnetic, and transport properties, making them promising candidates for spintronics applications. In this work, we investigate the effect of magnetic Mn doping on the structural stability, electronic structure, magnetism, and intrinsic anomalous Hall effect of the half-Heusler compound HfPtSi using first-principles density functional theory (DFT) calculations. Phonon dispersion calculations confirm the dynamical stability of both pristine and Mn-doped HfPtSi. The calculated electronic band structure shows that pristine HfPtSi exhibits semiconducting behavior. However, substitution of Mn at the Hf site significantly modifies the electronic structure and induces a ferromagnetic ground state with a magnetic moment of 3 μB per unit cell. As a result, the doped system exhibits half-metallic behavior, where the spin-up channel becomes metallic while the spin-down channel remains insulating. The emergence of ferromagnetism together with strong spin–orbit coupling (SOC) gives rise to a pronounced anomalous Hall effect originating from enhanced Berry curvature near the Fermi level. The calculated anomalous Hall conductivity reaches approximately 200 Ω^{-1} cm^{-1} at the Fermi level and increases to about 500 Ω^{-1} cm^{-1} at 100 meV above the Fermi level, which is comparable to several reported half-metallic ferromagnets. These results suggest that Mn-doped HfPtSi is a promising candidate for next-generation spintronic devices.

sciforum-179238: Bismuth Chalcogenide Nanoparticles for Eco-Friendly Optoelectronic Devices

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Bismuth-based compounds (Bi_2X_3, where X = O, S, Se, Te) are promising materials for optoelectronic and solar energy applications. They have the potential to replace toxic lead in hybrid perovskites [1-3]. Hybrid lead perovskites ($MAPbI_3$), when degraded, can release toxic Pb^{2+} into the environment, posing serious risks to human health and ecosystems. To overcome this, lead-based perovskites can be replaced with bismuth-based chalcohalides ($MABiXI_2$, X = O, S, Se, Te), which offer similar properties with lower toxicity and improved stability. Bismuth chalcohalides can be synthesized using bismuth chalcogenides. In this study, we discuss the synthesis and optoelectronic characterizations of bismuth chalcogenides Bi_2X_3 nanoparticles. These were synthesized via a simple solvothermal method and characterized using structural, optical, and electrical techniques. X-ray diffraction confirmed high-purity nanoparticles with hexagonal, orthorhombic, or tetragonal crystal structures and good crystallinity. Crystallite sizes, calculated using the Scherrer equation, ranged from 15 to 20 nm. Raman spectroscopy revealed distinct vibrational modes corresponding to each phase. Temperature-dependent resistivity measurements confirmed semiconducting behavior, with Bi_2Te_3 showing the highest resistivity and activation energy. The direct band gaps of bismuth chalcogenides were measured in the range of 1.7 eV to 2.9 eV. Electrical analysis based on the Poole-Frenkel model provided insights into the energy barrier that electric charge carriers have to cross to move in the material and also the dielectric constant. These results highlight the potential of Bi_2X_3 nanoparticles in optoelectronic and solar energy devices.

sciforum-176996: Characterization of the mechanical performance of epoxy resin composites containing graphene powder

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This research addresses the critical challenge of energy conversion and hydrogen storage as a key low-carbon energy carrier for modern transportation. The primary objective of this study is to provide a comprehensive analysis of the thermomechanical properties and molecular-level interaction mechanisms of a novel composite material, designed to optimize the operational performance and enhance the structural integrity of hydrogen transport pipelines and storage vessels within next-generation energy systems. The study involved the fabrication of five composite series with reduced graphene oxide (rGO) contents ranging from 0 to 2 wt%, utilizing a strategic partial curing agent substitution to examine its impact on the cross-linking density and thermomechanical performance of the epoxy matrix. A comprehensive experimental methodology was applied, including static flexural (ISO 178) and compression (ISO 604) strength tests, Vickers hardness measurements (ISO 6507), and differential scanning calorimetry (DSC) analysis. These empirical investigations were complemented by advanced quantum chemical simulations using the PM6 semi-empirical method within the Scigress software, facilitating the analysis of macromolecular electron distribution and physicochemical interactions at the epoxy-graphene interface. The results demonstrate a dual effect of the nanofiller: at low concentrations (0.25 wt%), increased material plasticity was observed due to reduced cross-linking density, whereas higher concentrations (≥ 0.5 wt%) led to significant mechanical reinforcement and restricted polymer chain mobility. Although rGO integration reduced flexural strength by 1.3-6.6%, the 2 wt% loading enhanced Vickers hardness by 7.5% and Young's modulus by 6.9%, reducing deflection by 22.2%. Integrated DSC and mechanical analyses identified 0.5 wt% as the critical threshold, where peak crystallinity optimized compressive strength to 89.7 MPa, notwithstanding a 5°C depression in the glass transition temperature (Tg). This phenomenon, combined with the "labyrinth effect" providing a superior diffusion barrier, significantly enhances the durability of hydrogen installations.

sciforum-176980: Electrolessly Deposited Transition Metal Phosphide Catalysts for Hydrogen Generation from Hydrolysis of Sodium Borohydride

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Hydrogen (H_2) is regarded as a significant and environmentally sustainable energy carrier due to its high energy efficacy, zero toxicity, and pollution-free combustion, making it a potential long-term substitute for fossil fuels. However, efficient hydrogen storage remains a challenge. Among chemical hydrides, sodium borohydride ($NaBH_4$) is attractive due to its high hydrogen content (10.8 wt%) and environmentally favorable hydrolysis products. Nevertheless, its hydrolysis in water is slow and requires efficient catalysts to enhance hydrogen generation. Herein, cobalt-phosphorus (Co-P) catalysts with varying phosphorus contents were investigated for hydrogen generation via the hydrolysis of alkaline $NaBH_4$ solutions. The catalysts were fabricated on copper substrates through an electroless metal plating technique, with sodium hypophosphite (NaH_2PO_2) utilized as the reducing agent. The Co-P catalysts with different P amounts of 3, 5, 8, and 11 wt.% were obtained. The morphology, structure, and elemental composition of the prepared catalysts were characterized using a variety of analytical techniques, including scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDX), inductively coupled plasma optical emission spectroscopy (ICP-OES), X-ray diffraction (XRD), and X-ray photoelectron spectroscopy (XPS).

The hydrogen generation rate was evaluated in a solution containing 5 wt.% $NaBH_4$ and 0.4 wt.% NaOH at temperatures ranging from 313 to 343 K. The results indicate that Co-P catalysts have notable catalytic activity toward the hydrolysis of $NaBH_4$. The hydrogen generation rate exhibited a range from 1 to 10 L min^{-1} g^{-1} at 343 K, while the activation energy demonstrated a range from 49 to 85 kJ mol^{-1}, dependent on the phosphorus content. Specifically, the Co-P catalyst containing 11wt.% phosphorus was identified as the most efficient catalyst, exhibiting a hydrogen generation rate of 10.05 L min^{-1} g^{-1} at 343K. The excellent catalytic performance and cost-effectiveness of the electroless-deposited Co-P catalysts highlight their potential for efficient hydrogen production via $NaBH_4$ hydrolysis.

sciforum-178943: Fabrication and characterization lanthanide doped perovskite solar cell

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In recent years, perovskite solar cells have been expected to become an alternative to silicon solar cells due to their high-power conversion efficiency and low production costs. However, the formation of PbI_2 during long-term storage, the resulting decrease in conversion efficiency, and the decrease in FF due to defects in the perovskite layer are challenges. In this study, rare-earth co-doped perovskite solar cells (Ce, Nd, Gd, Er, Yb) were fabricated to address these challenges. Rare earth elements are characterized by high localization of 4f orbitals and strong Lewis acidity. A decrease in trap density was observed in the Gd-doped device. In addition, an increase in (100) orientation and an increase in crystal size were observed after ~4 months of storage at room temperature and humidity in a dark place. As a result, the fill factor increased to 0.640. In addition, Gd-doped device was stored in a dark room temperature and humidity for ~4 months, and the conversion efficiency was greatly maintained without degradation. This study shows that rare earth-doped perovskite solar cells are effective in suppressing PbI_2 formation due to long-term storage, the resulting decrease in conversion efficiency, and the reduction of FF due to grain boundary defects, providing a new strategy for perovskite solar cells.

sciforum-177263: Improved Dielectric and Nonlinear Properties of Doped $CaCu_3Ti_4O_{12}$ Ceramics for High-Efficiency Energy Storage Applications

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Abstract (≈250 words)

A comprehensive study was conducted on the phase structure, microstructure, dielectric properties, and nonlinear current–voltage (J–E) behavior of doped $CaCu_3Ti_4O_{12}$ (CCTO) ceramics prepared using the conventional solid-state reaction method. The investigated compositions, including pure CCTO and Zr/rare-earth co-doped samples (Zr–Sc, Zr–Sm, Zr–Gd, and Zr–La), were sintered at 1080 °C for 8 h. X-ray diffraction analysis confirms that all ceramics crystallize in a cubic perovskite structure with the space group Im–3, indicating that the crystal structure remains stable after doping.

Microstructural observations reveal the formation of dense ceramics with a significant reduction in grain size as a result of Zr/rare-earth substitution. This grain refinement plays an important role in modifying the electrical behavior of the materials. Dielectric measurements show that the doped ceramics maintain a high relative permittivity ($\varepsilon' > 3.5 \times 10^3$). In particular, the Zr–Sc composition exhibits excellent thermal stability, with a permittivity variation ($\Delta\varepsilon'$) of less than ±15% up to 160 °C. Additionally, the dielectric loss ($\tan\delta$) is significantly reduced to 0.02 at 0.1 kHz at room temperature.

A remarkable enhancement in the breakdown electric field is also observed, reaching values more than 38 times higher than that of pure CCTO in the Zr^{4+}/Sc^{3+} co-doped composition. Furthermore, the doped ceramics exhibit an energy efficiency exceeding 98%, demonstrating their strong potential for high-efficiency energy storage applications. These improvements in dielectric and nonlinear properties are mainly attributed to the increase in grain boundary resistance (Rgb), which is closely related to the reduction of oxygen vacancies in the doped ceramics.

sciforum-165063: Investigation of Non-Aqueous Solvent Decomposition Mechanism on Mg Metal Anode Employing XPS Characterization

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Magnesium batteries (Mg-battery) can offer higher volumetric energy density than lithium ion batteries. However, the challenge is to establish the stable electrochemical interface (i.e. electrode-electrolyte interface) that can facilitate Mg^{2+} ion diffusion while impeding electronic transport that can trigger electrolyte decomposition process. Such a designer interface can help us enhance the charge rate, lifetime, operating voltage, and safety of the Mg-battery. However, the main knowledge gap is a predictive understanding of electrochemical interphase formation, especially at Mg-metal anode. Currently, very few non-aqueous solvents were identified as compatible for Mg-battery application due to their ability to withstand both the Mg plating and stripping process. For example, 1-Methoxy-2-(2-methoxyethoxy)ethane (diglyme) being an ethereal solvent, is considered less volatile and reasonably stable against Mg reduction. In order to understand and interpret the reactions and subsequent interphase layer evolution from possible diglyme interaction with Mg-metal anode, *in situ* X-ray photo electron spectroscopy (XPS) measurements were performed at Pacific Northwest National Laboratory. In the current study, the vapor of diglyme solvent is exposed Mg-metal single crystal substrate and subsequently analyzed using high resolution X-ray photo electron spectroscopy. Detail reaction mechanisms and pathways based on core-level spectra will be discussed in this presentation.

sciforum-179649: Mesoporous CeO_2-Supported Ni Catalysts: Tuning Nickel Dispersion for CO_2 Methanation

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Due to the growing concern over global warming, significant efforts are being directed toward the production of green fuels obtained via the hydrogenation of captured CO_2 using hydrogen from renewable sources. Methane represents one of the most relevant e-fuels and can be produced through the Sabatier reaction. Among the various catalytic systems, Ni-based catalysts are widely investigated due to their high activity, good selectivity at relatively low temperatures, and lower cost compared to noble metal-based alternatives. Their performance is often enhanced by the presence of supports or promoters such as CeO_2.

In this work, composite catalysts consisting of a NiO active phase dispersed on mesoporous CeO_2 were developed. The mesoporous structure enables a high dispersion of NiO as ultra-small nanoparticles, improving catalytic efficiency while minimizing the amount of active phase.

NiO was deposited on the support using both impregnation and self-combustion methods, yielding catalysts with Ni loadings of 5, 10, and 15 wt%. XRD analysis indicates that NiO is highly dispersed, particularly at low loading, where no distinct crystalline phases are detected. This is supported by HR-TEM, EDX/EELS mapping, H_2-TPR, and H_2 chemisorption, confirming increased dispersion at lower Ni content.

Catalytic tests reveal high CO_2 conversion (80–85 mol%) for CeO_2-supported samples with near-complete CH_4 selectivity. Notably, catalytic activity is only weakly dependent on Ni loading, highlighting that a low Ni content (5 wt%) is sufficient to achieve high performance due to an improved dispersion. This is particularly relevant for reducing the use of Ni, a critical and potentially hazardous material, without compromising efficiency.

sciforum-179587: Microwave-Assisted rGO Coupling for Stabilizing a V-Doped Co-Free Li-Rich Layered Cathode with High Discharge Capacity at 5C and 10C

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Co-free Li-rich layered oxides are promising cathodes for high-energy lithium-ion batteries, but their practical use is limited by structural degradation, voltage decay, and poor cycling stability at high rates. Here, we investigate microwave-assisted coupling with reduced graphene oxide (rGO) as a strategy to stabilize a V-doped Co-free Li-rich layered cathode, $Li_{1.2}Ni_{0.3}Mn_{0.49}V_{0.01}O_2$, using a composite containing 1 wt% rGO. Thermal analysis showed that 1 mol% V does not significantly modify the formation range of the layered phase, supporting calcination at 800 C for 12 h. Raman spectroscopy and X-ray diffraction confirmed preservation of the layered framework after both $Li_{1.2}Ni_{0.3}Mn_{0.49}V_{0.01}O_2$ and microwave-assisted rGO coupling. Rietveld refinement revealed very similar lattice parameters for the $Li_{1.2}Ni_{0.3}Mn_{0.49}V_{0.01}O_2$ and $Li_{1.2}Ni_{0.3}Mn_{0.49}V_{0.01}O_2$@rOG samples, indicating that the rGO treatment does not induce structural collapse. A low but measurable amount of Ni in the Li layer was detected in both samples, consistent with moderate antisite disorder. Electrochemically, V doping alone improved the high-rate response but reduced cycling stability. After microwave-assisted anchoring with 1 wt% rGO, the composite recovered the lost stability while maintaining strong rate capability. The $Li_{1.2}Ni_{0.3}Mn_{0.49}V_{0.01}O_2$@rGO cathode delivered 84.85% discharge-capacity retention after 80 cycles, compared with 79.63% for the $Li_{1.2}Ni_{0.3}Mn_{0.49}V_{0.01}O_2$ sample, and achieved discharge capacities of 148.47 and 113.58 mAh g^{-1} at 5C and 10C, respectively. These results show that microwave-assisted rGO coupling is an effective route for stabilizing a V-doped Co-free Li-rich layered cathode under demanding rate conditions. Vanadium improves bulk kinetic behavior, whereas rGO enhances interfacial charge transfer and electronic connectivity, thereby improving cycling stability and enabling high discharge capacities at 5C and 10C.

sciforum-176521: $NaNbO_3$ synthesis by combined EDTA/Citrate complexation

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The synthesis methodologies and reaction parameters, affect directly the structure and morphology of materials as perovskite-type compounds. In this work, sodium niobate ($NaNbO_3$), were produced by the combined EDTA/citrate complexation method, with ratios of 1:1:3 metal ions (sodium and niobium): EDTA: citric acid, and pre-treatment with 230 °C and temperature calcination 700 °C. The sample was analyzed by XRD with Rietveld refinement, and UV-Vis ERD. The study revealed that the material has an orthorhombic crystal structure and a $P2_1ma$ space group identified by the CIF 9014103. Based on the atomic positions obtained from Rietveld refinement, it is observed that each $NaNbO_3$ sample maintains the basic the perovskite network, particularly the BO_6 polyedra centered on niobium cation site, with lattice parameters a = 5.565Å, b = 7.774 Å and c = 5.521 Å. The crystallite size of sodium niobate was obtained using a Scherrer-type relationship, with values 169.91 nm. But the synthesis method promotes significant distortions within the NbO_6 coordination polyhedra. The bandgap value obtained is 2.69 eV, which are lower than those reported in the literature (~3.4 eV). These variations can be attributed to changes in the crystalline structure and particle morphology which may undergo phase transitions that affect its electronic properties and, consequently, its bandgap. Therefore, the synthesis method used is effective in producing $NaNbO_3$ with tunable properties, expanding its potential for technological applications as hydrogen porduction and storage.

sciforum-176427: Natural Anthocyanin-Sensitized DSSCs with Optimized TiO_2/Nb_2O_5 Photoanode Architecture

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In this study, a functional experimental model of dye-sensitized solar cells (DSSCs) based on natural anthocyanin dyes was developed, optimized, and evaluated under under simulated solar irradiation using a solar simulator. The photoanode architecture was optimized using a nanostructured TiO_2 film deposited on ST-FTO substrates, followed by controlled thermal treatment to improve adhesion, porosity, and electron transport. The influence of the number of TiO_2 layers on photovoltaic performance was investigated by comparing configurations with one, two, and three layers. In addition, a thin Nb_2O_5 interfacial layer was introduced to reduce electron recombination and improve charge transfer at the TiO_2/conductive substrate interface, while also acting as a light-scattering layer. Natural anthocyanin dyes extracted from various plant sources were used as photosensitizers. The assembled DSSC devices were tested using a solar simulator. The results demonstrated that the photovoltaic performance strongly depends on the photoanode architecture and the type of dye used. Increasing the number of TiO_2 layers enhanced the generated power due to improved dye adsorption and larger active surface area, while the introduction of the Nb_2O_5 layer significantly reduced recombination processes and improved charge transport.

The optimized DSSC configuration, consisting of three TiO_2 layers, an intermediate Nb_2O_5 layer, anthocyanin dye extracted from blackberries, an iodide/triiodide electrolyte, and a graphite counter electrode, demonstrated stable and reproducible photovoltaic response. These results confirm the potential of natural anthocyanin dyes as sustainable sensitizers for environmentally friendly DSSC devices.

sciforum-141515: Physical properties of the new double perovskite oxides Sr2BPO6 (B = Al, Ga) by ab initio calculations

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In this study, ab initio density functional theory (DFT) calculations were conducted to comprehensively investigate the structural, mechanical, electronic, and optical properties of the double perovskite oxides Sr2PAlO6 and Sr2PGaO6. The structural analysis, supported by the Goldschmidt tolerance factor, confirms that both compounds adopt a stable perovskite structure. Furthermore, their calculated negative formation energies (–3.059 eV for Sr2PAlO6 and –3.367 eV for Sr2PGaO6) strongly indicate excellent thermodynamic stability, making them promising candidates for practical applications. Mechanical stability is verified through elastic constant calculations, which fully satisfy the Born and Huang mechanical stability criteria for cubic systems. The absence of any imaginary frequencies in the phonon dispersion spectra further confirms the dynamic stability of both structures. In terms of mechanical behavior, these materials demonstrate anisotropic and brittle characteristics, as evidenced by anisotropy factors deviating from unity and Poisson's ratio values below 0.26. Electronic structure calculations reveal that both Sr2PAlO6 and Sr2PGaO6 exhibit semiconducting behavior with direct band gaps of 2.860 eV and 3.027 eV, respectively. Such values suggest they are suitable for use in optoelectronic devices operating in the visible to ultraviolet range. The optical properties, derived from the complex dielectric function, show strong and broad absorption features across the energy range of 0 to 12 eV, indicating their potential for efficient light-harvesting and energy conversion applications. In conclusion, the combined structural, mechanical, electronic, and optical analyses highlight that Sr2BPO6 (B = Al, Ga) double perovskites are promising multifunctional materials with significant potential for deployment in future optoelectronic and photovoltaic technologies.

sciforum-176970: Plasmonic Poynting vector vortices for uniform coupling to photocatalytic coatings

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Plasmon-assisted photocatalysis often suffers from spatial nonuniformity in electromagnetic energy distribution, leaving significant portions of adjacent catalytic coatings weakly activated. A more effective approach involves modes that confine energy uniformly along the entire metal-catalyst interface. In the present research, we propose using Poynting vector vortices (PVV) for photocatalytic activation. These vortices arise from surface plasmon polariton-like waves that circulate along the nanorod boundaries, analogous to whispering-gallery modes [1,2], and distribute electromagnetic energy uniformly around the rod perimeter. Unlike asymmetric excitations that localize fields on the illuminated side, these modes create a homogeneous electromagnetic environment along the full interface, which is particularly beneficial for activating conformal photocatalytic coatings.

We investigate these PVV modes in periodic arrays of Au and Ag nanorods coated with a photocatalytic film and supported on a dielectric SiO2 substrate. Using full-field finite-element simulations, we characterize the emergence of these PVV modes and evaluate the optical power dissipated within the surrounding catalytic layer. The circulating energy flow establishes a chiral electromagnetic topology that introduces local optical handedness even in geometrically symmetric structures. Such chiral field distributions may be relevant for catalytic processes sensitive to electromagnetic handedness, including emerging approaches to enantioselective photochemistry [3]. These findings highlight the potential of PVV modes for achieving more uniform and controllable photocatalytic activation across extended metal – catalyst interfaces.

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sciforum-176955: Schiff Base Metal Complexes as Efficient Catalysts for Energy-Related Applications

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New oxovanadium(V) Schiff base complexes were successfully synthesized and characterized as potential catalytic materials for environmentally friendly oxidation processes. Two dinuclear water-soluble oxovanadium(V) complexes, $[(L1H)VO(\mu\text{-}O)]_2$ (C1) and $[(L2H)VO(\mu\text{-}O)]_2$ (C2), were prepared by refluxing vanadyl sulfate ($VOSO_4$) with the corresponding tetradentate Schiff base ligands in methanol under controlled conditions. The formation of the complexes was confirmed using several physicochemical characterization techniques, including Fourier-transform infrared spectroscopy (FT-IR), UV–visible spectroscopy, and elemental analysis, which provided evidence for the coordination of the Schiff base ligands to the vanadium center.

The catalytic performance of the synthesized complexes was evaluated in the oxidation of olefins in aqueous medium. Water was employed as a green and environmentally benign solvent in order to develop a more sustainable catalytic process. Different oxidizing agents were investigated to determine their influence on catalytic efficiency and product selectivity. The results demonstrated that the oxovanadium(V) complexes exhibit high catalytic activity toward olefin oxidation, affording excellent product yields under mild reaction conditions. Furthermore, the catalysts showed remarkable stability and recyclability, maintaining their catalytic performance over several successive reaction cycles without significant loss of activity.

These findings highlight the potential of dinuclear oxovanadium(V) Schiff base complexes as efficient and sustainable catalysts for oxidation reactions. The use of water as a solvent and the good recyclability of the catalysts make these systems promising candidates for green catalytic processes and environmentally friendly chemical transformations with potential relevance to energy-related and sustainable chemistry applications.

sciforum-179561: Single-Crystal X-ray Diffraction Study of Doped $CaKFe_4As_4$: Structural Distortions.

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Iron-based superconductors, discovered in 2008, have attracted considerable attention due to their promising superconducting properties and their potential for high-field applications.

They share a FeAs or FeSe structural building blocks and exhibit a wide variety of structural families. Among them, the 1144 phase ($AAeFe_4As_4$ A=Alkaline and Ae=Alkaline earth metal), discovered in 2016, has attracted particular interest due to its robust superconducting properties. Within this family, $CaKFe_4As_4$ is considered one of the most promising compounds. The synthesis of these materials in polycrystalline form, relevant for superconducting wire applications, strongly affects their superconducting performance. In particular, intergrain properties, secondary phases, grain-boundary chemistry, and microstructural features such as porosity and density play a crucial role.

Chemical substitutions have been explored to optimize its superconducting properties, with partial replacement of Ca and K by elements with similar ionic radius (Na, La, Pr, Sr, and Ba). Previous studies on polycrystalline samples suggested that doping induces lattice distortions affecting the superconducting critical temperature (T_c), and enhancing the critical current density (J_c), although microstructural effects could not be excluded.

To distinguish intrinsic effects from microstructural contributions, single crystals of pristine and doped $CaKFe_4As_4$ were grown and investigated by single-crystal X-ray diffraction, from which the corresponding CIF files were obtained. Complementary morpho-structural and superconducting measurements were also performed to correlate the crystal structure with the physical properties.

The combined analysis highlights a clear correlation between structural modifications and superconducting behavior. Furthermore, the structural analysis suggests that defects introduced by doping act as effective pinning centers, explaining the observed enhancement of J_c.

sciforum-174125: Solubility of Metals in Semiconductors: Insights from Iron Silicide System

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Iron silicide is an earth-abundant and environmentally friendly material system that crystallizes in several phases, including metallic ε-FeSi and α-Fe_2Si_5, and semiconducting β-$FeSi_2$. Among them, β-$FeSi_2$ has attracted considerable interest for optoelectronic, photovoltaic, and thermoelectric applications due to its tunable electrical conductivity. Both n-type and p-type conduction can be achieved through transition-metal doping; however, performance optimization is often limited by dopant solubility and the emergence of secondary metallic phases. Previous studies mainly inferred solubility limits from lattice parameter shifts or qualitative phase identification, with a lack of quantitatively correlating bulk phase fractions and local elemental distribution.

Polycrystalline $Fe_{1-x}M_xSi_2$ (M = Mn, Co, Ni) samples were prepared by arc melting followed by a two-step heat treatment to promote the formation of the β phase. Dopant concentrations were systematically varied within controlled ranges. Phase identification and quantitative analysis were performed using X-ray diffraction combined with Rietveld refinement, while microstructure and elemental distributions were examined by SEM-EDS at multiple locations to evaluate reproducibility and local dopant incorporation.

The evolution of phase fractions reveals that increasing dopant concentration promotes the formation of metallic ε and α-phases. Although the β-phase remains dominant (>95%) over a finite composition range, local compositional analysis indicates earlier saturation of dopant incorporation within the β-matrix. The estimated solid-solution limits are approximately 6.3% for Mn and 8.8% for Co, while Ni exhibits significantly lower solubility. Beyond these limits, excess dopants segregate and contribute to metallic phase formation, which correlates with degradation in thermoelectric performance. The combined bulk and local analyses provide a practical strategy to evaluate dopant solubility and phase stability in β-$FeSi_2$, offering guidance for optimizing transition-metal doping in semiconductor-based energy materials.

sciforum-179670: Strontium Hydrides for Hydrogen Storage and Strain-Enhanced Hydrogen Desorption near Room Temperature

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Metal hydrides are promising candidates for hydrogen storage due to their high volumetric hydrogen density. In this study, Sr_2H_4, a strontium-based hydride, is investigated using first-principles density functional theory (DFT) within the PBEsol generalized gradient approximation as implemented in CASTEP. The optimized structure exhibits a trigonal crystal system with lattice parameters a = b = 4.07 Å and c = 5.53 Å. Its negative formation energy confirms thermodynamic stability, while the absence of imaginary phonon modes indicates dynamical stability, mechanical stability is also ensured through the satisfaction of Born stability criteria. Electronic structure calculations reveal that Sr_2H_4 is a semiconductor with an indirect band gap of 1.109 eV, and optical analysis demonstrates favorable absorption and refractive properties, highlighting its potential for optoelectronic applications. From a hydrogen storage perspective, Sr_2H_4 shows a relatively high desorption temperature (~1008 K), a gravimetric capacity of 2.25 wt%, and a volumetric hydrogen density that meets U.S. Department of Energy targets. To improve its performance, strain engineering is applied, and the results indicate that compressive strain effectively weakens the Sr–H bonds and significantly reduces the desorption temperature, enabling hydrogen release near room temperature. These findings provide valuable insights into the design of efficient hydrogen storage materials and highlight the role of strain engineering as a practical strategy to optimize their performance under near-ambient conditions.

sciforum-176543: Synthesis, Characterization and Dielectric Properties of Aegirine

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This study focuses on the low-temperature synthesis and characterization of aegirine ($NaFeSi_2O_6$) to investigate its structural, optical, and electrical properties. FTIR analysis reveals the characteristic vibrational signatures of the pyroxene framework, particularly the Si–O–Si bands (1000–1100 cm^{-1}), bending modes or Si–O–Fe linkages (~700 cm^{-1}), and Fe–O vibrations in the octahedral sites (540 and 470 cm^{-1}), confirming the formation of the crystalline silicate structure. Scanning electron microscopy shows well-crystallized grains with relatively smooth surfaces, indicating satisfactory crystallinity of the synthesized material.

UV–Visible spectroscopic analysis performed in the 250–650 nm range reveals absorption bands between 300 and 400 nm, associated with electronic transitions of Fe^{3+} ions located in octahedral coordination sites. The optical band gap energy, estimated to be approximately 3.0 eV using the Tauc method, confirms the semiconductor nature of the synthesized aegirine, supporting its suitability for electronic charge transport processes.

Dielectric measurements conducted over the frequency range of 0.1 Hz to 10^6 Hz show very high real permittivity values at low frequency (≈1.75×10^5), followed by a gradual decrease until reaching an almost constant plateau within the 10^1–10^6 Hz interval, reflecting the dominance of interfacial polarization. The dielectric loss tangent exhibits a relaxation peak of approximately 10, consistent with the Maxwell–Wagner–Sillars relaxation mechanism.

Frequency-dependent conductivity remains relatively stable between 10^1 and 10^3 Hz and increases at higher frequencies, with a room-temperature conductivity of approximately 1.3×10^{-5} $S\cdot m^{-1}$. Temperature-dependent conductivity measurements (50–200 °C) show non-monotonic values ranging from 3.25×10^{-6} to 2.25×10^{-6} $S\cdot m^{-1}$, suggesting thermally assisted charge transport. Nyquist impedance plots exhibit semicircular arcs characteristic of grain-dominated electrical response according to an RC-type equivalent circuit model. The resistance values vary with temperature, decreasing from approximately 2.75×10^6 Ω at room temperature to 5.5×10^4 Ω, 5.4×10^4 Ω, 5.7×10^4 Ω and 3.5×10^5 Ω at 50, 100, 150 and 200 °C, respectively.

Overall, low-temperature synthesized aegirine exhibits semiconductor behavior and dielectric properties strongly dependent on frequency and temperature, highlighting its potential for silicatebased functional materials for electronic and energy applications.

Session 6. Crystal Engineering

sciforum-162850: Crystallographic Principles Explored via Immersive and Non-Immersive Virtual Reality Tools

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Introduction: The visualization of crystallographic structures is essential for understanding lattice geometry, symmetry, and atomic arrangements. However, traditional two-dimensional depictions often fail to provide the spatial insight required for mastering these concepts. To address this challenge, we developed an immersive and non-immersive Virtual Reality Learning Environment (VRLE) designed to facilitate intuitive exploration of foundational crystallographic principles, including the 14 Bravais lattices, crystallographic directions, planes, plane families, and interstitial sites.

Methods: The application was implemented both as immersive and non-immersive VRLE. The VRLE is structured as a virtual museum consisting of five interactive stations, each dedicated to a specific crystallographic topic. Users can manipulate 3D models through rotation, translation, zooming, selective hiding or highlighting of elements, and guided structural walkthroughs.

Results: The application successfully conveys geometric and structural features that are typically difficult to interpret from traditional representations. Users can examine unit cells and extended lattices, visualize the orientation of crystallographic directions and planes, and explore families of Miller-indexed elements. The dynamic rendering of tetrahedral and octahedral voids provides a clear illustration of their distribution and coordination within the lattice. Preliminary use in educational settings indicates enhanced spatial comprehension and improved conceptual retention.

Conclusions: The immersive and non-immersive VRLE offers an effective and accessible platform for understanding crystallographic principles. Its interactivity, modular structure, and real-time visualization capabilities make it a valuable tool for both guided instruction and independent learning.

sciforum-179576: Anti-Electrostatic Anion–Anion Interactions in Halogen Oxyanions: Are X···O Contacts Really Halogen Bonds?

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Introduction: Noncovalent interactions act as a chemical glue that binds molecular entities and governs the formation of sophisticated functional materials. Beyond classical hydrogen bonding, halogen bonding, and related directional contacts involving elements across the periodic table, anti-electrostatic interactions have recently emerged as an unusual class of intermolecular interactions. These involve contacts between like-charged species that are expected to be repulsive based on simple electrostatic considerations, yet are frequently observed in crystalline solids.

Halogen oxyanions such as XO_3^- provide a particularly intriguing platform for examining such behavior. Numerous crystal structures display short X···O contacts between anions, often interpreted as halogen bonding. However, whether these contacts represent genuine attractive interactions or arise from environment-induced polarization remains unclear.

Results and discussion: In this work, we examined a series of anion–anion assemblies involving halogen oxyanions using density functional theory in both gas and solution phases. The optimized structures reveal that several systems stabilized in solution exhibit short X···O contacts that resemble halogen bonds. However, SAPT energy decomposition analysis shows that these interactions are characterized by large positive electrostatic contributions, and the total interaction energies are also positive when evaluated in the gas phase.

These findings indicate that the apparent stabilization of the dimers does not originate from intrinsic attractive halogen bonding. Instead, the structures are maintained by solvent screening and polarization effects that reduce Coulomb repulsion and allow weaker induction and dispersion contributions to shape the geometry. The persistence of these motifs in crystalline materials therefore arises from collective influences, including counterions, packing constraints, and polarization, rather than from intrinsic attractive forces between the isolated anions. These aspects are discussed in detail.

sciforum-176136: CFD Design of a NETmix Crystalliser for Struvite Precipitation from Sidestream Digestate

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Precipitation is an extensively used unit operation that involves mixing concentrated soluble reactants to form a sparingly soluble product. In wastewater treatment, it has recently been employed to recover nutrients from the liquid fraction obtained after dewatering digested sludge in wastewater treatment plants. Phosphorus (P) and nitrogen (N) are precipitated as struvite crystals upon addition of a concentrated magnesium solution, and subsequently used as slow-release fertilisers.

NETmix is a well-established static mixer and reactor. Owing to its distinct geometry, it surpasses most state-of-the-art technology for mixing and heat transfer and has been successfully used for the production of several crystalline compounds, including hydroxyapatite nanocrystals. This success motivated its application for the production of struvite crystals. This process requires mixing three liquid streams: the effluent stream (P and N source); a stream consisting of a concentrated magnesium (Mg) solution; and one consisting of a pH-controlling solution.

Two concentrated streams (Mg and pH-controlling solutions) are separately injected at low flowrate ratios relative to the main feed flowrate (effluent) directly into selected chambers along the NETmix reactor. This work assesses the effect of injection chamber position on the mixing performance of the reactor through the Computational Fluid Dynamics (CFD) simulation of passive tracer mixing experiments.

The topology of injection was found to have significant impact on mixing. Micromixing performance was quantified using the intensity of segregation. For all configurations studied, the intensity of segregation decreased along the NETmix network, indicating progressive homogenisation of the streams. The optimised injection scheme reduced the intensity of segregation by 99.9 %. It also ensured comparable mixing degrees for both tracers (Mg and pH-controlling solutions) at the outlets.

These results are highly relevant for crystalliser design, since mixing directly influences supersaturation, chemical reaction, nucleation and crystal growth during precipitation processes.

sciforum-172991: Control of photoreactivity in organic solids through large synthons

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Controlling photoreactivity in organic solids have attracted significant interest from chemists and material scientists for a long time. Although the pioneering works in this field dates back to 1970s when Schmidt formulated the topochemical principle based on cinnamic acid derivatives, the advent of the subject crystal engineering allowed to tune photoreactivity in a supramolecular way using hydrogen bonding and other non covalent interactions. The design of organic solids became easier with the formulation of the concept of supramolecular synthons. However, with the years it is realized that small synthons despite capturing necessary chemical and geometric details are often insufficient to provide sufficient control in many design strategies. In this context, the idea of large synthons was coined. Large synthons, in the present context, represent modular synthons often involving composite interactions which contain sufficient chemical and geometrical information for a targeted design and provides sufficient structural insulation that makes the strategy robust and general. These modular large synthons are often considered as starting point in Long Range Synthon Aufbau modules (LSAM) based design strategies. Despite their potential in crystal design, robust large synthons are often difficult to implement in design strategies as they are generally formed by combined effects of weak interactions and may lack in recurrence. This talk will focus on how a robust large synthon can be helpful especially in the context of bi-component crystal design, based on benzilic acid and stilbazole derivatives. Benzilic acid, a well-known molecule in the context of Benzil-Benzilic acid rearrangement, also contains intriguing supramolecular features that help in large synthon formation. The key focus of the talk will address: (i) crystal design with diverse photoresponses, (ii) tuning photoreactivity/photoresponses in the respective solids through a large synthon approach (iii) role of modularity of such large synthons in crystal design.

sciforum-179585: Coupling Between Br-Hexahelicene Molecules through Br···Br and Br···H Bonds

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Non-covalent interactions, particularly halogen–halogen and halogen–hydrogen bonds, play a fundamental role in supramolecular chemistry and are key determinants in the design and stabilization of hierarchical molecular architectures. In this work, we investigate in detail the intermolecular interactions governing the formation and stabilization of a dimer composed of two bromine-substituted hexahelicene (Br-Hexahelicene) molecules, which are inherently chiral helical systems built from six fused aromatic rings.

Geometry optimizations were carried out using the semi-empirical MOPAC method, revealing the presence of two enantiomeric forms, denoted M and P. These enantiomers can self-assemble into energetically equivalent homo-chiral dimers (MM and PP), highlighting the role of molecular chirality in the organization of supramolecular systems. To better understand the origin of stability, an energy decomposition analysis was performed, showing that the dimers are stabilized by a combination of directional short-range interactions and dispersive forces.

In particular, characteristic contacts such as C–Br···Br–C (3.55 Å) and C–Br···H–C (2.97 Å) were identified, together with significant van der Waals contributions. The computed interaction energies (–4.50, –3.33, and –5.44 kcal/mol) clearly indicate that halogen–halogen and halogen–hydrogen bonding interactions constitute the dominant driving forces in the self-assembly process. Additionally, advanced topological and electronic analyses, including the Interaction Region Indicator (IRI), electrostatic potential mapping, and bond-path analysis using Multiwfn, provide a clear visualization and confirmation of the interaction regions, revealing the presence of triangular Br···Br···H binding motifs.

Overall, these results demonstrate the strong propensity of Br-Hexahelicene molecules to form well-organized supramolecular assemblies, emphasizing the crucial role of halogen bonding in the rational design of functional chiral materials with promising applications in nanoscience and surface-based molecular engineering.

sciforum-179537: Crystal Engineering of Quinazoline Derivatives: Impact of Chalcogen Substitution and Substituent Bulk on 3D Architecture and Intermolecular Interactions

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The design of crystalline materials with tailored properties requires a profound understanding of molecular self-assembly principles. Quinazoline derivatives are essential pharmacophores [1]; however, the influence of specific substituents on their solid-state packing remains insufficiently explored. This study investigates the "chalcogen-switch" strategy, examining how substituting sulfur with oxygen and modifying the hydrocarbon radical volume serves as a directional mechanism for controlling supramolecular architecture. Three quinazoline derivatives—benzylthio-, methylthio- and ethoxy-substituted—were characterized via single-crystal X-ray diffraction. Structural refinement was performed using the Olex2 software package [2]. To visualize and quantify the competition between π···π stacking of the quinazoline cores and directional chalcogen-mediated contacts, Hirshfeld surface analysis and 2D fingerprint plots were generated using CrystalExplorer [3] . The compounds crystallize in the monoclinic system (P21 and P21/c) with very good quality (R1: 2.09%–3.96%). Hirshfeld surface analysis (dnorm) revealed that while H···H contacts dominate (45–55%), chalcogen-mediated interactions primarily dictate the crystal growth direction. Thio-derivatives exhibit diffuse yet numerous S···H contacts, promoting flexible packing. In the ethoxy-derivative, the presence of the rigid, highly electronegative oxygen atom leads to shorter and more directional O···H contacts, significantly altering the fingerprint plot landscape by shifting the "spikes" toward lower di/de regions. Our study demonstrates that subtle structural modulation, such as replacing sulfur with oxygen or increasing substituent bulk from methyl to benzyl, can fundamentally redirect the supramolecular landscape of quinazolines. These findings establish a predictive framework for using selective chalcogen substitution as a crystal engineering tool to design heterocyclic materials with controlled physicochemical properties.

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sciforum-179526: Crystallization behaviour of phage shock protein: morphological analysis and growth mechanisms

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Introduction: The phage shock protein (Psp) system is essential for maintaining membrane integrity under stress conditions in bacteria. Determining its three-dimensional structure requires well-ordered crystals, typically obtained through controlled crystallization methods. In this manuscript we present a range of crystal morphologies, reflecting variations in nucleation and growth conditions.

Methods: Crystallization was performed using the sitting drop vapor diffusion technique. A drop containing purified phage shock protein mixed with precipitant solution was equilibrated against a reservoir with higher precipitant concentration. Vapor diffusion gradually increased protein supersaturation within the drop, promoting nucleation and subsequent crystal growth. Experimental parameters such as protein concentration, precipitant composition, pH, and temperature were systematically optimized.

Results: Multiple crystal of the same protein appear under different condition. Well-defined hexagonal crystals indicate highly ordered growth under near-equilibrium conditions. Rod-shaped crystals suggest anisotropic growth along a preferred axis, while dendritic and clustered structures are indicative of rapid nucleation at high supersaturation. Regions containing numerous microcrystals suggest excessive nucleation with limited crystal growth.

Discussion: Crystal formation can be interpreted using thermodynamic principles, where the Gibbs free energy change is given by:

Δ=Δ+

Here, represents the bulk free energy change, γ is the interfacial surface tension, is the nucleus volume, and A is the surface area. The presence of well-formed hexagonal crystals suggests minimized free energy and stable growth conditions, whereas dendritic and clustered morphologies indicate kinetically dominated regimes. These observations highlight the importance of controlling supersaturation to balance nucleation and growth, ultimately improving crystal quality for structural analysis

sciforum-177609: Crystallo-Co-Agglomeration as a Crystal Engineering Strategy for Tailoring Pharmaceutical Crystal Properties and Enhancing Drug Processability

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Crystal engineering plays a crucial role in controlling the structure, morphology, and functional properties of crystalline materials across multiple disciplines, including pharmaceutical science. Among various particle engineering techniques, crystallo-co-agglomeration (CCA) has gained significant attention as an innovative method for tailoring the physicochemical and mechanical properties of crystalline drug substances. By combining crystallization and agglomeration in a single process, CCA enables the formation of spherical crystalline agglomerates with improved particle size distribution, flowability, and compressibility.

The technique typically employs a ternary solvent system consisting of a good solvent, an anti-solvent, and a bridging liquid that promotes crystal agglomeration during nucleation and growth. Through careful control of process parameters such as solvent composition, agitation intensity, temperature, and bridging liquid concentration, the morphology and internal structure of crystalline agglomerates can be precisely engineered. This approach enables the production of functional crystalline particles with enhanced downstream processing characteristics.

From a crystal engineering perspective, CCA offers unique opportunities to manipulate crystal habit, surface properties, and interparticle interactions. The method also allows the incorporation of excipients or secondary components to produce composite crystalline materials with tailored dissolution and mechanical behavior. Recent studies have further demonstrated the potential of integrating advanced analytical techniques and computational tools to understand and optimize agglomeration mechanisms. Consequently, CCA provides an effective strategy for designing advanced crystalline pharmaceutical materials while contributing to broader developments in crystal engineering and materials science.

sciforum-176638: Design and Crystal Engineering of a Photonic Crystal Fiber for Optical Pressure Sensing

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Photonic crystal fibers (PCFs) have attracted considerable interest due to their unique microstructured geometry and their ability to manipulate optical properties through structural design. In this work, a novel photonic crystal fiber configuration is proposed and investigated for pressure sensing applications. The structure is based on a silica background with a periodic arrangement of air holes forming a photonic crystal cladding. By engineering the geometrical parameters of the microstructured lattice and selectively infiltrating water into the air holes, the optical behavior of the fiber can be significantly modified.

Numerical simulations were carried out to analyze the influence of pressure variations on the chromatic dispersion characteristics of the proposed structure. The study demonstrates that the infiltration of water into the microstructured regions strongly affects the dispersion profile and shifts the zero-dispersion wavelength of the fiber. This behavior highlights the strong interaction between the guided optical field and the infiltrated medium, which can be exploited for sensing purposes.

Furthermore, the pressure sensitivity of the proposed sensor was evaluated by analyzing the variation of chromatic dispersion at different operating wavelengths. The results indicate that the sensor exhibits enhanced sensitivity at longer wavelengths, demonstrating the potential of the proposed design for high-precision pressure detection.

Compared with previously reported photonic crystal fiber sensors, the engineered structure shows improved sensing performance due to the optimized microstructured design and the interaction between the optical field and the infiltrated liquid. These findings demonstrate that crystal-engineered photonic crystal fibers can provide an effective platform for the development of highly sensitive optical pressure sensors for various scientific and industrial applications.

sciforum-176804: ESTANPy Toolbox for Assessing and Enhancing Data Information Content: Application to Paracetamol Batch Cooling Crystallization

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Introduction. The pharmaceutical industry is transitioning from quality-by-test (QbT) to quality-by-design (QbD) and quality-by-digital-design (QbDD) paradigms, necessitating built-in quality assurance throughout the product lifecycle [1]. High-fidelity mathematical models are critical for reliable process design, optimisation, and control [2]. However, robust model establishment is challenged by scarce experimental data and inadequate assessment of data information content, hindering parameter estimation and undermining predictive capability [3]. Crystallisation processes exemplify this difficulty, as complex mechanisms (nucleation, growth, agglomeration, polymorphism) yield high-dimensional population balance models with extensive parameter sets, which demands substantial experimental resources yet often yields information-deficient data [4,5].

Methods. We developed ESTANPy, a Python-based web application integrating global sensitivity analysis with sequential orthogonalisation to quantify data information content, diagnose non-estimable parameters, and guide information-rich experimental design.

Results. Applied to a 16-parameter paracetamol batch cooling crystallisation model, ESTANPy identified 10 estimable parameters from preliminary data; estimability-guided model-based design of experiment (MBDoE) subsequently yielded an optimally designed experiment, increasing this to 12 [4]. Compared with traditional full factorial design requiring 16 runs minimum, the proposed approach achieves equivalent estimability with 3 runs (more than 80% reduction in experimental burden), whilst markedly curtailing material consumption, energy usage, and environmental impacts.

Conclusions. ESTANPy enables efficient, targeted model development by identifying information-deficient parameters and guiding information-rich experimental design. This capability directly supports QbDD implementation in pharmaceutical processes, delivering substantial reductions in experimental burden without compromising model reliability.

sciforum-176885: Facile hydrothermal synthesis of $Zn_{1-x}Fe_xO$ nanoparticles

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Even if the ZnO NPs were widely investigated extensively, they are still relevant given their versatility on various fields of application. Hence the necessity of advancing techniques to synthesize it in a highly controlled manner to enhance their properties.

It is well known that the properties of nanoparticles depend mostly on the size and the homogeneity of the crystalline structure. Hydrothermal synthesis is a promising technique, as it promotes a highly controlled synthesis of nanoparticles at low temperatures and short reaction times, without the need for expensive equipment and the production of polluting effluents.

This study achieved not only the synthesis of ZnO NPs but also the crystallization of the $Zn_{1-x}Fe_xO$ solid solution NP with an inclusion of Fe^{2+} ions in quantities from 1 to 10% in the zinc oxide wurtzite structure. These nanoparticles were synthesized through hydrothermal reactions, carried out on Teflon-lined stainless-steel autoclaves at temperature of 160 °C on reaction time of only 1 hour using $Zn(NO_3)_2$ $6H_2O$, as zinc ions precursor, $FeCl_2{\cdot}4H_2O$ as iron atoms source and NaOH solutions as hydrothermal media.

The synthesized nanoparticles were analyzed by XRD which presented highly defined peaks proving the exclusive crystallization of ZnO NPs and their gradual shift to lower angles matching with the expansion of the lattice of the unit cell, from 45 nm to 53 nm with 10% Fe^{2+} substitution. Also, the $Zn_{1-x}Fe_xO$ nanoparticles exhibited a notable change in colour hue relative to the ZnO NPs. Finally, DLS indicated the size of about 60 nm and high homogeneity of the NPs of the NPs. Meanwhile the UV-Vis spectroscopy indicated the formation of $Zn_{1-x}Fe_xO$ nanoparticles.

sciforum-179643: Identifying Key Drivers of Nanobody Crystallization using Machine Learning

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Antibody-based therapeutics represent an important class of biopharmaceuticals [1]. Crystallization of antibodies is essential for structural characterization and holds potential for applications in downstream processing and drug formulation [2]. However, crystallization of antibodies remains challenging due to the large size, conformational flexibility, and complex intermolecular interactions of antibodies [3]. Predicting mutations that influence crystallizability could facilitate rational design of crystallization strategies, yet the limited availability of structural data has restricted the development of robust predictive models. In this study, we combine computational modelling with machine learning to identify descriptors associated with crystallization in nanobodies as a proof-of-concept system, given the scarcity of crystallized full-length monoclonal antibodies. Monomeric nanobody structures were curated and analysed to identify crystal interface residues, which were classified as crystal-site or non-crystal-site residues. Each residue was represented using a multidimensional set of physicochemical and structural descriptors capturing both intrinsic residue properties and features of the surrounding structural environment. Several machine learning algorithms were evaluated for residue classification, among which XGBoost demonstrated the best predictive performance. Here, we present our preliminary analysis revealing structural characteristics associated with crystallization propensity, providing insights into residue-level determinants of crystal formation. This is one of fundamental first steps towards a framework aimed at enhancing crystallization of antibodies through mutation-driven crystal contacts engineering.

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sciforum-176976: Impurity Aware Route Design for Mefenamic Acid Crystallization using Computer Aided Retrosynthesis

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The presence of impurities during the crystallisation of active pharmaceutical ingredients is a major process engineering challenge because they can affect product purity, safety, efficacy, and consistency.[1,2] In mefenamic acid (MFA) manufacture, impurities inherited from reaction steps can influence crystal quality attributes.[3] The current MFA synthesis relies on a Buchwald coupling, that also generate benzoic acid through dehalogenation, and relies on excess toxic 2,3-dimethylaniline, both known impurities to affect MFA crystal morphology.

This study leverages state-of-the-art computer-aided retrosynthesis (CAR),[4,5] to develop a greener-by-design and safer multistep synthesis for MFA. The main objective is to identify an effective, greener, and feasible route for the selected API while avoiding the presence of impurities that are toxic and affect crystal quality attributes.

The CAR identified two viable routes. The first is similar to the current synthesis. However, when constrained against toxic and crystallisation relevant compounds, the CAR proposed a one-step route for MFA from safe building blocks, eliminating the need to remove hazardous materials and simplified the purification to the final crystal product. In addition, as the CAR route avoids 2-chlorobenzoic acid, the formation of benzoic acid impurity that affect the crystal morphology is minimized.

In summary, CAR identified a synthetic route for MFA that eliminated the use of hazardous and toxic compounds, improving the safety and greenness of the reaction. By reducing impurity inheritance upstream, the proposed route offers process advantages, lowering the burden on downstream purification and enabling more robust crystallisation with improved control of final crystal quality.

Acknowledgement:

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sciforum-179428: Insights into the supramolecular architecture of xanthene derivatives

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Introduction: Xanthenes are important representatives of oxygen-containing tricyclic compounds. Several xanthene derivatives, including 9H-xanthene, xanthydrol, and xanthene-9-carboxylic acid, display diverse biological activities such as neuroprotective, antiparasitic, cytotoxic, and antibacterial. In this study, two xanthene-1,8(2H)-diones bearing 3-chloro-4-hydroxyphenyl (**1**) and 3,5-dibromo-4-hydroxyphenyl (**2**) groups in position 9 were synthesized via condensation of dimedone with the corresponding benzaldehydes. Their crystal structures were determined and analysed through the identification and quantification of simple dimeric motifs arising from distinct intermolecular interactions, thus extending our ongoing crystallographic studies on structurally related small molecules of pharmacological interest.

Methods: The structures were confirmed by spectroscopic methods. The single crystals suitable for X-ray diffraction were obtained by slow evaporation from ethanol. Data collection was performed on an Oxford Gemini S diffractometer. The computational calculations were conducted with Gaussian 09 and CrystalExplorer 21.5. These compounds were also examined with SwissADME and PreADMET *in silico* tools

Results: Both compounds share the same conformation, with a central shallow boat and twisted outer rings. Compound **1** forms chains along the *a*-axis via C–H···O interactions, which further assemble into zig-zag double chains through O–H···O hydrogen bonds and Cl···π interactions. In compound **2**, alternating asymmetric units are connected by O–H···O, C–H···O, and Br···Br interactions and form chains, with additional C–H···O and C–H···π contacts extending the network. Both compounds display similar distributions of H···H, O···H and C···H contacts, although X···H and X···C interactions are more pronounced in **2**. Based on the values of the molecular descriptors, these compounds meet all the necessary empirical criteria, which qualify them as interesting drug candidates.

Conclusions: These compounds demonstrate the potential of xanthene-1,8-diones as versatile building blocks for constructing interesting supramolecular structures of pharmaceutical relevance.

sciforum-179453: Mechanistic Role of Shear Rate on Transport-Controlled Crystal Growth in Antisolvent Crystallization

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Introduction

Hydrodynamics plays a central role in antisolvent crystallization by governing mixing and supersaturation generation, which in turn controls crystal growth [1]. While previous studies report distributions of flow and crystallization fields, the mechanistic role of shear rate in governing growth through transport phenomena remains insufficiently understood.

Methods

A coupled computational fluid dynamics–population balance model (CFD-PBM) is employed to investigate the influence of shear rate on crystal growth under steady-state laminar conditions [2]. A two-dimensional axisymmetric configuration is considered for nickel sulphate hexahydrate ($NiSO_4.6H_2O$) crystallization using ethanol as the antisolvent. Supersaturation is generated by the reduction in solubility caused by the addition of an antisolvent to the initially saturated aqueous salt solution at a constant temperature. The size-independent growth rate is applied to the crystal growth.

Results

Shear-induced mixing modifies the spatial distribution of supersaturation and thereby controls growth dynamics. Increasing shear rate enhances convective transport, producing sharper supersaturation gradients and stronger spatial confinement of the growth zone near the mixing interface. In contrast, lower shear conditions result in broader supersaturation fields and more distributed growth regions. The magnitude of the crystal growth rate correlates directly with local supersaturation.

Conclusions

Shear does not intrinsically alter growth kinetics but acts indirectly through transport modulation. This study provides a mechanistic framework for understanding shear-mediated transport effects in growth-dominated antisolvent crystallization systems, connecting hydrodynamic shear to crystal growth and distribution.

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sciforum-176666: Modelling of molecular crystals habit under growth, equilibrium and milling conditions from crystal structure

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Crystal habit both underpins many advanced simulations (powder packing, mechanical behavior, sorption) and provides a sensitive benchmark for evaluating in silico models for molecular crystals. Small changes in crystallization conditions alter habit, so a model that captures the relevant physical and chemical effects should reproduce experimentally observed morphologies. Habits also evolve during growth, as crystals approach equilibrium, and after milling.

Here we present an integrated, computational workflow that simulates growth, equilibrium, and milled habits directly from crystal structure. The approach decomposes the crystal into strongly bound building units and evaluates pairwise interactions using quantum-chemical calculations combined with molecular dynamics to account for crystal environment, solvent, supersaturation, and thermodynamics. Monte Carlo crystal collection under high- and low-oversaturation profiles at fixed thermodynamic conditions produces growth and equilibrium morphologies, respectively. Resulting face areas feed an in-house fragmentation model that uses interlayer attachment energies and the initial habit to simulate breakage during milling. The workflow is computationally efficient and scalable, yielding distinct, physically consistent habits corresponding to different crystallization and milling conditions. The method provides practical, reliable input morphologies for downstream simulations and supports validation of atomistic crystal models against experimentally observed habit variations. Additional validation and benchmarking studies are ongoing to further refine the approach.

sciforum-176988: Organoboronic Acids as Co-formers in Pharmaceutical Crystal Engineering

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Introduction: The ability to predict non-covalent interactions is a major driving force behind the development of multi-component crystals of pharmaceutical compounds. Organoboronic acids have a distinctive hydrogen bonding profile, but their potential as co-formers of a variety of different active pharmaceutical ingredients is still an area of active research. This current work is dedicated to the supramolecular potential of a selection of different boronic acid derivatives as potential tools in the creation of new crystalline forms.

Methods: In order to explore the potential of these compounds as co-formers, a number of experiments were conducted with several different pharmaceutical compounds and a selection of different organoboronic acids, including phenylboronic acid and several phenyl-substituted derivatives thereof. In order to understand the process of molecular assembly, a detailed analysis of the Cambridge Structural Database was conducted to understand the interplay between homosynthons and heterosynthons within the context of boronic acid-based compounds.

Results: The results demonstrate the prevalence of strong self-associating motifs within boronic acids that can significantly impact the API-co-former interplay. The findings indicate that specific steric and electronic characteristics of the organic boronic acid compounds under investigation affect the lattice stability. The study provides a structural rationale for the observed crystallization behavior, emphasizing the role of synthon competition in the design of pharmaceutical co-crystals.

Conclusions: The work provides critical insights into the crystal engineering process mediated by boronic acids and serves to clarify the structural requirements for successful supramolecular synthesis. These results are essential for refining the selection criteria used to identify co-formers in future attempts to optimize the crystallization conditions of new multicomponent pharmaceutical phases.

sciforum-178679: Polymorphism and structural studies of N-[(2-hydroxyphenyl)methylene]-2-chlorobenzohydrazide

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Polymorphism is a phenomenon of fundamental importance in solid state chemistry and crystallography, chemical and pharmaceutical industry. The understanding and controlling this process are crucial for crystal engineering and materials chemistry. The existence of different solid forms of the same compound - such as polymorphs, solvates and hydrates, as well as co-crystals - creates both scientific challenges and opportunities. Changes in crystal structure can lead to undesirable, unintended alterations in properties. On the other hand, polymorphism offers excellent possibilities for tuning the physicochemical properties of functional materials and provides a unique opportunity to study structure-property relationship.

The general aim of this study was to search for new polymorphs of biologically active compound from the group of N^1-acylhydrazones, N-[(2-hydroxyphenyl)methylidene]-2-chlorobenzohydrazide. Another goal was to study the molecular and crystal structure of the resulting polymorphs, to establish the main intermolecular interactions and supramolecular synthons, as well as to correlate those data with thermal and thermodynamic stability of the crystals. To achieve this, several crystallization techniques were employed, including: (i) slow solvent evaporation from solution at room temperature, (ii) cooling crystallization, (iii) vapor-diffusion and (iv) antisolvent crystallization, using several organic solvents with different polarities.

The research carried out confirmed the existence of three polymorphic modifications of the compound. In each polymorph, the molecules adopt a similar conformation, but their arrangement in the crystal is slightly different. In turn, the DSC analyses and VT PXRD data revealed the phase transitions between polymorphs.

sciforum-176859: Robust, Safer and More Sustainable Crystallisation of Meloxicam Through Multicriteria Solvent Selection, Real-Time Monitoring and High Throughput Experimentation

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Crystallization is a cornerstone of pharmaceutical manufacturing because it strongly influences product quality attributes.[1] However, identifying suitable crystallization conditions through trial-and-error requires exploring a large design space, substantial time and resources.[2,3] This work presents an integrated methodology combining solvent selection, high-throughput screening, and AI-driven analysis to optimise the crystallization of meloxicam (MLX).

A multicriteria solvent screening approach based on Hansen solubility parameters and Environmental, Health, and Safety criteria was applied to identify suitable solvents for MLX crystallization. This analysis revealed dimethyl sulfoxide (DMSO) as the most promising solvent. Experimental validation was performed using a high-throughput platform equipped with turbidity measurements and high-resolution imaging. AI-based image analysis enabled real-time monitoring of morphological changes during crystallization. These results confirmed DMSO as the most suitable solvent, providing a favourable balance between solubility, controllable supersaturation, induction time, and acceptable EHS performance.

Cooling crystallization of MLX in DMSO, however, produced elongated agglomerated needles with broad size distributions and fouling, while the relatively low slope of the solubility curve limited yield. To overcome these limitations, the methodology was extended to antisolvent crystallization. Water was identified as the most suitable antisolvent, and the DMSO:H2O system was investigated experimentally. Temperature cycling improved crystal habit, transforming needle shaped crystals into more compact quasi equant forms, although some agglomeration remained. The addition of polyvinylpyrrolidone further reduced agglomeration and produced well defined quasi equant crystals with smaller particle size.

Overall, this integrated methodology laid strong foundation for systematic optimisation of the crystallization recipes toward safer and more sustainable pharmaceutical manufacturing and provides a scalable framework for robust pharmaceutical process development.

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sciforum-179455: SolECOs: A Data-Driven Platform for Sustainable Solvent Selection in Single and Binary Crystallization Systems

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Solvent selection plays a critical role in pharmaceutical crystallization, affecting product quality, manufacturability, regulatory compliance, and environmental impacts. With the growing emphasis on sustainability and life cycle assessment (LCA) in regulatory frameworks, solvent design must go beyond thermodynamic considerations to actively incorporate environmental responsibility. However, current practices still heavily rely on expert heuristics and trial-and-error experimentation, which are time-consuming and difficult to scale. Although methods such as Computer-Aided Molecular Design and other commercial tools are available, they often suffer from high complexity, limited usability, and inadequate integration of sustainability metrics. To address these limitations, we developed a hybrid, data-driven framework with two primary goals: (a) to identify green solvents or binary mixtures that meet solubility, sustainability, and uncertainty criteria for a given API; and (b) to provide a user-friendly, computationally efficient platform for pharmaceutical engineers. The framework includes a solubility database of over 60,000 data points across 1,183 solvent systems, integrated with sustainability assessments based on ReCiPe 2016 and the GSK Solvent Sustainability Guide. Machine learning models - including a multi-task polynomial regression network, a temperature-adjusted solubility predictor, and a binary solvent model - were combined with Monte Carlo uncertainty quantification to enable robust solvent recommendation. The entire workflow is encapsulated in SolECOs, an interactive GUI that supports model execution, solubility curve visualization, and dynamic sustainability analysis. A case study on cytarabine demonstrated the platform's value under different cooling profiles and sustainability priorities. The model consistently identified 1,2-dimethylbenzene as a primary solvent, with polar co-solvents like dichloromethane and ethanol enhancing solubility. However, high predicted solubility did not always align with favorable environmental scores, underscoring the need to balance performance and sustainability. Case studies on four APIs, including cytarabine, under varying cooling gradients and sustainability priorities validated the model's accuracy and robustness, further demonstrating SolECOs's ability to support reliable, goal-oriented, and sustainability-aware solvent selection.

Session 7. Crystalline Metals and Alloys

sciforum-177003: Activation-Free Hydrogen Storage in a Nanostructured TiVCrMn Medium-Entropy Alloy Processed by High-Pressure Torsion

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High and medium-entropy alloys are promising candidates for solid-state hydrogen storage; however, their practical implementation remains constrained by demanding activation procedures, limited understanding of long-term cyclic stability, and the necessity for precise microstructural optimization to ensure favorable hydrogen sorption kinetics and reversible storage performance. This study evaluates the effect of microstructure on the hydrogen storage performance of a quaternary, medium-entropy TiVCrMn alloy under moderate pressure and temperature conditions.

Calphad simulations predict a dual-phase BCC + C14 Laves phase microstructure for TiVCrMn below 800 °C. The alloy was produced by arc-melting and characterized by XRD, SEM-EDS, and STEM-EDS, confirming the predicted phase constitution. Disks cut from the as-cast ingot were processed by high-pressure torsion, HPT (5 GPa, 1 rpm, 10 turns), leading to ultrafine microstructures with crystallite sizes of 20-50 nm.

Hydrogenation experiments demonstrated that the HPT process improved the resistance to deactivation. The HPT-processed medium-entropy alloy absorbed 1.6 wt.% hydrogen at 45 °C without requiring any prior activation treatment, exhibiting rapid kinetics (~50 min to reach saturation) and full reversibility in two stages: one at room temperature and the other at 300 °C.

The results indicate that hydrogen absorption occurs predominantly in the BCC phase and that nanostructuring via severe plastic deformation enhances hydrogen uptake and stability against deactivation, highlighting its potential to tailor medium-entropy alloys for hydrogen storage applications.

sciforum-178690: Crystallography and Structural Evolution of Iron Ore Minerals in Banded Iron Formations: Implications for Geometallurgy

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Banded Iron Formations (BIFs) represent one of the most important Precambrian sources of iron ore and consist predominantly of iron oxide minerals such as hematite, magnetite, and goethite, whose crystallographic characteristics significantly influence ore quality and processing behavior. This review synthesizes current knowledge on the crystallography and structural evolution of iron-bearing minerals in BIF-hosted deposits and evaluates their implications for geometallurgical performance. The crystal structures, lattice parameters, and symmetry of hematite, magnetite, and goethite control important physical properties including hardness, density, magnetic behavior, and grain boundary characteristics. Geological processes such as diagenesis, metamorphism, hydrothermal alteration, and supergene enrichment lead to mineral transformations, particularly the conversion of magnetite to hematite and goethite, which modify the crystalline framework and microstructural textures of the ore. These structural modifications influence ore liberation, beneficiation efficiency, and metallurgical performance during processing. The review also highlights the role of crystallographic defects, mineral intergrowths, and trace element substitution in governing the stability and transformation pathways of iron oxide minerals. By integrating mineralogical, crystallographic, and geometallurgical perspectives, this study provides a comprehensive understanding of how structural attributes of BIF minerals affect ore quality and industrial processing. Such insights are essential for improving beneficiation strategies and optimizing the sustainable utilization of iron ore resources.

sciforum-179022: Effect of heterogeneous interfaces on the mechanical characteristic and deformation behavior of metals Bilayers

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This study investigates the nanoindentation response of Ag coating deposited on Cu (111) substrate using molecular dynamics (MD) simulations, with a particular focus on the role of crystallographic orientation and loading conditions. Three different Ag bilayer orientations, namely Ag (100), Ag (110), and Ag (111), are systematically analyzed to evaluate how heterogeneous interfaces affect the deformation mechanisms and mechanical behavior at the nanoscale. The results demonstrate that the Ag (111)/Cu (111) configuration produces a higher indentation force compared to the Ag (100)/Cu (111) and Ag (110)/Cu (111) systems, indicating enhanced resistance to deformation. This behavior is attributed to the lower lattice mismatch and better atomic registry at the Ag (111)/Cu (111) interface, which promotes stronger interfacial bonding and improved load transfer. Furthermore, the influence of indentation velocity is examined for the Ag (111)/Cu (111) bilayer by varying the velocity from 120 m/s to 200 m/s. The simulation results reveal a clear trend of increasing force and hardness with higher indentation velocities, suggesting a strain-rate-dependent strengthening effect. At elevated velocities, limited time for atomic relaxation leads to increased resistance against plastic deformation. Dislocation extraction analysis (DXA) further supports these findings by revealing the nucleation and evolution of dislocations and defects, particularly near the interface region. The density and complexity of dislocation structures increase with both improved interface coherence and higher indentation velocities, providing deeper insight into the fundamental mechanisms governing the mechanical performance of Ag/Cu bilayer systems.

sciforum-176929: Investigation of Crystal Deformation by X-ray Diffraction Method

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Additively manufactured (AM) AlSi10Mg aluminum alloy exhibits highly anisotropic microstructures that depend on process parameters and build orientation design. The process optimization and parts-building orientations influence the mechanical properties of the materials. In this investigation, we studied the influence of build orientation, such as 0°, 60°, and 90° relative to the build platform, on the crystalline deformation mechanisms of AM-processed AlSi10Mg. We used the X-ray diffraction (XRD) method to characterize the Charpy test specimens. The Charpy test is one of the most popular impact experiments that provides a measurement of impact energy absorption behavior and toughness of the tested parts. The XRD experiment provides characteristics build-orientation dependent behavior of the Charpy tested parts. We used the Williamson–Hall method to study the XRD spectrum of the parts produced at different build orientations. Williamson–Hall (WH) method is one of the renowned methods to investigate the stress-strain behavior of crystals. We used three WH methods, which are known as the Uniform deformation model (UDM), the Uniform stress deformation model (USDM), and the Uniform deformation energy density model (UDEDM), for studying the crystal size, lattice stress, and strain. The results demonstrate that XRD is a powerful tool for finding the fundamental relationships between the additive manufacturing process parameters and the resulting crystal lattice integrity. It also provides crucial insights for the process optimization and mechanical performance prediction of AlSi10Mg components. We found that the 0° (horizontal) samples exhibited a different deformation behavior compared to the 60° and 90° (vertical) samples, which correlates with previously reported mechanical anisotropy of the materials.

sciforum-168914: Molecular dynamics analysis of TiNi thin-film growth on a Ni substrate: effect of incident energy and substrate temperature

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TiNi alloy thin films have attracted significant attention in both research and industrial applications owing to their remarkable functional properties. These include the shape memory effect and superelasticity, which originate from the reversible phase transformation between martensite and austenite. In addition, TiNi thin films exhibit excellent corrosion resistance, good biocompatibility, and superior damping capacity. Consequently, the investigation of the physical conditions enabling the achievement of these properties requires a thorough understanding of the production processes of these thin films. At present, experimental characterization techniques alone are not sufficient to fully elucidate the mechanisms governing thin film growth at the nanoscale. Implementing advanced simulation techniques, such as molecular dynamics (MD), offers an effective solution to this issue. In this study, we investigated the atomic-scale growth of TiNi films using MD method. The effects of the incident energy and substrate temperature are explored in details from the atomic scale. The films deposited with an incidence energy of 0.1 eV show a rough morphology due to their low surface mobility. However, as the energy increased from 1 to 15 eV, the morphology became smoother. This is explained by the high mobility of deposited atoms, which inhibits cluster formation on the surface. Increasing the substrate temperature from 300 to 600 K slightly reduces the film roughness. This is due to the enhanced agitation of the atoms, which also promotes the filling of surface voids. The results also show that at energies above 5 eV, at the film-substrate interface, some atoms from the film penetrate the upper layers of the substrate, while some atoms from the substrate are ejected into the film. The average atomic stress was calculated and found to be consistent with the experimental stress values.

sciforum-179289: Optical properties of non-centrosymmetric Th-based superconductors: a density functional theory study

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Non-centrosymmetric superconductors are the subject of intensive study because the lack of an inversion center can lead to mixed spin-singlet and spin-triplet pairing states[1]. Here, we investigate the optical properties with the help of electronic transitions for non-centrosymmetric superconductors based on Th with the stoichiometry Th_7T_3 (T=Fe, Co, Ni) [3-5], which exhibit weak electron correlations. The full potential linear augmented plane wave (FP-LAPW) method was employed, as well as scalar and fully relativistic treatments. The Th_7T_3 compounds crystallize in the hexagonal Th_7Fe_3 -type structure (space group $P6_3mc$) and undergo a superconducting transition at Tc≈2TK. The crystal unit cell contains three inequivalent thorium positions (Th1, Th2 at 6c, Th3 at 2b) and one transition metal position (6c). By replacing the Fe with Co or Co with Ni, one additional electron is added to the system. This substitution of one transition metal atom for another, along with the change in atomic masses and the role of the relativistic effect of the thorium atoms, leads to interesting properties in the electronic and optical structures of the Th_7T_3 compounds. We emphasize the role of the ASOC strength since anisotropic spin splitting, both in the band structure and optical properties emerge when one takes into account the spin-orbit coupling in the calculations. By providing the frequency-independent dielectric function calculations at 2, 10, and 50 K temperatures, we assume that transitions between Th-6d and T-d valence electrons are mainly responsible for the superconducting properties.

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sciforum-178107: Simulation of recrystallization in polycrystalline materials

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The microstructure evolution plays an important role in the process of static recrystallization occurring during heat treatment following plastic deformation. The process is affected by the deformation energy stored in the material and the temperature of the heat treatment of finite duration. Key parameters are the density and spatial distribution of nucleation sites in the initial polycrystalline microstructure. Similarly, key modelling assumptions are the distribution of the moving speed of the recrystallization front, and whether nucleation is site-saturated or continuous.

The simulations are done on three-dimensional rectangular subblocks using the principles of Monte Carlo Potts model. The effect of the previous deformation was defined by the elongated shape of grains in the initial microstructure. The nucleation happens with a defined probability for internal cells, surfaces and edges on the grain boundaries, and triple junctions. Outer surfaces are defined as either periodic or rigid boundary conditions. Continuous nucleation is defined as a constant generation possibility on each unrecrystallized cell over time.

The JMAK (Johnson–Mehl–Avrami–Kolmogorov) theory describes recrystallization kinetics using a shape exponent and a scale parameter. An important result is finding the relation between the coefficients in the general JMAK model, and the parameters of the current simulation with various initial assumptions. Simulations with site-saturated nucleation precisely reproduce the JMAK model with three-dimensional growth, while continuous nucleation causes higher exponents, similarly to the theoretical values.

The developed model can simulate the static recrystallization of the crystalline materials, with a good correlation to measured recrystallization fraction from measured hardnesses. A further aim is taking into consideration the effect of the grain boundary misorientation and the orientations of the grains on the nucleation process.

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