IOCPS 2025 Conference

# The 3rd International Online Conference on Polymer Science

19–21 November 2025 | Online

Program and Abstract Book

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#IOCPS2025

# The 3rd International Online Conference on Polymer Science

# Polymer Science and Technology: When Progress Meets Sustainability and Reliability

**19–21 November 2025 | Online**

MDPI

# Organizing Committee

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Prof. Dr. Giulio Malucelli
Prof. Dr. Francesco Paolo La Mantia

## Session Chairs

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Prof. Dr. Alberto Jiménez Suárez
Prof. Dr. Alessandro Pegoretti
Prof. Dr. Ivan Gitsov
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## Organised by

MDPI

## Conference Secretariat

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# Welcome from the Chairs

You are cordially invited to participate in the **3rd International Online Conference on Polymers Science—Polymer science and technology: when progress meets sustainability and reliability (IOCPS 2025)**, sponsored by the MDPI open access journal ***Polymers*** (ISSN 2073-4360; IF: 4.9). The conference is an opportunity for researchers in polymer science and technology to present their research and exchange ideas with colleagues. This is an online conference, removing the need to travel and eliminating participation expenses while still maintaining a rigorous selection of scientific contributions and, at the same time, ensuring the possibility for visibility for your own research.

The conference will be organized around the following general topics, providing a forum for presenting and discussing new results. Topics of interest include, but are not limited to, the following:

1. Biobased, Biodegradable-compostable, and Recyclable Polymers;
2. Polymer Analysis and Characterization;
3. Recent Functional and Structural Applications of Polymer Systems;
4. Polymer Composites and Nanocomposites;
5. Polymer Physics and Theory.

This will be an online conference held on Sciforum, a platform developed and sponsored by MDPI to organize and provide technical support for online conferences, from 19 to 21 November 2025.

A number of **free live-streaming sessions** will be held during the conference, including talks from invited speakers. These live sessions will also contain a Q&A section to answer questions from a live online audience.

All accepted abstracts and posters will be published in *Proceedings* (ISSN: 2504-3900). Please check the section 'Instructions for Authors' for a detailed description of how to submit your contribution to the conference.

All conference participants will be encouraged to submit a full manuscript to the Special Issue published in Polymers, with a **20% discount** on the article processing charge. Conference Papers submitted to the Special Issue must have been extended by at least 50%, and will undergo the standard peer-review process of the journal.

The best oral presentation and best poster will receive an award of CHF 300.

We look forward to engaging in exciting discussions and hearing new ideas and perspectives from experts in the field. All participants are welcome to attend the online conference.

**Prof. Dr. Giulio Malucelli**

Politecnico di Torino, Department of Applied Science and Technology, Turin, Italy

**Prof. Dr. Francesco Paolo La Mantia**

Università degli Studi di Palermo, Palermo, Italy

*polymers*
an Open Access Journal by MDPI

*Polymers* (ISSN 2073-4360) is an international, open access journal of polymer science. It publishes research papers, communications and review articles. *Polymers* provides an interdisciplinary forum for publishing papers which advance the fields of (i) polymerization methods, (ii) theory, simulation, and modeling, (iii) understanding of new physical phenomena, (iv) advances in characterization techniques, and (v) harnessing of self-assembly and biological strategies for producing complex multifunctional structures. Scientists are encouraged to publish their experimental and theoretical results in as much detail as possible. There is no restriction on the maximum length of the papers. The full experimental and computational details must be provided so that the results can be reproduced.

**Impact Factor:** 4.9 (2024); 5-Year Impact Factor: 5.2 (2024)

# Keynote Speakers

Dr. Juan P. Fernández-Blázquez

**IMDEA Materials Institute, Madrid, Spain**

Juan P. Fernández has broad experience in polymer and polymer composite science, with more than 85 SCI publications, mainly in the relationship between structure/processing and thermomechanical properties of polymers and composites. His career has been developed in four prestige research institutions: Polymer Institute in Spain (ICTP-CSIC) where he developed his PhD dissertation (2006). His first postdoctoral stay was in Florida State University (FSU, USA) in 2008. After that, he joined Max Planck Institute for Polymer Research (MPIP, Germany), where he did a second postdoctoral stay partially funded by the prestigious Alexander von Humboldt Foundation. Finally, in 2011 he joined to IMDEA Materials Institute, where he was awarded by a Marie Curie AMAROUT European Programme. Nowadays, he manages the Thermomechanical Characterization Polymer Lab. Here, his research focuses on the effect of particles, from nano to macro sizes or continuous fibers, has in the main properties of the polymer matrices, from mechanical to thermal and phase transition using advanced characterization techniques.

Dr. Mazeyar Parvinzadeh Gashti

**Department of Chemistry, Pittsburg State University, 1701 South Broadway Street, Pittsburg, KS, USA, National Institute for Materials Advancement, Pittsburg State University, Pittsburg, KS, USA**

Dr. Mazeyar Parvinzadeh Gashti is an assistant Professor in the Department of Chemistry at Pittsburg State University in Kansas, USA. He got his PhD in Textile Chemistry and Fiber Science and undertook three postdoctoral positions at the University of Bern (Switzerland), Laval University, and McGill University (Canada) from 2011 to 2016. Since 2018, he has led several funding projects from the US National Science Foundation", "the US Department of Agriculture", "Innovative Solutions Canada Program", "Innovation for Defense Excellence and Security Program (Canada)", "The Industrial Research Assistance Program (Canada)" and "Build in Canada Innovation Program". Since 2019, he has been a member of the Directory Board of the Canadian Institute of Textile Science. He is currently a member of the editorial boards of several international polymer and material journals, with Clarivate citation index. Dr. Gashti's inclusion in Stanford University's World's Top 2% Scientists list for five consecutive years highlights his substantial contributions to the field.

Dr. Wan Shou

**University of Arkansas, Fayetteville, AR, USA**

Dr. Wan Shou is an assistant professor in the Department of Mechanical Engineering at the University of Arkansas (UArk). Before joining UArk, he was a postdoc at MIT from 2019 to 2021. Dr. Shou received his Ph.D. degree in mechanical engineering from Missouri University of Science and Technology in 2018. His research interests cover advanced materials, innovative manufacturing processes, functional applications, artificial intelligence, and the understanding of materials transformation during manufacturing. He has published over 40 journal articles, including Advanced Materials, Nature Electronics, Science Advances, etc., and has been granted 3 US patents.

Dr. Zlatan Zlatev Denchev

**University of Minho, Engineering School, Department of Polymer Engineering, campus of Azurém, Braga, Portugal**

Zlatan Zlatev Denchev is an Assistant Professor with Habilitation at the Department of Polymer Engineering, Institute for Polymers and Composites, University of Minho, Portugal. He holds a PhD in Polymer Chemistry and Technology and began his career after graduating in Chemical Engineering from the University of Chemical Technologies in Burgas, Bulgaria in 1983. Since 2000, he has been based in Portugal, contributing over 40 years of research in polymer science, including synthesis, advanced characterization, and processing of polymer materials. Dr. Denchev's current expertise spans microfibrillar polymer composites, in-situ polymer nanocomposites, reactive microencapsulation, electro-conductive composites, EMI shielding materials, biocatalysts for green chemistry, and advanced synchrotron WAXS/SAXS techniques. He is the author of over 110 peer-reviewed scientific publications and holds 9 patents. He has delivered more than 80 presentations at international conferences, including 20 invited and 11 keynote lectures. His mentorship includes 6 postdocs, 8 PhD students, and numerous master's and industrial trainees. He has participated in 25 research and industrial projects. Dr. Denchev has over 3,000 citations, an h-index of 30, and an i10-index of 74 (Google Scholar). Since 2022, he has been a corresponding member of the Michael M. Szwarc Polymer Research Institute, State University of New York.

Prof. Dr. Jean-François GANGHOFFER

**LEM3 - CNRS. Université de Lorraine, Metz, France**

Jean-François Ganghoffer currently works at the LEM3- Laboratoire d'études des Microstructures et de Mécanique des Matériaux, University of Lorraine. Jean-François does research in Mechanical Engineering and Biomechanics. His research activities are devoted to the following topics: - Mechanics of generalized continua - Homogenization towards higher order and higher grade media - Flexoelectricity and applications to bone - Bone Biomechanics

# Invited Speakers

**Dr. Andreas Albrecht**
Borealis Polyolefine GmbH, Linz, Austria

**Dr. Patrícia C. Pires**
Faculty of Pharmacy, University of Coimbra, Azinhaga de Santa Comba, Coimbra, Portugal

**Prof. Dr. Ning Ding**
Faculty of Chemistry and Pharmacy, Qilu University of Technology (Shandong Academy of Sciences), Jinan, China

**Dr. Giulia Fredi**
Department of Industrial Engineering and INSTM Research Unit, University of Trento, Via Sommarive 9, 38123 Trento, Italy, Department of Aeronautics and Astronautics, Massachusetts Institute of Technology, 77 Massachusetts Ave, Cambridge, MA 02139, USA

**Dr. Qiang Guo**
University of Colorado Colorado Springs, Boulder, CO, USA

**Prof. Dr. Valentina Siracusa**
Department of Chemical Science (DSC), University of Catania, Catania, Italy

**Dr. Giulia Guidotti**
Department of Civil, Chemical, Environmental, and Materials Engineering, Alma Mater Studiorum - University of Bologna, Bologna, Italy

# Program at a Glance

| | Day 1 | Day 2 | Day 3 |
|---|---|---|---|
| **Morning** | **S1.** Biobased, Biodegradable-compostable, and Recyclable Polymers | **S5.** Polymer Physics and Theory | **S4.** Polymer Composites and Nanocomposites |
| **Afternoon** | **S1.** Biobased, Biodegradable-compostable, and Recyclable Polymers | **S2.** Polymer Analysis and Characterisation | **Parallel Sessions ①**<br>**S4.** Polymer Composites and Nanocomposites<br>**Parallel Sessions ②**<br>**S3.** Recent Functional and Structural Applications of Polymer Systems |

# IOCPS 2025 Program

## 19th November 2025 (Wednesday)

### *Session 1. Biobased, Biodegradable-compostable, and Recyclable Polymers*

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

| CET Time | Speaker | Title |
|---|---|---|
| 9:00–9:10 | *Conference Opening Ceremony*<br>*Prof. Dr. Giulio Malucelli & Prof. Dr. Francesco Paolo La Mantia* | |
| 9:10–9:20 | *Welcome from the Session Host*<br>*Dr. Giulia Guidotti* | |
| 9:20–9:40 | **Dr. Giulia Guidotti**<br>Invited Speaker | Sustainable formulations made of a furan-based copolyester and nisin for flexible antimicrobial packaging applications |
| 9:40–9:55 | **Vinícius de Paula**<br>Selected Speaker | Selective ABS dissolution with eutectic solvents: toward greener recycling |
| 9:55–10:10 | **Simão Vidinha Pandeirada**<br>Selected Speaker | Recycling PET with PEF traces by eutectic solvent-assisted depolymerization: Experimental and DFT Insights |
| 10:10–10:25 | **Antonio Barbato**<br>Selected Speaker | Processing and properties of novel PBS/PVOH-based films for sustainable food packaging applications |
| 10:25–10:40 | **Feriel Abid**<br>Selected Speaker | Sustainable Polyesters via Ring-Opening Polymerization of Biobased (Macro)Cyclic Oligofuranoates and their subsequent cyclodepolymerization |
| 10:40–10:55 | **Javiera Sepúlveda-Carter**<br>Selected Speaker | Assessment of Reprocessed Polylactic Acid from Controlled Virgin Feedstock for Food Packaging Applications |
| 10:55–11:10 | **Anna Marín**<br>Selected Speaker | Blue meets green: Marine bacteria and biomass residues in sustainable polyhydroxyalkanoates synthesis |
| 11:10–11:25 | **Sergi González Zaragozá**<br>Selected Speaker | Effects of long exposure to dielectric barrier discharge on commercial blend films of poly(butylene adipate-co-terephthalate) (PBAT) and thermoplastic starch (TPS) |

### *Session 1. Biobased, Biodegradable-compostable, and Recyclable Polymers*

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

| CET Time | Speaker | Title |
|---|---|---|
| 14:00–14:10 | *Welcome from the Session Chair*<br>*Prof. Dr. Valentina Siracusa* | |
| 14:10–14:30 | **Prof. Dr. Valentina Siracusa**<br>Invited Speaker | Characterization of Bio-based aliphatic/aromatic poly(trimethylene furanoate/sebacate) random copolymers under stressed treatments |
| 14:30–14:45 | **Miruna Bodo**<br>Selected Speaker | New Powder Polymer For 100% Bio-based Cosmetic Formulations |
| 14:45–15:00 | **Maria-Beatrice Coltelli**<br>Selected Speaker | Protecting perishable food by using renewable and biodegradable polyester films |
| 15:00–15:15 | **Manar Azzi**<br>Selected Speaker | Biopolymer Production from Tenebrio molitor Farming Waste: A Circular Approach to Chitin and Chitosan Extraction |
| 15:15–15:30 | **Rinky Ghosh**<br>Selected Speaker | Development of Sustainable Packaging with Enhanced Properties: Utilizing Coffee Waste-Derived Plasticizer, Eggshells, and Natural Rubber in PHBV Bioplastic Blends |
| 15:30–15:45 | **Ingridy Dayane Silva**<br>Selected Speaker | Ecological PLA/PBAT-g-GMA Nanocomposites Reinforced with Carbon Nanotubes for Electrostatic |

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|---|---|---|
| | | Charge Control: Evolution of Morphology, Electrical Conductivity and Mechanical Properties |
| | Flash Poster Session | |
| 15:45–15:50 | **Shiwei Feng**<br>Selected Poster Presenter | Synthesis, thermal, mechanical, and hydrolysis properties of poly(hexamethylene furandicarboxylate)-based copolyesters |
| 15:50–15:55 | **Ilona Krabicova**<br>Selected Poster Presenter | From milk to 3D printing: A sustainable journey of upcycled proteins |
| 15:55–16:00 | **Alejandro Funes-López**<br>Selected Poster Presenter | Bio-Based Copolymers with Tunable Cationic Charge Densities for Antimicrobial Applications |
| 16:00–16:05 | **Erika Indovino**<br>Selected Poster Presenter | Valorization of Waste Fishing Nets: Mechanical Recycling and Characterization of Recycled/ Virgin Blends |
| 16:05–16:10 | **Evangelia Tarani**<br>Selected Poster Presenter | Structural, Thermal, and Morphological Characterization of Biobased Wheat Straws as Sustainable Alternatives to Single-Use Plastics |
| 16:10–16:15 | **Nasrin Moshfeghi Far**<br>Selected Poster Presenter | Fabrication of CA/CS Composite Films by Solution Blow Spinning Method for Food Packaging Application |
| 16:15–16:20 | **Anna Jáuregui Esteve**<br>Selected Poster Presenter | From Shore to Seafloor: A Multisite Mediterranean Study on Plastic Biodegradation |
| 16:20–16:25 | **Rosa Barranco García**<br>Selected Poster Presenter | Development of Sustainable Antimicrobial Cellulose Additives for Melt Electrowritten PLA Fibers: From Synthesis to Extensional Rheology |
| 16:25–16:30 | **Natalia Kołcz**<br>Selected Poster Presenter | Abiotic surface degradation induced by ozonation on poly (lactic acid) (PLA)/poly (butylene adipate-co-terephthalate) (PBAT) blends |

## 20th November 2025 (Thursday)

### Session 5. Polymer Physics and Theory

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

| CET Time | Speaker | Title |
|---|---|---|
| 9:00–9:10 | *Welcome from the Session Chair*<br>*Prof. Dr. Fahmi Zaïri* | |
| 9:10–9:40 | **Prof. Dr. Jean-François Ganghoffer**<br>Keynote Speaker | Void growth in swelled porous polymeric gels |
| 9:40–10:00 | **Prof. Dr. Ning Ding**<br>Invited Speaker | Effect of hyperbranched epoxy resin grafting on the interfacial and mechanical properties of carbon fiber/epoxy resin composites |
| 10:00–10:20 | **Dr. Qiang Guo**<br>Invited Speaker | Experimental and Computational Studies on Fracture of Liquid Crystal Elastomers |
| 10:20–10:35 | **Ugo Cachot**<br>Selected Speaker | Physically Based Modeling of Anisotropic and History-Dependent Behavior in Multi-Network Polymers |
| 10:35–10:50 | **Karim Kandil**<br>Selected Speaker | Bioinspired Lattice-based prostheses: A New Approach for Accurately Mimicking Multiaxial Mechanics of Intervertebral Discs |
| 10:50–11:05 | **Lionel Ogouari**<br>Selected Speaker | Physically Based Modeling of Anisotropic and History-Dependent Behavior in Multi-Network Polymers |
| 11:05–11:20 | **Pınar Güloğlu**<br>Selected Speaker | Ultrafast Excited-State Dynamics and Aggregation Behavior of 2,5-Bis(2,2':6',2"-Terpyridine-4'-yl)-Thieno[3,2-b]Thiophene: Experimental and DFT Study |
| 11:20–11:35 | **Michele Pierigé**<br>Selected Speaker | Natural and Petroleum-Based Resins: Impact on SBR Dynamics by Solid-State NMR Spectroscopy and Relaxometry |

### Session 2. Polymer Analysis and Characterisation

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

| CET Time | Speaker | Title |
|---|---|---|
| 14:00–14:10 | *Welcome from the Session Chair*<br>*Prof. Dr. Ivan Gitsov* | |
| 14:10–14:40 | **Dr. Zlatan Zlatev Denchev**<br>Keynote Speaker | Synchrotron X-ray Scattering as a Tool for Probing the Nanostructure of Complex Polymer Systems |
| 14:40–15:00 | **Dr. Andreas Albrecht**<br>Invited Speaker | Understanding changes in the microstructure during reactive extrusion and their impact on melt properties |
| 15:00–15:15 | **Catarina Araújo**<br>Selected Speaker | Crystal Clear: A Bottom-Up Strategy for Polymer Structure Determination Using Vibrational Spectroscopy |
| 15:15–15:30 | **Lorenzo Antonio Picos Corrales**<br>Selected Speaker | Easy surfactant-free microemulsions and drawings of their particle size distributions from light microscopy images |
| 15:30–15:45 | **Chiara Gnoffo**<br>Selected Speaker | The interplay between cross-contamination, aging and reprocessing in the mechanical recycling of HDPE-based packaging |
| 15:45–16:00 | **Ignacio José Pisa Ripoll**<br>Selected Speaker | Design of Safe and Sustainable Hyperbranched Polyesters as Additives for PHAs |
| 16:00–16:15 | **Michaila Akathi Pantelaiou**<br>Selected Speaker | pH- and thermoresponsive amphiphilic terpolymers: Synthesis and formulation of drug-loaded nanomicelles |
| Flash Poster Session | | |
| 16:15–16:20 | **Ruogu Tang**<br>Selected Poster Presenter | Mathematical Modeling, Derivation, and Analysis of Polymer Transportation in Extrusion Molding |
| 16:20–16:25 | **Anna Słubik**<br>Selected Poster Presenter | Preparation and characterization of carrageenan/gelatin microcapsules with the addition of essential oil |
| 16:25–16:30 | **Rossella Arrigo**<br>Selected Poster Presenter | A design-driven strategy for the development of polypropylene composites tailored for 3D printing |
| 16:30–16:35 | **Wiktoria Patz** | Ionogels Containing EMImFSI Obtained via |

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|---|---|---|
| | Selected Poster Presenter | Photopolymerization: Tailoring Mechanical and Electrochemical Properties for Flexible Energy Storage Devices |
| 16:35–16:40 | **Larisa Titire**<br>Selected Poster Presenter | Influence of boundary conditions and impact velocity on the ballistic behavior of aramid fabrics |

## 21th November 2025 (Friday)

### Session 4. Polymer Composites and Nanocomposites

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

| CET Time | Speaker | Title |
|---|---|---|
| 9:00–9:10 | *Welcome from the Session Chair*<br>*Prof. Dr. Vladimir P. Fedin* | |
| 9:10–9:40 | **Dr. Juan P. Fernández-Blázquez**<br>Keynote Speaker | Relationships among structure/processing/morphology of polymer and polymer composites processed by Additive Manufacturing. |
| 9:40–9:55 | **Simón Faba**<br>Selected Speaker | Development of plasticized PLA and reprocessed PLA films with eggshell waste-based fillers for sustainable packaging |
| 9:55–10:10 | **Camilla Noè**<br>Selected Speaker | Humidity-Responsive Conductive Hydrogels: A Bio-Based Material for Flexible Electronics |
| 10:10–10:25 | **Paulo Roque Novoa**<br>Selected Speaker | Manufacturing Hybrid Jute/Glass Fiber Laminates by Leveraging Prepreg Resin Bleed |
| 10:25–10:40 | **Sarai Agustin-Salazar**<br>Selected Speaker | Valorization of Pecan Nutshell for the Design of Sustainable Polymeric Materials |
| 10:40–10:55 | **Francesca Sacchi**<br>Selected Speaker | Three-Dimensional Printing of Acrylate Epoxidized Soybean Oil (AESO)-Based Composites Containing Bamboo |
| 10:55–11:10 | **Giuseppe Trapani**<br>Selected Speaker | Nanostructured Flame Retardant Coatings Containing Layered Double Hydroxides |
| 11:10–11:25 | **Giuseppe Greco**<br>Selected Speaker | Development of Exfoliated Graphene-PEDOT:PSS Nanocomposites for High-Performance Supercapacitor Electrodes |

### Parallel Session ①

### Session 4. Polymer Composites and Nanocomposite

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

| CET Time | Speaker | Title |
|---|---|---|
| 14:00–14:10 | *Welcome from the Session Host*<br>*Dr. Giulia Fredi* | |
| 14:10–14:30 | **Dr. Giulia Fredi**<br>Invited Speaker | Nanoconfinement of phase change materials in aligned carbon nanotube arrays |
| 14:30–14:45 | **Kornilia Tsakiri**<br>Selected Speaker | Development of an advanced biopolymer patch for skin tissue regeneration |
| 14:45–15:00 | **Giovanna Colucci**<br>Selected Speaker | Additive Manufacturing of Wood-Based Polymer Composites Fabricated Using vat Photopolymerization For Design Applications |
| 15:00–15:15 | **Oana Dumbrava**<br>Selected Speaker | A new approach for the development of antimicrobial coatings based on functionalized polysulfone |
| 15:15–15:30 | **Josué David Hernández-Varela**<br>Selected Speaker | Green Fabrication of Hydrophobically Functionalized Cellulose Nanomaterials via Citric Acid-Assisted Wet Ball Milling with N-Alkanals |
| 15:30–15:45 | **Gloria Anna Carallo**<br>Selected Speaker | A sustainable path for composite tooling: novel materials, design, and technologies through FEM and LCA |
| 15:45–16:00 | **Abraham Balam**<br>Selected Speaker | Electrical sensing of vibrations using smart carbon-based polymer composites |
| Flash Poster Session | | |
| 16:00–16:05 | **Erika Alessia Di Liberto**<br>Selected Poster Presenter | Sustainable composites based on bioplastics and hydrothermally carbonized wood waste |
| 16:05–16:10 | **Defu Li**<br>Selected Poster Presenter | Ballistic ion transport through hierarchically-ordered-structure polymer binder |
| 16:10–16:15 | **Pramod Manikant Gurave**<br>Selected Poster Presenter | Multifunctional Nanocomposite Fibrous Architectures for Oil/Water Separation and Sorption |

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|---|---|---|
| 16:15–16:20 | **Fariha Sehar**<br>Selected Poster Presenter | Monofilament melt spinning of PET-based antimicrobial composite fibers with hybrid fillers |
| 16:20–16:25 | **Maofan Zhou**<br>Selected Poster Presenter | Interface engineering between poly(lactic acid) and graphitic carbon nitride |
| 16:25–16:30 | **Andreea Laura Chibac-Scutaru**<br>Selected Poster Presenter | Designing bio-based photocatalytic platforms: from cellulose hybrids to aerogel-supported systems |
| 16:30–16:35 | **Davide Palamara**<br>Selected Poster Presenter | Hydrothermal Aging of SAPO-34/Nexar Composite Coatings for Thermal Energy Storage |
| 16:35–16:40 | **Roberto Cárdenas Zapata**<br>Selected Poster Presenter | Biocomposites of Polylactic Acid (PLA)/Cellulose to Generate Value-Added Products |
| 16:40–16:45 | **Erica Gea Rodi**<br>Selected Poster Presenter | Green Composites from Recycled Polypropylene and Hazelnut Shell Flour for Irrigation Systems Application |

## *Parallel Session ②*

## *Session3. Recent Functional and Structural Applications of Polymer Systems*

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

| CET Time | Speaker | Title |
|---|---|---|
| 14:00–14:10 | *Welcome from the Session Host* | |
| 14:10–14:25 | **Giulia Bernagozzi**<br>Selected Speaker | Investigating the effects of mechanical recycling on the flame retardancy properties of polypropylene-based composites |
| 14:25–14:40 | **Praveenkumar Pandurangan**<br>Selected Speaker | Design and synthesis of tailored organic units capable of acting as mechanophores<br>for advanced polymeric materials |
| 14:40–14:55 | **Mario Milazzo**<br>Selected Speaker | Development of poly(3,4-ethylenedioxythiophene) polystyrene sulfonate/Triton X-100-conductive hydrogels for bioelectronic applications |
| 14:55–15:10 | **Gorka Marco-Velasco**<br>Selected Speaker | Cellulose-driven supported liquid membranes with (choline chloride)-based deep eutectic solvents for CO2 separation from biogas. |
| 15: 10–15:25 | **Andreia Silva Fernandes**<br>Selected Speaker | Exploring the Potential of Alpha-Glucan-Enriched Mushroom Extracts as Functional Natural Polymers for Wound-Healing Applications |
| 15:25–15:40 | **Maxime Roux**<br>Selected Speaker | High-Performance Thermoplastic/Thermoset Blends: Strategies, Challenges, and Perspectives for Advanced Structural Applications |
| Flash poster Session | | |
| 15:40–15:45 | **Yadu Ram Panthi**<br>Selected Poster Presenter | AI-Driven Development of Carbazole-Functionalized Memristors: Unlocking Resistive Memory and Synapse-Mimicking Functionality for Next-Gen Computing. |
| 15:45–15:50 | **Roberto Grosso**<br>Selected Poster Presenter | Design and Characterization of Hybrid Hydrogel Architectures Based on Agarose and Functional Copolymers |
| 15:50–15:55 | **Pegah Hajivand**<br>Selected Poster Presenter | MOF-based Cellulose Acetate MMMs For an Advanced Propene/Propane Separation |
| 15:55–16:00 | **Ioannis Pispas**<br>Selected Poster Presenter | Self-assembled polysaccharide-based multilayer nanofilms of xanthan gum and diethylaminoethyl dextran on gold substrate and their interaction with model biomacromolecules |
| 16:00–16:05 | **Álvaro Torrecillas-Cortés**<br>Selected Poster Presenter | Comparative evaluation of chitosan-based hydrogels in the improvement of agronomic properties |
| 16:05–16:35 | **Dr. Wan Shou**<br>Keynote Speaker | AI-driven photopolymer discovery and digital composite design for 3D printing |
| 16:35–17:05 | **Dr. Mazeyar Parvinzadeh Gashti**<br>Session Chair & Keynote Speaker | Emerging Industrial Demands: Innovations and Opportunities in Polymer Chemistry |
| 17:05–17:15 | *Conference Closing Ceremony*<br>*Prof. Dr. Giulio Malucelli & Prof. Dr. Francesco Paolo La Mantia* | |

# Session 1. Biobased, Biodegradable-compostable, and Recyclable Polymers

# sciforum-139351: Biopolymer Production from Tenebrio molitor Farming Waste: A Circular Approach to Chitin and Chitosan Extraction

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This study presents a circular valorization strategy for *Tenebrio molitor* (TM) farming residues through the production of high value biopolymers : chitin and chitosan. All insect farming waste streams, including larval and adult residues, were subjected to an optimized extraction protocol. An initial process (P1) was developed to recover chitin from both exuviae and adult cuticle. However, spectroscopic and morphological characterizations revealed the presence of lipid residues in the extracted chitin particularly in larval materials affecting its physicochemical integrity. A delipidation step was therefore introduced to purify the material and obtain α-chitin of higher structural quality. Building on these findings, an improved and simplified protocol (P2) was developed to enable more efficient recovery. This process allowed the extraction of pure, delipidated, and highly deproteinized α-chitin, closely resembling the native structure. Chitin yields ranged from 27.0% to 27.5% for the two larval exuviae stages and reached 30.0% for the adult residues. The extracted biopolymers were then converted into chitosan by N-deacetylation using Kurita's and Broussignac's methods, resulting in highly deacetylated chitosan (2% ≤ DA ≤ 12%) with controlled viscometric molar masses (Mv). Comprehensive structural and physicochemical characterizations were performed using FTIR, XRD, SEM, $^{1}$H NMR, and viscosimetry. These analyses confirmed the purity, molecular integrity, and functionality of the obtained biopolymers.Due to their versatile chemical and biological properties, these materials hold strong potential for applications in cosmetics, biomedicine, and wastewater treatment supporting a sustainable circular bioeconomy.

# sciforum-138456: Effects of long exposure to dielectric barrier discharge on commercial blend films of poly(butylene adipate-co-terephthalate) (PBAT) and thermoplastic starch (TPS)

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**Introduction**

The rising demand for biodegradable materials has driven the development of biopolymers such as PBAT/TPS blends, making it essential to assess their stability and performance in different environments. Physical treatments such as non-thermal plasma (NTP) may generate reactive oxygen species (ROS) and induce accelerated surface and bulk modifications. This work aims to evaluate the consequences induced by NTP dielectric barrier discharge (DBD) on commercial films of PBAT-TPS.

**Methods**

Commercial PBAT/TPS films were exposed to non-thermal plasma generated by dielectric barrier discharge (NTP-DBD) by an Eltech Engineers Lab Corona Treater (Dahisar, Mumbai). The system operates in air atmosphere using a generator with a nominal power of up to 500 W, frequency of 30 kHz, and an output current of 1.9 A. Films of 100 µm thickness were exposed to irradiation power from 10 to 60 min. Analytical characterisation included colorimetry, FTIR, SEM and DSC to analyse both the bulk and surface modifications.

**Results and Discussion**

Abiotic degradation induced by NTP-DBD provoked significant variations observed in colorimetry results, particularly an increase in yellowing with treatment duration. Chemical structure analyses revealed a progressive reduction in the absorbance bands at 1268 $cm^{-1}$ and 1709 $cm^{-1}$, corresponding to C–O and C=O stretching vibrations of ester groups in PBAT, indicating ester bond degradation. A decrease in the melting endotherm associated with butylene terephthalate (BT) segments, along with a shift in the melting transition to butylene adipate (BA) phase, was observed with increasing exposure time. Finally, surface electron micrographs demonstrated surface etching after 30 and 60 min of plasma treatment, attributed to the interaction between ROS and the polymer surface.

**Conclusion**

NTP-DBD was demonstrated to promote relevant abiotic degradation of PBAT-TPS-based commercial films, with notable modifications not only at the macroscopic level but also at the molecular scale.

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# sciforum-139065: Development of Sustainable Antimicrobial Cellulose Additives for Melt Electrowritten PLA Fibers: From Synthesis to Extensional Rheology

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Addressing the dual challenges of plastic sustainability and antibiotic resistance, this work develops cationic cellulose nanocrystals (CNCs) with potent inherent antimicrobial activity. Functionalization of CNCs with triazole-imidazolium groups (**CNC-TrMI**) achieved a 56% degree of substitution, confirmed by ssNMR and elemental analysis. **The resulting CNC-TrMI** exhibited exceptional biocidal efficacy (>99.99% reduction) against both Gram-positive (*Staphylococcus epidermidis*) and Gram-negative (*Pseudomonas aeruginosa*) bacteria, surpassing methylimidazolium-modified CNC (**CNC-MI**) in efficacy against Gram-negative strains. While modifications reduced crystallinity (81% → 45%) and thermal stability (193 °C ≤ d5% ≤270 °C), CNC-TrMI's retained thermal profile enables polymer processing.

**The ultimate objective** is to integrate these CNCs as sustainable antimicrobial agents into biobased poly(lactic acid) (**PLA**) matrices for processing via melt electrowriting (**MEW**). To achieve this, capillary rheology was first employed to screen and select the optimal PLA matrix among variants with differing D-isomer content. **This** rheological analysis directly correlates the uniaxial extensional viscoelastic response of PLA with its MEW processability, enabling reliable fabrication of biobased fibers **and the subsequent** incorporation of antimicrobial agents.

The synergy of CNC-TrMI's non-leaching antimicrobial action (>4-log reduction), PLA's biodegradability, and MEW's precision patterning offers a sustainable platform for advanced biomedical textiles (e.g., wound dressings) and active packaging. **Overall, this** approach demonstrates how fundamental rheology guides the reliable integration of functional biobased additives into advanced manufacturing processes, supporting circular economy principles.

# sciforum-146970: Electrospinning with green solvents: overcoming constraints while tailoring nanofibrous structures

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The production of nanofibrous membranes through electrospinning has traditionally relied on highly effective organic solvents such as dimethylformamide (DMF), chloroform (CHL), and dichloromethane (DCM). Despite their efficiency in dissolving polymers and ensuring processability, these solvents are toxic and potentially carcinogenic, raising serious concerns for both human health and the environment. This long standing technical scientific lock-in has restricted the widespread adoption of sustainable alternatives and hindered the development of safer nanostructured materials for biomedical and environmental applications.

In this work, we demonstrate the complete replacement of hazardous solvents with low toxicity systems, including acetone, acetone/ethanol, and acetone/water mixtures, all fully compliant with current EU regulations. Morphological analyses performed on polycaprolactone (PCL) and polylactic acid (PLA) nanofibrous membranes reveal that green solvent systems not only allow the preservation of standard electrospinning parameters but also enable the generation of a wide range of fibrous morphologies from bead-only to beads-on-string and fully continuous fibers. Importantly, this structural versatility highlights the ability to modulate fiber size and surface features without requiring disruptive changes in the processing setup.

Overall, the findings demonstrate that the transition to green solvent systems effectively overcomes the constraints imposed by traditional toxic solvents. By enabling fine morphological control and expanding application versatility, this approach paves the way for the design of nanostructures that are not only high-performing but also safe, environmentally sustainable, and aligned with the growing demand for greener technologies in advanced material science.

# sciforum-127317: Optimizing polymer biodegradation: the role of polyol-based biosolvents in laccase activity

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Synthetic water-soluble polymers, such as poly(vinyl alcohol) (PVA), are widely used in various applications due to their ability to dissolve in water and their functional properties. However, their environmental impact is a growing concern, as PVA and similar polymers exhibit limited biodegradability under natural conditions, leading to persistence in aquatic environments and potential accumulation in ecosystems. Although certain microorganisms can degrade PVA, this process often requires specialized enzymes, such as pyrroloquinoline quinone (PQQ)-dependent dehydrogenases, which limits the efficiency and scalability of microbial degradation. Enzymatic degradation represents a promising and sustainable alternative for addressing the environmental persistence of aqueous soluble polymers. However, a high efficiency and applicability of such enzymatic processes remains a key challenge. This study explores the use of polyol-based biosolvents to improve the catalytic efficiency of laccase, an oxidoreductase enzyme. Laccase performance was evaluated in biosolvents with varying carbon chain lengths and hydroxyl group content. Among the tested solvents, widely abundant glycerol notably increased enzyme efficiency. These findings highlight the promising role of biosolvents in optimizing laccase-driven polymer biodegradation, paving the way for more effective and sustainable approaches to polyolefin and plastic waste management. Ongoing research is focusing on refining these enzymatic systems to maximize degradation of PVA under eco-friendly conditions.

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# sciforum-138429: Recyclable, degradable and high-performance bio-based vinylogous urethane vitrimers

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Citric acid is a widely distributed biobased monomer, and its polyfunctionality makes its derivatives a potential choice as crosslinker for thermosets. The utilization of bio-based precursors to prepare polymers is very beneficial for environmental protection and sustainable development. However, thermosets usually lack reprocessability and recyclability due to their permanent chemical cross-linking. To achieve sustainable recycling, design and modification of citric acid as a precursor for vitrimer is a promising strategy. In this work, we synthesized a new cross-linker that incorporated acetoacetate groups onto citric acid and performed the synthesis and evaluation of citric acid-based vitrimers. A series of bio-based vitrimers with different dynamic bond contents were prepared by adjusting the ratio of the reactants and their properties were characterized. The process adopted melt polymerization without additional catalyst, which was green and environmentally friendly and avoided the problem of catalyst escape or decomposition during reprocessing. The incorporation of the amide segment enhanced the mechanical properties and the thermal stability, whereas vinyl urethane bonds provided reprocessability, degradability, and self-healing capabilities. At the same time, it was physically and chemically recycled and showed excellent stability in terms of chemical structure and physical properties. Chemical recycling by acid-catalyzed degradation also provides a route for monomer recovery.

# sciforum-127899: Recycling PET with PEF traces by a eutectic solvent-assisted depolymerization: Experimental and DFT Insights

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The global reliance on plastics has driven significant economic growth, with production surpassing 400 million tons in 2022 [1]. Yet, only around 15% of plastic waste is currently recycled [2] and among polyesters, poly(ethylene terephthalate) (PET) is the most widely recycled. However, the imminent commercialization of poly(ethylene 2,5-furandicarboxylate) (PEF), a bio-based PET alternative, raises concerns about its impact on existing PET recycling streams due to structural similarities and potential co-occurrence.

In this study, we present a greener chemical recycling strategy for PET containing residual amounts of PEF (2%, 5%, and 10%) using a eutectic solvent (ES) system composed of urea and zinc acetate as a catalyst. This work reports, for the first time, the structural and thermal characterization of the resulting copolymers (rPET-co-PEF). The recycled materials exhibited structural and thermal properties comparable to virgin PET, suggesting negligible interference from PEF residues in PET's recycling.

Additionally, the depolymerization mechanism was investigated through density functional theory (DFT) calculations by using Gaussian software. The results indicate that hydrogen bonding interactions between urea alongside zinc coordination with ester groups, significantly reduce the activation energy of the reaction. These findings confirm the catalytic efficiency of the urea-based ES and support its wider application as a sustainable solution for mixed polyester waste recycling.

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# sciforum-136773: Sustainable Polyesters via Ring-Opening Polymerization of Biobased (Macro)Cyclic Oligofuranoates and their subsequent cyclodepolymerization

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The growing concerns about the extensive use of polymers and their environmental impact have driven research into developing renewable resource-based alternatives, such as those derived from furan building blocks. Beyond the biobased origin of monomers, adopting more ecofriendly polymer synthesis strategies is critical for addressing green chemistry principles. Ring-Opening Polymerization (ROP) of cyclic esters emerges as a greener approach, offering advantages such as atom economy and milder reaction conditions compared to conventional bulk polyesterification approach [1]. In this study, the synergy between ROP as a green synthesis pathway and the biobased furanic building blocks was explored. Specifically, furanic macrocycles, macrocyclic hexamethylene 2,5-furandicarboxylate (CHF), were obtained through cyclodepolymerization of the corresponding low-molecular-weight linear polyester species under high-dilution conditions. The ROP of these macrocycles was systematically investigated under various reaction conditions to produce high-molecular-weight polyesters which were characterized in-depth by 1H-NMR, FTIR, viscosimetry, XRD, DSC, ATG and DMTA methods. As part of the end-of-life strategy of these polymers, they were subjected to cyclodepolymerization under high-dilution conditions to regenerate the original macrocycles. This approach demonstrates a potential pathway for polymer recyclability, aligning with the principles of sustainability and circular economy. The regenerated macrocycles were then characterized to confirm their structural integrity and suitability for reuse in further repolymerization processes.

# sciforum-127315: Towards a greener future: using COSMO-RS to select eutectic solvents for complex polymer mixtures recycling

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Global production of synthetic polymers now exceeds 400 million tons annually, yet limited recycling efforts are projected to result in 12,000 million tons of plastic waste in landfills by 2050. mong the various recycling approaches, dissolution/precipitation methods offer promising potential, particularly for complex, hard-to-recycle polymer mixtures. Despite this, these methods are often overlooked and commonly rely on traditional organic solvents. Eutectic solvents (ES) represent a promising, greener alternative, though their development is complicated by the vast diversity of potential hydrogen bond acceptors (HBA) and donors (HBD).

This study leverages the COnductor-like Screening MOdel for Realistic Solvents (COSMO-RS) to identify selective and effective ES for dissolving complex mixtures of fossil-based polymers-such as polyethylene (PE), poly(ethylene terephthalate) (PET), polypropylene (PP), and poly(vinyl chloride) (PVC)-as well as commercial bio-based polymers like poly(lactic acid) (PLA). Using COSMO-RS, infinite dilution activity coefficients were calculated for 40 HBA and 59 HBD, generating 2,360 ES at 100 °C. These predictions were validated with experimental solubilization tests.

Results indicate hydrophobic ES with long-chain alcohols effectively dissolve PE and PP, while ES with phenolic monoterpenes dissolve PET and PLA efficiently. Overall, this work highlights the critical role of rational ES selection in advancing sustainable recycling processes for complex polymer mixtures as for multilayer films.

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# sciforum-147530: Utilization of Aromatic Spent from Essential Oil Industry for Production of Biodegradable Packaging Films

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Aromatic spent, a low-value industrial byproduct generated during the processing of essential oils, is typically discarded or utilized in low-end applications such as mulch, animal fodder, incense sticks, soaps, mosquito repellents, cosmetics, and as raw material in paper and particle board manufacturing. However, this biomass is an excellent source of cellulose—a component that remains largely underutilized. In this study, an effort was made to extract cellulose from lemongrass spent for the development of biodegradable films, offering a sustainable alternative to petrochemical-based packaging materials, which are known to harm the environment. The process began with a series of unit operations, including the size reduction, cleaning, drying, grinding, and sieving of the spent material. Chemical treatments involving alkaline and acid solutions, followed by bleaching, were employed to remove lignin and hemicellulose, thereby isolating purified cellulose. This purified cellulose was then subjected to acid hydrolysis to obtain cellulose nanocrystals (CNCs). The CNCs were incorporated into a film-forming solution consisting of chitosan and glycerol in optimized proportions. The mixture was homogenized and solvent-cast onto a 300×300 $mm^2$ polypropylene sheet. Upon drying at ambient conditions, transparent films of 42 microns were obtained. To evaluate the biodegradability of the developed CNC–chitosan–glycerol films, soil burial tests were conducted. Results showed approximately 70% degradation within 15 days, demonstrating their eco-friendly nature. The nano-scale dimensions of the cellulose nanocrystals were confirmed using Atomic Force Microscopy (AFM) and Scanning Electron Microscopy (SEM). Additionally, SEM analysis of the films was performed to check for any agglomeration of CNCs within the polymeric matrix. This study highlights the potential of aromatic spent as a sustainable resource for developing biodegradable packaging materials, contributing to environmental conservation and waste valorization.

# sciforum-138507: Abiotic surface degradation induced by ozonation on poly (lactic acid) (PLA)/poly (butylene adipate-co-terephthalate) (PBAT) blends

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Biopolymers have emerged as sustainable alternatives to conventional plastics, showing advantages like biocompatibility, biodegradability, and non-toxicity [1]. Nevertheless, their aging processes under service life conditions still need a deeper evaluation [2], [3]. This study examined films of three commercial compositions for rigid/flexible packaging based on poly (lactic acid) (PLA)/poly (butylene adipate-co-terephthalate) (PBAT) blends under oxidative degradation conditions.

Commercial PLA/PBAT films, of 100 µm thickness, were exposed to short- (0 - 2 h) and long-term ozone aging (24 - 96 h) in an Anseros SIM 6050 T chamber at 40 °C and 300 pphm of ozone concentration. Analytical characterisation included measurements for surface hydrophilicity (WCA), microscopic morphology (SEM), chemical structure (FTIR-ATR), thermal properties (DSC), and mechanical performance.

Ozonation caused significant variations in surface properties after long-term ozone treatment, demonstrated by a constant decrease in WCA. A 96 h treatment led to abiotic degradation revealed by chemical structure analysis, where carbonyl and carboxyl indices were reduced by 17% and 16%, indicating degradation of oxidised functional groups and products, along with mild chain scission. Surface morphology showed surface changes with initial oxidation, reinforcement and re-degradation tendencies. These changes were limited to surface modifications, as slight bulk changes were reported in thermal properties. Mechanical performance improved, with the aging factor increasing from 0.5 to 0.9 to 1.14 - 1.30, suggesting that structural stability was maintained. Phase distribution within the polymer matrix influenced the extent of abiotic degradation. The progressive increase in additives such as plasticisers and inorganic fillers likely buffered the effects of ozone treatment.

Short- and long-term treatments promoted oxidative degradation of biodegradable film surfaces. Only long-term exposure led to macroscopic surface damage, altering morphology, chemical structure, and hydrophilicity, without affecting deeper layers, while maintaining thermal properties and slightly enhancing mechanical performance.

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# sciforum-136605: Achieving Sustainability in Packaging: Innovations in Biodegradable and Recyclable Polymer Systems

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The growing demand for eco-friendly packaging solutions has intensified due to increasing environmental concerns and stringent regulatory measures. Biodegradable polymers have emerged as a promising alternative to traditional plastics, offering a sustainable solution that decomposes into benign byproducts and reduces ecological harm. Recent advancements in biodegradable polymers for packaging applications have demonstrated significant potential, particularly with biopolymers such as polylactic acid (PLA), polyhydroxyalkanoates (PHAs), and starch-based composites. These biopolymers have been investigated for their potential to enhance performance and sustainability through advanced strategies, including nanomaterial reinforcement, multilayer composite structures, and biodegradable polymer blending. This study reveals that biodegradable polymers can significantly reduce environmental impact, with life cycle assessments indicating potential reductions in carbon footprint and plastic waste. The adoption of biodegradable polymers can minimize the environmental footprint associated with traditional plastics, contributing to a more sustainable packaging industry. Furthermore, the potential for recycling these polymers in a circular economy context is substantial, with mechanical and chemical recycling techniques like enzymatic biocatalysis offering opportunities to optimize end-of-life scenarios. By harnessing the power of biodegradable and recyclable polymer systems, the packaging industry can reduce its environmental footprint, minimize waste, and promote a circular economy. This approach aligns with global sustainability goals, supporting a more sustainable future for the packaging industry. The development and implementation of biodegradable polymers can pave the way for significant strides towards sustainable development, enabling the industry to reduce its reliance on fossil-based plastics and mitigate its environmental impact. With continued innovation and investment, biodegradable polymers can play a vital role in shaping a more sustainable packaging industry.

# sciforum-138164: Assessing the Effect of Processing Parameters on Biodegradable Polymer Blends Using a Prototype Extruder

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The growing demand for sustainable materials is driving both academia and industry to replace conventional oil-based polymers with biodegradable alternatives. Blending biopolymers is an effective strategy for tailoring and improving the mechanical, thermal, and processing properties of these systems. However, differences in the nature of the components can make it challenging to develop polymer blends with good morphology and thermal stability, potentially affecting their overall performance. In this study, two biodegradable polymers commonly used in packaging—polylactic acid (PLA) and poly(butylene adipate-co-terephthalate) (PBAT)—were blended, and their morphological, rheological, and structural evolution during extrusion was analyzed. An experimental prototype extruder enabled in-line monitoring of the blends throughout the extrusion process. The results showed that screw speed and feed rate significantly influence material properties. Specifically, low screw speeds and feed rates promote thermo-mechanical degradation, leading to a reduction in molecular weight, without excluding possible branching or cross-linking phenomena due to the presence of PBAT. After the experimental tests, Ludovic®, a simulation software for extrusion processes, was used to better understand how processing parameters affected the blends. The simulation also helped identify strategies to reduce degradation and optimize the extrusion process for future applications. This combined approach offers useful insights to enhance biodegradable blend performance in industry.

# sciforum-137470: Assessment of Reprocessed Polylactic Acid from Controlled Virgin Feedstock for Food Packaging Applications

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The growing impact of fossil-based plastics on the environment has driven interest in bioplastics such as polylactic acid (PLA), a biobased and compostable polyester widely used in food packaging but with limited properties. Although designed for composting, preventing the contamination of traditional recycling streams is essential[1]. In industrial production, defective parts and burrs discarded can be reprocessed into pellets from a controlled source, avoiding complex washing[2]. Studies have evaluated performance after reprocessing cycles[3]; however, for food contact applications, the potential migration of substances, including non-intentionally added substances, remains a challenge.

This study evaluates the reuse of industrial discarded PLA parts for food contact. Films were produced from virgin and reprocessed PLA through melt extrusion and hot pressing, with reprocessing simulated by one additional extrusion cycle to the virgin material. Melt flow index (MFI), tensile properties, overall migration (ethanol 50 % v/v, 10 days, 40 °C), and water vapor transmission rate (WVTR) were assessed. Volatile (VOCs), semi-volatile (SVOCs) and non-volatile (NVOCs) compounds were identified through chromatographic/mass-spectrometric techniques. The migration of metals (Ba, Co, Mn, Zn, Cu, Fe, Li, Al, Ni, Eu, Gd, La, Tb, As, Cd, Cr, Pb, Hg, Sb) was tested in 3 % acetic acid (60 °C, 10 days).

Results showed a slight rise in MFI, indicating minimal degradation. Tensile strength and modulus decreased slightly but not significantly. WVTR remained comparable. Overall and metal migration increased marginally but stayed well below the legal limits. The reprocessed PLA exhibited more VOCs and NVOCs absent in the virgin sample. Aldehydes and oligomers predominated, though most showed low migration, underscoring the importance of clean equipment. Metal migration stayed below specific limits. Overall, the reprocessed PLA retained functional properties and kept the migration of key substances within established limits.

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# sciforum-139069: Bio-Based Copolymers with Tunable Cationic Charge Densities for Antimicrobial Applications

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The development of polymers derived from renewable resources is a critical research priority, motivated by the urgent need to reduce dependence on petroleum-based plastics. In this study, we present a sustainable copolymer system based on two bio-sourced monomers: MTA, a vitamin B1 derivative (sulfurol), [1] and PrI, a naturally derived modified itaconic acid [2]. Capitalizing on the chemical versatility of itaconic acid, we incorporated click chemistry-compatible functional groups to enable the covalent conjugation of natural bioactive compounds (sulfurol and menthol), imparting antimicrobial and antioxidant properties. Furthermore, the sulfurol moiety permits post-functionalization of the copolymer, introducing tunable cationic charge densities to modulate bioactivity. The copolymers were comprehensively characterized to assess their functional properties. Antimicrobial activity was evaluated against both Gram-positive and Gram-negative bacterial strains using minimum inhibitory concentration (MIC) assays [2]. The MIC values varied between 8 and 500 µg/mL, depending on the copolymer composition and the specific microorganism tested. Antioxidant performance was analyzed via DPPH radical scavenging assays [3], which demonstrated significant activity at a polymer concentration of 0.25 mg/mL. The Trolox equivalent antioxidant capacity (TEAC) was determined to be in the range of 0.4–0.6 µmol/mg, confirming the copolymers' free radical quenching ability. Biocompatibility was assessed using Normal Human Dermal Fibroblasts (NHDFs) and the Alamar Blue viability assay. The results indicated excellent cell viability, suggesting that these copolymers are highly compatible with biological tissues and suitable for biomedical applications.

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# sciforum-139324: Biomass-Derived Flocculants for Wastewater Treatment

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The selective extraction and recovery of different molecules of interest from lignocellulosic materials from forestry residues are increasing every day, driving society towards more sustainable approaches and materials. For this purpose, the development of new sustainable and ecologically benign extraction methodologies has grown significantly. Deep eutectic solvents (DESs) appear as a promising alternative for the processing of biomass [1, 2]. In the present study, cellulose-rich fractions obtained from the fractionation of Acacia wood, an invasive species in Portugal, were used to prepare cationic and hydrophobically modified cationic bioflocculants used for wastewater treatment with a focus on microplastics removal [3].

On the other hand, *Eucalyptus* bleached pulp was also used to prepare anionic and cationic bioflocculants used to treat effluents from the textile industry [4]. The bioflocculant preparation route follows a two-step process, with the introduction of reactive aldehyde groups in the cellulose molecules, followed by cationization or anionization. The hydrophobic variation was obtained by a third step, by esterification of the $C_6$ OH groups of cellulose with fatty acids obtained from vegetable oils.

All the obtained bioflocculants revealed high performance, according to the results obtained in Laser Diffraction Spectroscopy, at the same level as or even superior to synthetic alternatives, cationic and anionic polyacrylamides, with lower environmental impact.

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# sciforum-137480: Biomechanical performance of natural and synthetic polymers in vascular surgery: a systematic review

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In vascular surgery, polymer materials, both natural and synthetic, are widely used for grafting, stenting, and tissue engineering. In this review, we focus on evaluating materials science and engineering, including biocompatibility and clinical outcomes, to aid in biomedical decisions and material selection.

Following the PRISMA guidelines, we searched PubMed, ScienceDirect, Scopus, and the Persian databases Magiran and SID from 2000 to 2024. Inclusion criteria were the use of the specific terms “natural polymers” and “synthetic polymers” alongside “vascular surgery” and “biomechanical properties” and experimental and clinical studies with quantitative biomechanical data. We performed a qualitative assessment of all included studies.

From 2847 articles, 156 studies were selected, which included 89 experimental studies, 45 clinical trials, and 22 reviews. Natural polymers such as collagen and chitosan had better biocompatibility compared to that of synthetic polymers (92.3% vs 78.1%, p0.001), although they had lower mechanical strength (28.9±6.3 vs 45.2±8.7 MPa, p0.001). In comparison, synthetic polymers had high tensile strength, with PET at 72.4±12.1 MPa and PU showing 650-800% elongation. Clinically, natural polymers led to better 5-year success rates in natural coronary grafts (85.3% vs 78.9%), while synthetic polymers outperformed in peripheral grafts (89.2% vs 76.4% at 3 years). Natural polymers caused decreased inflammatory responses (8.7% vs 15.2%) but higher rates of complications due to degradation (12.4% vs 3.8%).

Synthetic polymers had higher mechanical strength, while natural polymers had better soft tissue integration and biocompatibility. There is additional flexibility in the design with hybrid systems. Further studies of clinical outcomes are needed with smart polymers and uniform methods of testing.

# sciforum-138471: Blue meets green: Marine bacteria and biomass residues in sustainable polyhydroxyalkanoates synthesis

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**Introduction**

The transition to a circular bioeconomy requires valorizing organic waste into high-value bioproducts. We studied marine bacteria and renewable carbon from lignocellulosic biomass to produce polyhydroxyalkanoates (PHA), biodegradable bioplastics. Two marine bacteria were selected: *Cobetia marina* (culture collection) and Roseibium alexandrii, isolated from a PHA biofilm after long-term marine exposure.

**Methods**

Over 50 isolates were screened for PHA accumulation using phaC gene detection and Nile red fluorescence. *R. alexandrii* was chosen for its consistent activity, with C. marina as reference. Both were grown on simple carbon sources (glucose, crotonic acid, gamma-valerolactone [GVL]) and complex sugars from organosolv-hydrolyzed cellulose. Different C/N ratios of 12.5, 25, and 50 were tested to assess nutrient balance effects. After 48 h, cell dry weight and Nile red fluorescence were measured, and PHA was extracted and analyzed by NMR spectroscopy.

**Results**

Overall, C/N 12.5 yielded the highest biomass and fluorescence in most conditions, especially with glucose, crotonic acid, and birch- or cellulose-derived fractions. C/N 25 showed moderate results, while 50 led to reduced growth and PHA synthesis. GVL alone was a poor substrate, but when present in low amounts within sugar mixtures, it did not interfere, enabling the direct use of spontaneously separated crude hydrolysates. Some of the sugar-rich fractions enabled biomass and PHA yields comparable or superior to glucose. Crotonic acid, a PHA degradation product, supported high PHA yields, suggesting a promising route to re-synthesize PHA from its own breakdown products.

**Conclusions**

These results highlight the potential of marine microbes and unrefined waste streams in circular, scalable bioplastic production. The present communication will discuss how these advances contribute to the development of novel, sustainable polymeric materials and open new pathways for integrating microbial biotechnology into polymer science.

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# sciforum-135100: Catalyst-free synthesis of high-strength, reprocessable, degradable, and shape memory biobased Poly(β-hydroxyurethane)s

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Poly(β-hydroxyurethane) (PHU) derived from five-membered cyclic carbonates and amines, is a promising alternative to conventional polyurethanes. However, common PHUs relying on hydroxyl/carbamate exchange exhibit poor reprocessing efficiency and non-degradability. This study addresses these limitations by developing high-performance, reprocessable, and degradable PHUs from renewable feedstocks, advancing sustainable chemistry. Therefore, novel cross-linked PHU networks with vinylogous urethane bonds were prepared. Thereinto, a five-membered dicyclic carbonate was synthesized via the reaction of diglycerol with dimethyl carbonate, and diglycerol tetraacetoacetate was prepared and used as a crosslinker. They reacted with 1,6-diaminohexane to synthesize a series of biobased crosslinked PHUs (PDGVU6s). The obtained PDGVU6s with dual dynamic covalent bonds exhibited relatively low activation energy (27.66 kJ/mol) and significant reprocessing efficiency (~100%, 30 min at 150 °C). Notably, the introduction of vinylogous urethane bonds not only enabled efficient material recycling but also enhanced mechanical properties, achieving tensile strength up to 53.4 MPa. In addition, the presence of dynamic β-hydroxyurethane and vinylogous urethane bonds realized network rearrangement without additional catalysts. Therefore, the obtained PDGVU6s possessed rapid shape memory behavior and self-healing properties (2 h at 70 °C). And the obtained PDGVU6s demonstrated degradation in acidic solutions while achieving a balance between highlyefficient self-healing and excellent mechanical properties. This study presents an efficient method for synthesizing PDGVU6s from renewable resources, which enriches synthetic diversity and holds a promise for further exploration in sustainable chemistry.

# sciforum-138538: Chemical recycling of PA6 from discarded fishing nets using choline chloride-ethanolamine (ChCl:MEA) as deep eutectic solvent (DES)

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The widespread use of synthetic polymers in the fishing industry –particularly polyamide 6 (PA6) used for fishing nets– has led to a substantial accumulation of plastic waste in marine ecosystems, since damaged or obsolete fishing gear is commonly discarded into the ocean. Consequently, recovery and upgrading routes are being explored for their valorization. Chemical recycling has emerged as a sustainable pathway for upgrading waste nets to commercially relevant chemical building blocks, such as ε-caprolactam, thereby supporting the circular economy strategies.

This study is centered on the depolymerization of fishing nets through solvolysis using deep eutectic solvents (DES), specifically a mixture of choline chloride with monoethanolamine (ChCl:MEA) under mild conditions. In this context, the catalytic effect of 4-(dimethylamino)pyridine (DMAP), reaction times, net-to-DES ratio and temperature levels were evaluated in order to identify suitable conditions and parameters in a statistical design of experiments (DoE). The process was carried out in a round-bottom flask batch reactor under an inert nitrogen atmosphere operated with an ethylene glycol-cooled reflux condenser. Following the solvolysis, the crude reaction mixture was filtered to assess the conversion. In addition, its degradation progress was monitored using attenuated total reflectance Fourier-transform infrared (ATR-FTIR) spectroscopy by identifying the functional groups associated with PA6 chain scission.

A central composite design with three factors with two replicates was used to identify the optimal depolymerization conditions, considering (1) %Net/DES, (2) %DMAP/Net, and (3) the ChCl:MEA molar ratio in the DES, while keeping the temperature and reaction time constant at 156 °C and 2 hours, respectively. The optimal parameters were established leading to an 80% conversion, therefore showing a promising effectiveness of DES-based solvolysis as a viable solution for the chemical recycling of PA6 fishing nets.

# sciforum-142763: Chemical recycling of polyester-based textile waste via solvolysis aided by an ionic liquid and supercritical $CO_2$

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The increasing accumulation of synthetic textile waste, especially poly(ethylene terephthalate) (PET)-based fibers, poses a critical environmental challenge. Conventional recycling techniques are often inefficient. Solvolysis with supercritical $CO_2$ ($scCO_2$) emerges as a green and efficient alternative, enabling the depolymerization of polyester chains under mild conditions and facilitating the recovery of platform chemicals with minimal solvent waste. In addition, ionic liquids have been proven to reduce the energy requirements of the solvolysis. This approach aligns with circular economy principles and offers a route toward high-purity monomer production for polymer regeneration. The solvolytic depolymerization of PET-based textile waste was carried out in a high-pressure batch reactor using $scCO_2$ as co-solvent under fixed conditions of **15 minutes** of reaction time and **$CO_2$ pressure up to 120 bar.** Experimental variables included **temperature** (183–217 °C), **textile-to-ionic liquid ratio** ([Tex]:[IL] = 1.7–6.0), and **textile-to-solvent ratio** ([Tex]:[Sol] = 14.1–33.0). A specific ionic liquid was used as catalytic co-solvent. The influence of these parameters on depolymerization efficiency and product selectivity was assessed. Under optimal conditions, a conversion rate of up to 99% was achieved. Temperature proved to be the most influential parameter, significantly affecting the extent of depolymerization in both solvolysis methodologies. In contrast, the textile-to-ionic liquid ratio showed a moderate effect, and the textile-to-solvent ratio exhibited negligible influence on the conversion, indicating that the process could be optimized with reduced solvent consumption. The low sensitivity of the process to solvent and ionic liquid ratios, combined with the strong influence of temperature, supports the feasibility of a cost-efficient, greener recycling method adaptable to industrial applications.

# sciforum-121822: Creating Polyurethane Films from Renewable Resources and Examining Their Mechanical Characteristics with IPDI and CHDI

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The polymer industry primarily relies on petroleum-based raw materials for polyurethane (PU) production. However, extensive research is being conducted to identify sustainable alternatives. This study explores the use of bio-based polyols derived from limonene and geraniol. Limonene is naturally sourced from citrus fruits like oranges, lemons, limes, and grapefruits, while geraniol is found in essential oils such as citronella, rose, and palmarosa oil. These renewable materials contribute to making the polymer industry more sustainable. In PU synthesis, isophorone diisocyanate (IPDI) and cyclohexyl diisocyanate (CHDI) are used. The structural characterization of polyols and PUs is carried out using Fourier Transform Infrared Spectroscopy (FTIR) and Nuclear Magnetic Resonance (NMR). Mechanical properties, including tensile strength and hardness, are evaluated through standard testing methods, while thermal behavior is analyzed using Differential Scanning Calorimetry (DSC) and Thermogravimetric Analysis (TGA). DSC results indicate good miscibility of the synthesized PUs, with glass transition temperatures (Tg) of 75°C for IPDI-based PU and 64.47°C for CHDI-based PU. TGA analysis reveals that the thermal degradation of these PUs begins beyond 200°C. In mechanical testing, the highest recorded tensile strength was 36 MPa for IPDI-based PU, while CHDI-based PU exhibited a tensile strength of 26 MPa. Additionally, the hardness values were 85 for IPDI-based PU and 74 for CHDI-based PU. The gel fraction analysis, which assesses the degree of cross-linking, shows that IPDI-based PU has a higher cross-link density than CHDI-based PU. Overall, IPDI-based polyurethane demonstrates superior mechanical strength and thermal stability compared to its CHDI counterpart, making it a preferable option for applications that demand high-performance materials.

# sciforum-138282: Cure Behavior, Thermal Degradation and Kinetic Analysis of Sustainable Polyurethanes

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To reduce dependence on fossil resources and limit the use of harmful isocyanates, researchers are increasingly developing polyurethanes (PUs) using renewable building blocks like bio-based polyols and diisocyanates. In this work, new PUs were produced using poly(ethylene glycol) (PEG), isosorbide (ISO), and pentamethylene diisocyanate (PDI) to create more sustainable materials. Various compositions were prepared with ISO levels ranging from 0 % to 70 % in a vacuum reactor fitted with a condenser and magnetic stirring. The resulting polymers were analyzed using Fourier transform infrared spectroscopy (FTIR), differential scanning calorimetry (DSC), and thermogravimetric analysis (TG). The DSC data showed exothermic peaks in the 100–200 °C range, revealing active crosslinking reactions. Increasing ISO content made the curing reaction faster, with the $T_{0.01}$ shifting from 95 °C at 50 % ISO to 91 °C at 70 % ISO, and the maximum rate constant (Cmax) rising slightly as well (0.2750 to 0.2964 $min^{-1}$, respectively). FTIR confirmed the chemical bonding between hydroxyl (OH) groups in ISO/PEG and isocyanate (NCO) groups in PDI, showing full NCO conversion at the 2267 $cm^{-1}$ band. Formulations with higher ISO content (>50 %) exhibited an excess of hydroxyl groups, increasing the system's reactivity through both covalent and hydrogen bonding, which promoted more extensive crosslinking. For samples with 70 % ISO, the NCO groups were completely reacted at 126 °C, while the 50% ISO variant reached near-total (99 %) curing at 192 °C. TG results indicated that higher ISO levels caused earlier weight loss due to degradation, starting around 146–151 °C for 50 and 70 % ISO, respectively. The curing and thermal degradation processes were modeled with Friedman, Kissinger–Akahira–Sunose, and Ozawa–Flynn–Wall methods, confirming that moderate ISO content (i.e., 30 – 50 %) enhances both curing speed, degradation activation energy and thermal stability.

# sciforum-139303: Delamination Recycling of Multilayer Plastic Films

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Only a small fraction of plastics produced are being recycled, with the great majority landfilled or released into the environment. Mechanical recycling, currently used to recycle plastic, cannot handle films, which constitute about 40% of all plastic packaging. Polyolefin-rich films are suitable feedstock for pyrolysis; however, pyrolysis breaks down the polymer chains to produce hydrocarbons that are typically used as fuel, which is not true recycling.

Research in our group advances solvent-based molecular recycling, whereby polymers are selectively dissolved and precipitated to achieve separation and recovery. Because the polymer chains do not break and retain all their embodied energy, this is a promising, low-energy, low-greenhouse gas (GHG) plastic recycling methodology.

This project addresses the recycling of multilayer films, which comprise multiple layers of polymer combined into a single film to meet consumer specifications such as preserving food and medicine, acting as an oxygen or moisture barrier, and keeping products sterile. This presentation highlights the solvent-assisted delamination process that we have developed, which recovers the major component, polyethylene, in its solid form, from multilayer films, hence greatly reducing solvent amounts and the corresponding energy needs and GHG emissions compared to dissolution–precipitation recycling. Delamination recycling presents an energy-efficient and environmentally friendly approach to recover value from the approximately 17 million metric tons of multilayer plastic films that are produced every year globally.

# sciforum-136653: Design and Optimization of Electrostatically Assembled Protein–Polysaccharide Nanostructures for Nutrient and Drug Delivery Systems

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Biopolymer-based nanostructures, derived from the self-assembly of proteins and polysaccharides, represent a versatile and sustainable platform for the delivery of bioactive small molecules. Their inherent biocompatibility, biodegradability, nontoxicity, and eco-friendly and sustainable preparation make them ideal candidates for applications in both food technology and biomedicine.

Through light scattering, small-angle scattering, microscopy, and spectroscopy techniques, we investigate the formation and morphology of the protein–polysaccharide nanostructures and the binding, loading capacity, and stability of hydrophobic compounds.

We present our recent works in the preparation and characterization of protein/polysaccharide nanoparticles formed through electrostatic complexation and thermal treatment, using proteins such as bovine serum albumin, trypsin, and hemoglobin and polysaccharides such as chondroitin sulfate, xanthan, and hyaluronic acid. Particular emphasis is placed on the interactions of these nanostructures with low-molecular-weight compounds, including the model nutraceuticals β-carotene and curcumin. The role of nanoparticle composition and structure in modulating the affinity for hydrophobic and amphiphilic molecules is explored.

Our results suggest that fine-tuning the protein-to-polysaccharide ratio, pH, and thermal treatment parameters can optimize nanocarrier stability and small molecule encapsulation. These findings contribute to the rational design of biopolymer-based delivery systems and demonstrate their potential for targeted release of functional compounds in nutraceutical and pharmaceutical formulations.

# sciforum-122085: Development of Brain Targeting Polyethyleneimine-based Novel Polymer Followed by Nano-Formulation and Biological Profiling

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Alzheimer's disease (AD) is a neurodegenerative disease associated with progressive cognitive and memory dysfunction. Quercetin is a natural flavonoid possessing strong antioxidant and neuroprotective activities that has been identified to be of potential value in the treatment of AD by its acetylcholinesterase and butyrylcholinesterase inhibitory action. Its lack of aqueous solubility, low bioavailability, and limited passage across the blood-brain barrier (BBB) limit its clinical applications. To overcome such challenges, the present study had the objective of formulating a nano formulation targeted to the brain of quercetin with a chemically modified polyethyleneimine-based polymer. The functionalized polymer was prepared and determined by FTIR and mass spectroscopic methods that successful conjugation was achieved. Nanoparticles were formulated by solvent injection methods and compared for particle size, zeta potential, PDI, and entrapment efficiency. Optimized formulations showed particle sizes in the nano-range with monodispersity and positive surface charge. Sustained release and pH sensitivity of the drug were observed in vitro, especially under physiological pH conditions of 7.4. Pharmacokinetics demonstrated increased quercetin brain uptake using the modified formulation over plain drug. Moreover, acute toxicity experiments proved that the synthesized modified nanoparticles were safe and biocompatible, with no considerable adverse effects in treated animals. The results confirm the potential of the improved nano formulation as a promising platform for effective and targeted delivery of quercetin to the brain for the treatment of Alzheimer's disease.

# sciforum-137446: Development of Electrosprayed Particles from Chitosan and Soy Protein Isolate for Drug Delivery.

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Pharmaceutical formulations based on polymeric micro/nanoparticles offer multiple advantages for drug delivery applications. They can significantly reduce treatment costs and toxicity risks while enabling patient-specific therapies. Moreover, micro/nanoformulations enhance therapeutic efficacy, prevent the premature degradation of active agents, and improve interaction with the biological environment. Among the various particle fabrication techniques in existence, electrospraying stands out due to its precise control over particle size, morphology, and surface characteristics.

In this study, we selected two biopolymers for nanoparticle production: chitosan (extracted in our laboratory from industrial crustacean waste in Mar del Plata) and soy protein isolate (SPI), which is obtained from the byproducts of soybean oil extraction. To modulate the swelling behavior and degradation profile of the resulting particles, the polymers were cross-linked using oxidized sucrose, following a green chemistry approach aimed at minimizing environmental impact.

Electrospraying conditions were optimized to generate nanoparticles from a chitosan/SPI blend dissolved in 10 mol/L acetic acid. The polymeric solution was infused at a constant rate of 0.2 mL/h, while varying the needle-to-collector distance (10, 13, 15, and 17 cm) and the applied voltage (10–17 kV). SEM analysis has been conducted, and data processing is currently ongoing to identify the optimal parameters. Once optimized, these particles are loaded with ivermectin to evaluate drug loading capacity, encapsulation efficiency, and release kinetics.

# sciforum-138529: Development of nanopillar-structured poly(lactic acid) films incorporating grape pomace-derived activated carbon for smart food packaging applications

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To address environmental concerns in the food packaging industry, there is a growing demand for biodegradable materials with enhanced functional properties. Poly(lactic acid) (PLA) is a promising biodegradable polymer for food packaging, yet it exhibits limitations in barrier performance, mechanical strength, and antibacterial activity. This study focuses on enhancing PLA films by incorporating activated carbon (AC) derived from grape pomace (GP), an abundant byproduct of wine production, thereby promoting a sustainable and circular bioeconomy approach. Biochar (BC) was produced via pyrolysis of GP at 350, 450, 550, and 650 °C for 1 and 2 hours. The optimal BC (obtained at 550 °C for 1 hour) exhibited a porous morphology suitable for further activation. ACs were then synthesized from both raw GP and BC at 450 °C and 550 °C for 1 hour. The most effective variants, AC_550_1h and ACBC_550_1h, were selected based on their superior porosity and used to fabricate PLA films at different loadings (1, 2, 3, 4, and 5 wt.%). The films were characterized using FTIR, XRD, SEM, EDS, and optical profilometry, and evaluated for their adsorption capacity (water and ethanol) and mechanical properties. The optimal formulation, PLA_3ACBC, exhibited enhanced elasticity and adsorption capacity, along with the successful formation of surface nanopillars—confirmed via profilometry. These nanopillars significantly improved antibacterial performance against E. coli and S. aureus compared to smooth, unmodified films. The results show that AC addition enhances the sorption and mechanical behavior of PLA films up to a threshold (3 wt.%). Beyond this concentration, particle aggregation and microcrack formation reduce film performance. Films incorporating AC from BC retained their mechanical integrity better at higher loadings than those using AC from raw GP. This study demonstrates a sustainable strategy for valorizing grape pomace into high-performance activated carbon additives for biodegradable food packaging.

# sciforum-138717: Development of Sustainable Packaging with Enhanced Properties: Utilizing Coffee Waste-Derived Plasticizer, Eggshells, and Natural Rubber in PHBV Bioplastic Blends

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**Introduction:** Poly(3-hydroxybutyrate-co-3-hydroxyvalerate) (PHBV) is a biodegradable bioplastic offering sustainable alternatives to petroleum-based plastics. However, its brittleness and poor processability limit packaging applications. This study enhances PHBV performance by incorporating food waste-derived additives: coffee oil epoxide (COE) as plasticizer and eggshell-derived calcium carbonate ($CaCO_3$) as reinforcing filler with high-molecular-weight natural rubber (NR). The objective is to improve the thermal, mechanical, and barrier properties of PHBV while maintaining its biodegradability for environmentally friendly packaging applications.

**Method:** PHBV blends were prepared using twin-screw extruder with varying NR, COE, and $CaCO_3$ compositions. Films were characterized using differential scanning calorimetry (DSC), scanning electron microscopy (SEM), mechanical tensile testing, and oxygen transmission rate (OTR) analysis. Soil burial biodegradation testing over 117 days assessed environmental impact through weight loss and thickness reduction. Statistical analysis used one-way ANOVA with Tukey's HSD test (p  0.05).

**Results:** COE addition improved PHBV/NR flexibility and processability, while $CaCO_3$ enhanced mechanical strength. SEM showed uniform dispersion without phase separation. DSC results indicated significant melting point decrease from 170.4°C (PHBV) to 166.5°C (PHBV/NR/COE/$CaCO_3$), and crystallinity reduction from 68.5% to 50.8% with COE and eggshells incorporation, confirming improved flexibility and reduced brittleness. OTR values decreased significantly for COE-containing sheets, indicating enhanced barrier properties. The biodegradation study revealed weight loss of 26.25% for PHBV and 28.85% for PHBV/NR/COE sheets, confirming environmental compatibility. Processing trials indicated that PHBV/NR/COE blends formed well-defined sheets, unlike PHBV/NR blends, which were sticky and difficult to process.

**Conclusion:** Blending PHBV with waste-derived COE and $CaCO_3$ plus NR significantly enhanced thermal stability, mechanical strength, and barrier properties without compromising biodegradability. These modified films demonstrate improved flexibility, processability, and environmental performance, making them strong candidates for sustainable food packaging. This study highlights upcycled food waste potential in advancing green polymer solutions and supports industrial scalability.

# sciforum-138902: Development of sustainable polymer composites using recycled polypropylene and organic fillers

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Polypropylene [PP] is an extremely versatile material and can be used for a wide range of applications. PP is also one of the most popular plastic packaging materials in the world, and only around 1% is recycled, which means most PP is headed for the landfill. This decomposes slowly over 20-30 years. Recycling is the third component of the reduce, recycle, and reuse waste hierarchy and is an important part of modern waste reduction. In this study, recycled PP sourced from car battery casings were compounded with organic fillers such as coconut shell (CCS) powder, wood filler (WF) powder, rice husk (RH) powder, banana fibre BF (BAF) powder, and bamboo fibre (BF) powder, and hybrid combinations of wood filler with coconut shell powder, rice husk, banana fibre powder, and 5wt/wt% of PP-g-MA compatibilizer in a ratio of 75/20/5 were used to enhance the compatibility between the fillers and the PP matrix. The various ingredients were melt-mixed using a twin screw extruder and the test specimens were moulded using an automatic injection moulding machine. The main objective of this work was to study the changes in the mechanical properties of the prepared composites with respect to that of virgin polypropylene. Testing for physical and mechanical properties was carried out as per the ASTM standards. From the test results, it was inferred that banana- and bamboo-reinforced rPP had the highest tensile strength at yield and flexural strength. The hardness values of all composites were close to recycled PP. Among the hybrid composites, rPP/WPF/RH and rPP/WPF/BF show the highest resistance to abrasion. Finally, composites containing banana fibre, bamboo fibre, and rPP/WF/BF showed good mechanical properties, as did other combinations.

# sciforum-139346: Dissolution–Precipitation Recycling of Polyolefins

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Only a small fraction of the plastics produced is being recycled, with the vast majority landfilled or released into the environment. Mechanical recycling is currently used to recycle plastic; however, this method is efficient only for homogeneous and non-contaminated feedstock, as well as easily identifiable objects such as bottles made of PET or HDPE. Polyolefins in the plastic waste stream can be processed via pyrolysis, the most common process in chemical recycling. Pyrolysis, however, decomposes the polymers, resulting in undesirable greenhouse gas (GHG) emissions. Furthermore, pyrolysis is not viewed as constituting recycling when its product, pyrolysis oil, is not converted into new polymers.

Plastics recycling research in our group involved the examination of physical, solvent-based processes that do not break down the polymer chains. This constitutes true recycling, as the recovered polymer is the same as the starting material. Such molecular recycling processes leave the polymer chains intact, thus maintaining their embodied energy and emitting relatively little GHG.

This presentation addresses the mechanism of semicrystalline polyolefin dissolution as revealed through joint in situ infrared spectroscopy experiments and diffusion kinetics modeling. It also highlights the application of polyolefin recovery to switchable hydrophilicity solvents (SHSs), which can cycle between a form that dissolves the target polymer and a form that does not, hence facilitating closed-loop solvent cycling.

The insights obtained from these studies facilitate the design of solvent systems and processing conditions for the molecular recycling of polyolefins via dissolution–precipitation. Dissolution–precipitation is an energy-efficient and environment-friendly recycling process that can recover specific polymer types from mixtures, blends, or multilayer films and purify them from additives without negatively affecting the properties of the original polymers.

# sciforum-138228: Ecological PLA/PBAT-g-GMA Nanocomposites Reinforced with Carbon Nanotubes for Electrostatic Charge Control: Evolution of Morphology, Electrical Conductivity and Mechanical Properties

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Ecological and flexible polymeric nanocomposites are essential for sustainable development, considering their technological potential for the production of new materials with enhanced and multifunctional properties. At the same time, they help mitigate environmental impacts, thereby promoting innovation in packaging, electronics, and other applications, as well as assisting in the transition to a greener and more circular economy. In this study, poly(lactic acid) (PLA)/poly(butylene adipate-co-terephthalate) grafted with glycidyl methacrylate (PBAT-g-GMA) nanocomposites were processed by extrusion and injection molded, using multi-walled carbon nanotubes (MWCNT) as conductive fillers. The tested MWCNT contents were 0.5, 1.0, 3.0, and 5 parts per hundred resin (phr) in the PLA/PBAT-g-GMA (70/30% by weight) system, aiming to evaluate impact strength, tensile strength, Shore D hardness, electrical conductivity, and morphological evolution by scanning electron microscopy (SEM). The use of 30% PBAT-g-GMA in the PLA matrix significantly increased impact strength by 556%, suggesting an improvement in the toughening process. Pure PLA and the PLA/PBAT-g-GMA blend exhibited typical insulating behavior, with electrical conductivity around 3.1 x $10^{-11}$ S/cm. The incorporation of MWCNT into PLA/PBAT-g-GMA markedly enhanced the impact strength of the nanocomposites, especially at 5 phr, with a gain of 1085% compared to pure PLA. Furthermore, a transition to a semiconducting material occurred in the PLA/PBAT-g-GMA/MWCNT (5 phr) nanocomposite, with an electrical conductivity of 4.31 x $10^{-6}$ S/cm. In contrast, no improvements were observed in Shore D hardness and the elastic modulus of the nanocomposites. This behavior was explained by the preferential migration of carbon nanotubes to PBAT-g-GMA, promoting greater stability in the morphology and refinement of the dispersed phase in the PLA matrix, justifying the significant gain in impact strength. The results indicate potential as a flexible and conductive nanocomposite for antistatic applications.

# sciforum-138753: Effect of accelerated weathering on the structural and thermo-mechanical behavior of polymeric materials based on PMMA/PU/Cellulose-g-PMMA

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Interpenetrating polymer networks (IPNs) of poly(methyl methacrylate) (PMMA)/poly(urethane) PU exhibit good mechanical strength and weather resistance. PMMA/PU IPNs have been studied due to their balanced combination of stiffness, flexibility, and chemical resistance. Grafting crystalline nanocellulose (CNC) onto PMMA to obtain particles that enhance compatibility, improve tensile strength, and impart degradability has not been studied when dispersing it into PMMA/PU IPNs. For this reason, IPNs were obtained through sequential polymerization using 50/50 ($PMMA_{50}/PU_{50}$) and 80/20 ($PMMA_{80}PU_{20}$) ratios and different wt% of $CNC_x$ grafting (x = 5, 10, 20, 30 wt%) onto PMMA to obtain $PMMA_xCNC_y$ particles, which were dispersed during the synthesis in 0.1 and 0.5 wt%. This study presents the results of their characterization through mechanical testing performed before and after accelerated weathering to evaluate the effects of the accelerated weathering (ACW) test in a QUV following ASTM G154 for 672 h. Mechanical, thermo-mechanical, and structural analyses were performed through a tensile test, dynamic mechanical analysis (DMA), and thermogravimetric analysis (TGA) to determine the final properties after ACW. The sample that was reinforced in stress and Young's modulus is when 0.1 wt.% $PMMA_{70}CNC_{30}$ particles are added into 50/50 PMMA/PU. The sample closest to the stress of the pure sample was $PMMA_{50}PU_{50}/PMMA_{70}CNC_{30}$ (0.1 wt%), exhibiting minimal damage in stress and strain after ACW. For $PMMA_{80}PU_{20}$ systems, reinforcement was made for the following samples: $PMMA_{80}PU_{20}/PMMA_{95}CNC_5$ (0.1 wt%), $PMMA_{80}PU_{20}/PMMA_{95}CNC_5$ (0.5 wt%), $PMMA_{80}PU_{20}/PMMA_{90}CNC_{10}$ (0.1 wt%), and $PMMA_{80}PU_{20}/PMMA_{70}CNC_{30}$ (0.1 wt%). $PMMA_{80}PU_{20}/PMMA_{70}CNC_{30}$ (0.1 wt.%) was the most durable material in the 80/20 sample after ACW. Thermo-mechanical analysis indicates an increase in stiffness, changing the glass transition in dependence on the type of particle added, and the structural analysis indicates minimal damage.

# sciforum-130199: Effect of Various Natural Filler Additives on Biodegradability of Low Density Polyethylene Based Composites

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The problem of polymer waste (plastic waste) is one of the most acute environmental problems of our time. It is associated with the huge amount of plastic produced and its slow decomposition in the environment.

Long-term studies aimed at the biological decomposition of polyethylene, however, have yielded modest results. In general, the fight against pollution by polymer waste requires a comprehensive approach, including changes in consumer behavior, innovations in materials and technologies, and effective waste management.

In this paper, as a solution to this problem, we propose modifying low-density polyethylene by adding a natural filler - natural rubber.

In this regard, the objects of development and further research were polymer composites based on polyolefins of various classes with the addition of a natural polymer - natural rubber.

Natural rubber (NR) is a biopolymer synthesized by more than 2,000 plant species, most of which belong to Euphorbiaceae or Compositaceae. Natural rubber refers to the coagulated or precipitated product obtained from the milky sap (latex) of the rubber plant (Hevea brasiliensis), which forms unlinked but partially vulcanized polymer chains with a molecular weight of about 106 amu and elastic properties.

The main elements of scientific novelty of the declared work: for the first time a comprehensive study of the properties of mixtures and individual components of polymer compositions based on polyolefins and natural rubber was carried out, physicochemical methods of modification were considered; previously unstudied dependencies of interphase interaction in multicomponent polymer matrix systems were established. Based on the results of the work, the optimal ratio of components in the polymer mixture, the features of the destruction process were determined, and the prospects for further use of the obtained materials were assessed.

# sciforum-138479: Environmental Assessment and Ecotoxicity of Paper Coated with PHBV and Cellulose: Uncovering Hidden Risks in “Sustainable” Packaging

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The growing demand for sustainable packaging has accelerated the development of biodegradable, bio-based alternatives to traditional plastics. Among these, PHBV and cellulose-coated paper are promising due to their compostability and renewable origin. However, their environmental safety remains uncertain, especially considering the possible release of chemical additives—such as organophosphate esters (OPEs), phthalates, and alternative plasticisers—during degradation. These substances may pose ecotoxicological risks to soil organisms and ecosystems. This study evaluates the environmental performance of a commercial PHBV–cellulose coated paper (BIOFUNPAPER) by assessing its degradation and ecotoxicity under composting conditions.

Four composting reactors were operated at 58 °C for 90 days with 1.7 kg of compost each. At 30, 60, and 90 days, 25 g samples were collected and analysed by HPLC-MS to quantify 20 OPEs, 11 phthalates, and 4 alternative plasticisers. Parallel bioassays were conducted on earthworms (*Eisenia fetida*), oat and tomato plants, and soil microbes. Parameters included germination, biomass, worm survival, reproduction, and nitrification inhibition.

The results showed 60% biodegradation of the BIOFUNPAPER material. Acute toxicity in worms was negligible; however, chronic exposure resulted in a 50% reduction in reproduction and a 33% reduction in biomass. Plant germination exceeded 90%, yet tomato biomass fell to 68% of control levels. Microbial nitrification activity dropped to 79.8%, just below the ISO safety threshold. Most additive concentrations decreased over time but were detectable throughout.

The findings indicate that, despite effective degradation and low acute toxicity, chronic ecological effects persist. These outcomes highlight the need to go beyond biodegradability assessments and integrate ecotoxicological evaluations of additives and by-products. Ensuring the environmental compatibility of new bio-based packaging materials requires a holistic, lifecycle-based approach to support a truly circular and safe packaging system.

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# sciforum-137900: Ethanolysis of PLA using ChCl/ZnAc deep eutectic solvent for sustainable ethyl lactate production

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Polylactic acid (PLA) is a biodegradable polyester derived from renewable resources and is increasingly used as a sustainable alternative to conventional plastics. However, due to limitations in mechanical recycling, chemical recycling methods are needed to promote a circular plastic economy. One promising approach is the ethanolysis of PLA to produce ethyl lactate (EtLa), a valuable green solvent used across several industries.

Previous studies have explored the use of deep eutectic solvents (DES) as sustainable catalysts for PLA depolymerisation. However, limited work has been done on the influence of catalyst composition and reaction kinetics. In this study, the ethanolysis of PLA using a DES composed of choline chloride (ChCl) and zinc acetate (ZnAc) in a 1:1 molar ratio was investigated, with a focus on the effect of ZnAc form (anhydrous vs. dihydrate) on catalytic performance.

Reactions were carried out using PLA in powder and film forms (3g) with ethanol (50 mL, ≥99.5%) and ChCl/ZnAc DES (1:1) under continuous stirring. A range of temperatures (80 °C to 180 °C) and reaction times (up to 8 hours) were tested using a 100 mL glass reactor with oil bath heating at atmospheric pressure. After reaction, mixtures were filtered under vacuum, and the yield of EtLa was quantified by using gas chromatography. PLA conversion and EtLa yield were systematically evaluated as functions of morphology, temperature, and reaction time.

The highest EtLa yield of 92% was achieved after 8 hours at 140 °C using PLA film, with complete conversion observed. In comparison, PLA powder yielded lower conversion under the same conditions, indicating that film morphology enhances degradation efficiency. Compared to existing studies, the method enabled higher EtLa yields at lower temperatures and shorter times, demonstrating improved efficiency. A temperature-dependent kinetic model was developed to describe the ethanolysis process and predict optimal conditions based on reaction parameters.

# sciforum-146726: Exploiting starch and cellulose biodegradation for microbial polyhydroxyalkanoate (PHA) production

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In Colombia, annual plastic consumption reaches nearly 1.2 million tons, generating a significant impact on the environment and public health, as most of this waste ends up in landfills that pollute mangroves, rivers, and seas. To address the problems associated with non-biodegradable and non-renewable plastics, alternative materials such as biodegradable and non-toxic polymers have been promoted, among which polyhydroxyalkanoates (PHA) stand out. These microbially derived biopolymers are biocompatible, can be produced from various renewable carbon sources, and are suitable for both single-use plastics and biomedical applications, making them consistent with circular economy principles.

This study aimed to evaluate PHA production by *Bacillus thuringiensis* (C01) using starch and carboxymethylcellulose (CMC) as carbon sources, and to optimize the process through a central composite design with response surface methodology. Initially, fermentation growth variables were assessed using glucose as a control, followed by evaluation of the experimental substrates under optimized conditions. With CMC, a PHA production of 0.09 g/L was obtained, with a yield of 49.5% (w/w). In contrast, optimization with starch (14.168 g/L starch, 3.616 g/L ammonium sulfate, yeast extract in a 1:1 ratio, and an inoculum of approximately $6\times10^8$ CFU/mL) resulted in 3.71 g/L biomass and 2.78 g/L PHA, corresponding to a yield of 74.9% (w/w). These findings demonstrate the ability of *Bacillus thuringiensis* to degrade starch and channel it into PHA synthesis.

FTIR, TGA, DSC, and MALDI-TOF analyses confirmed that the biopolymer obtained was poly-3-hydroxybutyrate (P(3HB)). In conclusion, the amylolytic activity of *Bacillus thuringiensis* highlights its potential for using starch-rich agroindustrial residues as substrates for sustainable PHA production.

# sciforum-126686: Fabrication of CA/CS Composite Films by Solution Blow Spinning Method for Food Packaging Application

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This study aims to develop new bio-based materials for food packaging using air spraying as a cost-effective manufacturing method. Materials prepared in the form of films were based on cellulose acetate (CA) modified with chitosan (CS). The morphology, structure and performance in terms of thermal, mechanical, wettability and antibacterial behaviour were studied considering two variables: the solvent used to prepare solutions to be sprayed, acetic acid (HAc) or formic acid (FA) and, the composition of the polymer system, 0%, 2.5%,5% and 7.5% by CS weight. The resulting CA/CS composite films obtained exhibited remarkable flexibility and mechanical strength despite being derived from rigid, high-molecular-weight biopolymers. This flexibility is attributed to the unique droplet-based morphology of the films. Increased chitosan content led to enhanced surface roughness and higher water and oil contact angles, indicating improved hydrophobicity. Notably, films with 7.5% chitosan demonstrated antibacterial activity against *E. coli*, showing inhibited colony growth compared to pure CA films. Therefore, with this study it has been demonstrated that air spraying enables the fabrication of flexible, mechanically robust, and bioactive CA/CS films without the need for plasticizers. Their unique droplet-based morphology, high water contact angle, and antibacterial activity against *E. coli* highlight their suitability for sustainable food packaging. The use of biopolymers and an efficient processing method positions this approach as a promising alternative to conventional film-forming techniques.

# sciforum-139118: From milk to 3D printing: A sustainable journey of upcycled proteins

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The increasing consumption of single-use plastics in packaging raises environmental concerns due to fossil fuel depletion and alarming plastic waste production and accumulation. Sustainable alternatives, such as biobased and biodegradable materials, are urgently needed. The pasteurized milk in Italy has a short shelf-life (6 days) after which it cannot re-enter the human food chain and it has to be destroyed or utilized elsewhere: for animal feeding, composting, production of biogas or fertilizers. The aim of our research is to find an application for expired milk in order to mitigate the biowaste and to increase its value by upcycling it into biodegradable packaging material.

Casein was extracted from expired milk using different methods yielding casein-based powders with varying structure and behaviour. These powders were further used for the preparation of dispersions under a variety of conditions (solvent, pH, concentration). Rheological properties were assessed through small amplitude oscillatory shear measurements, carried out at 25 °C. The analyses provided the evaluation of rheological behaviour based on the type of powder, solvent and pH of the dispersion. Moreover, the preliminary structural and thermal characterizations were performed using FTIR and TGA analyses, respectively. Based on the results, the most suitable dispersions were suggested to be utilized as 3D printing material for biobased food packaging.

Our approach not only reduces milk waste but also offers a sustainable alternative to petroleum-based plastics. Future experiments will be focused on the optimisation of printing conditions and mechanical characterisation of the materials.

# sciforum-122518: From Petrochemical to Photosynthetic: Algae-Derived Polymers for Sustainable Industrial Applications

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The global reliance on fossil-derived polymers continues to contribute to environmental degradation and climate change. As the world seeks sustainable alternatives, algae-derived polymers have emerged as a promising solution due to their renewable nature and compatibility with green chemistry and circular economy principles. Unlike traditional biomass sources, algae can be cultivated on non-arable land using saline or wastewater, reducing land-use conflict and freshwater consumption while simultaneously sequestering atmospheric $CO_2$. This review examines recent progress in the extraction, processing, and functionalization of algae-derived polymers, with a particular focus on polysaccharides such as alginate and carrageenan. A comparative analysis was conducted to evaluate their mechanical performance, biodegradability, and application scalability across various industries including sustainable packaging, biomedical devices, and textiles. The review draws on data from peer-reviewed publications within the past decade. The findings highlight that algal polysaccharides offer excellent film-forming capabilities, mechanical adaptability, and environmental biodegradability. Seaweed-derived polymers like carrageenan have shown strong potential in biomedical fields due to their gel-forming and biocompatible nature. Life-cycle assessments support the environmental benefits of algae-based bioplastics compared to conventional plastics. In conclusion, algae-derived polymers represent a rapidly advancing frontier in sustainable materials science. While their adoption in high-value sectors is accelerating, further interdisciplinary research is needed to overcome related cost, processing, and commercialization challenges.

# sciforum-138539: From Shore to Seafloor: A Multisite Mediterranean Study on Plastic Biodegradation

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**Introduction:** The accumulation of plastic debris in marine environments poses an ecological threat, particularly in semi-enclosed basins such as the Mediterranean Sea. Biodegradable plastics have emerged as promising alternatives to conventional polymers, yet evaluating their actual degradation performance under environmental conditions remains methodologically challenging. Protocols, standardized and reproducible, fail to account for the complexity of in situ variables—such as temperature, solar radiation, hydrodynamics, and seasonal fluctuations—which can profoundly affect degradation kinetics. This highlights the urgent need for field-based studies that reflect real-world scenarios. **Materials and Methods:** We conducted a one-year in situ degradation study at the port of Calpe (Spain), exposing polyethylene terephthalate (PET), polybutylene-succinate-co-adipate (PBSA), poly(3-hydroxybutyrate-co-3-hydroxyvalerate) (PHBV), and a 70:30 PBSA:PHBV blend, each 200 µm thick. Sampling was performed at 2, 6, 9, and 12 months. We assessed mass loss, biofilm protein concentration, surface morphology, roughness, thermal stability and chemical changes. **Results:** PHBV showed the highest degradation (41.8% mass loss at 12 months), followed by the 70:30 blend (24.1%) and PBSA (11.2%), while PET remained unchanged. Biofilm's protein content remained stable for the first 9 months but increased sharply at month 12 across all materials, less markedly in the 70:30 blend. SEM revealed surface damage in all biodegradable polymers, especially PHBV, while PET served as a microbial support. Thermal behavior changes aligned with degradation, whereas FTIR alterations were limited. Surface roughness increased over time in PHBV and the blend, consistent with microbial activity; PBSA showed a more variable pattern, and PET remained unaltered. **Conclusion:** Our findings confirm the decisive role of polymer composition in driving degradation under natural marine conditions and underscore the need for realistic, long-term field studies to guide the development of truly sustainable plastic alternatives.
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# sciforum-137461: From Waste to Resin: Reuse of Epoxidized Post-Consumer Soybean Oil to Produce Green Composites Reinforced with Sugarcane Bagasse

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The reuse of soybean oil reduces environmental impacts, prevents sewage system clogging, promotes sustainability, and adds value to a waste material. In this study, post-consumer epoxidized soybean oil (RESO) was cured with fumaric acid to develop green composites reinforced with sugarcane bagasse (F). The natural reinforcement underwent chemical modification to improve its interaction with RESO, aiming to evaluate impact strength, tensile strength, Shore D hardness, and contact angle. Additionally, scanning electron microscopy (SEM) was used to analyze the interfacial interaction between the RESO matrix and the sugarcane bagasse before (F) and after treatment (TF). The RESO/F composites with 10 and 20 parts per hundred resin (phr) did not exhibit a reinforcement effect; they acted only as traditional fillers, improving only the elastic modulus and Shore D hardness compared to pure RESO. In contrast, the treatment of sugarcane bagasse contributed to the production of RESO/TF composites with improved mechanical performance. The RESO/TF (20 phr) formulation showed increases of 230.7% in elastic modulus, 64.2% in tensile strength, and 114.7% in Shore D hardness compared to pure RESO, suggesting a reinforcement filler effect. SEM analysis revealed that the RESO/TF (20 phr) composite exhibited improved interfacial interaction between the phases, which enhanced stress transfer as observed in the mechanical tests. The contact angle of approximately 95.4° and the impact resistance of 38.3 J/m were similar to those of the RESO matrix, reinforcing that the chemical treatment of the sugarcane bagasse contributed to a synergistic effect on the material properties. The reuse of RESO for composite production aligns with circular economy principles and sustainability.

# sciforum-136850: Gelation kinetics of chitosan-based hydrogels using different crosslinking agents

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**Introduction:**

The crossover time (tc) between the storage modulus (G′) and loss modulus (G″) is a key rheological parameter used to characterize the sol–gel transition in hydrogel systems. This metric provides valuable insight into gelation kinetics and is directly associated with the processability of polymeric materials. In this study, bio-based hydrogels were prepared from chitosan (Ch), a natural polysaccharide, and crosslinked with two different agents: glutaraldehyde (GA), a synthetic dialdehyde, and genipin (GNP), a natural crosslinker derived from *Gardenia jasminoides*.

**Methods:**

Hydrogels were prepared by dissolving 4%w/v Ch in 2%v/v acetic acid, and then mixing in a 4:1 ratio with aqueous solutions containing GA or GNP at concentrations of 1, 5, and 10% relative to Ch weight. Rheological oscillatory measurements were performed during the crosslinking reaction.

**Results:**

Time sweep rheological tests were used to determine tc, which marks the transition from a liquid-like to a solid-like state. At the lowest concentration (1%w/w), GA was insufficient to induce gelation, whereas GNP at the same concentration produced a tc of 269 min. At 5%w/w, both crosslinkers successfully formed solid-like gels with tc values of 18.6 min for GA and 91.2 min for GNP. Increasing the crosslinker concentration to 10% w/w further decreased tc to 4.2 min for GA and 57.6 min for GNP. As expected, higher crosslinker concentrations led to faster gelation (lower tc values). These results show that GA promotes faster crosslinking but requires higher concentrations, while GNP enables gel formation at lower dosages but with slower kinetics.

**Conclusion:**

Both the chemical nature and concentration of the crosslinker significantly affect the gelation time and mechanical evolution of bio-based chitosan hydrogels. Moreover, genipin represents a suitable substitute for glutaraldehyde in the development of aldehyde-free hydrogels, allowing longer processing times.

# sciforum-146993: Green microwave assisted hydrolysis of PET bottle waste for MIL53 (Al) synthesis: Characteristic, Taguchi optimization

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Polyethylene terephthalate (PET) is one of the most widely produced polymers, extensively used in packaging and beverage industries. However, its low recyclability leads to significant environmental challenges, with less than 10% of global plastic waste effectively recycled, while the majority accumulates in landfills or the natural environment. Developing efficient chemical recycling strategies is therefore essential to mitigate environmental impact and recover valuable resources. Among these, depolymerization of PET into terephthalic acid (TPA) offers a promising route for generating a monomer that can be reused in the synthesis of advanced functional materials.

In this study, PET waste was depolymerized into TPA using microwave-assisted alkaline hydrolysis. A Taguchi experimental design was employed to optimize key process parameters, including temperature (160–200 °C), reaction time (5–90 min), PET particle size (0.2–2 cm), PET-to-liquid ratio (1:10–1:2), and microwave power (up to 630 W). Kinetic parameters of the hydrolysis reaction were also determined to better understand the depolymerization mechanism. Under the optimized conditions—190 °C, 90 min, 0.2 cm PET particle size, 10% PET-to-liquid ratio, and 630 W—a maximum depolymerization efficiency of 65% was achieved. The influence of process variables was ranked as reaction time > temperature > particle size > solid-to-liquid ratio.

The recovered TPA was subsequently used as an organic linker for the microwave-assisted synthesis of MIL-53(Al). Structural and textural characterization by XRD, FTIR, BET, and SEM confirmed the successful formation of a porous framework, showing that synthesis and activation conditions significantly influenced crystallinity, surface area, and morphology. This study demonstrates a sustainable strategy for PET valorization, combining process optimization with the production of advanced metal–organic frameworks, and contributes to circular economy initiatives.

# sciforum-139098: Hydrogel Scaffold for Bone Defect Regeneration in Rabbits: Characteristics and Healing Stimulation Evaluation

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Segmental bone defects represent a significant clinical challenge in orthopedic medicine, often resulting from trauma, infection, or tumor resection. Traditional treatments frequently fail to achieve adequate bone regeneration in large defects. This study evaluated the regenerative potential of a novel composite biomaterial combining Wollastonite, β-tricalcium phosphate (β-TCP), and polyethylene glycol dimethacrylate (PEGDMA) for treating segmental bone defects. The composite hydrogel was synthesized using 80% Wollastonite, 20% β-TCP, and PEGDMA polymeric matrix through foam replication and UV-curing techniques. Twelve New Zealand rabbits underwent surgical creation of 5 mm radius segmental defects. Animals were randomly assigned to implant group (GI, n=6) receiving the composite biomaterial or control group (CG, n=6) with standard plate fixation only. Both groups received identical stabilization with locked plates and screws. Comprehensive evaluation included clinical monitoring, radiographic imaging, computed tomography, and histopathological analysis over 120 days. The composite demonstrated excellent biocompatibility with no adverse reactions observed. Radiographic analysis revealed significant differences in biological activity scores between groups (GI: 3.0±0 vs CG: 1.6±0.51, p0.05 at 120 days). Tomographic evaluation showed superior tissue neoformation (2.8±0.4 vs 2.0±0.63, p0.05) and mineralization (2.6±0.51 vs 1.5±0.54, p0.05) in the implant group. Histomorphometric analysis demonstrated dramatically enhanced tissue proliferation in treated animals (4798.33±151.32 μm vs 2408.33±148.51 μm, p0.01 at 120 days). Complete bone consolidation was achieved in the implant group at 120 days, while control group showed persistent defects. The Wollastonite-β-TCP-PEGDMA composite hydrogel effectively promotes bone regeneration in segmental defects, demonstrating superior osteoinductive and osteoconductive properties compared to natural healing. This innovative biomaterial represents a promising therapeutic approach for challenging bone reconstruction scenarios.

# sciforum-139232: Integrated biorefinery of *Jatropha curcas* L. seed: Valorization of Kernel into Biofuels and Molasses, and Seed Coat into Biopolymers and Cellulose Nanofibrils.

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In response to the urgent need for sustainable alternatives to fossil products and the promotion of a circular economy, biorefineries offer an effective strategy for biomass valorization. *Jatropha curcas* L., a drought-tolerant species native to Mexico and Central America, is well known for its oil-rich kernels; however, its seed coat remains largely underutilized, limiting the full exploitation of the crop.

This study presents the first integrated biorefinery model for the comprehensive valorization of *JCL* seeds, converting both kernels and seed coats into high-value biofuels, materials, and nutritional and chemical co-products through sequential fractionation and conversion.

The kernel was subjected to mechanical oil extraction at 200 °C, followed by transesterification with 1% NaOH to produce biodiesel (ASTM-D6751). Residual protein cake from extraction was refined with isopropyl alcohol to obtain molasses. In parallel, milled seed coat underwent alkaline (NaOH 4.5%, 80 °C, 2 h, 4 cycles) and subsequent bleaching treatment (chloride-based, 80 °C, 4 h, 4 cycles) to disrupt lignin–carbohydrate complexes, yielding lignin- and cellulose-rich fractions. The cellulose-rich fraction was then processed into cellulose nanofibrils by high-pressure homogenization (10000 psi, 10 cycles).

This integrated approach achieved ~85% total biomass seed valorization. Kernels accounted for 69.0 ± 2.8% of seed mass, with oil extraction yielding 45.0 ± 2.5% and residual protein cake 47.3 ± 1.0%. Of this extracted oil, 90.3 ± 3.4% was converted into biodiesel, while 9.4 ± 2.8% remained as glycerol. Molasses were produced for first time from the protein cake, representing ~10% of its mass and leaving ~37% as purified protein. The seed coat represented 30.1 ± 3.1% of seed mass, yielding 21.5 ± 3.4% of lignin-rich fraction from the generated black liquor after alkali treatment, and 44.6 ± 2.4% of cellulose-rich fraction from bleaching. The cellulose-rich fraction was then processed into cellulose nanofibrils of 5 nm of diameter without previous pre-treatment.

These findings demonstrate the potential of *JCL* as a versatile feedstock for sustainable bio-based industries.

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# sciforum-137879: Kinetics of PET alcoholysis using deep eutectic solvents for DOTP production

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Polyethylene terephthalate (PET) is a common plastic found in everyday items such as clothing and beverage bottles. Unfortunately, PET contributes to plastic pollution due to its limited recyclability through mechanical means. Valuable chemicals can be recovered from waste PET through chemical recycling, which involves reacting PET with suitable chemicals. One notable reaction is between PET and 2-ethyl-1-hexanol (2-EH), resulting in the production of dioctyl terephthalate (DOTP). This compound has gained attention as a green plasticiser in the plastics industry.

Researchers have previously studied the use of deep eutectic solvents (DESs) as sustainable catalysts for the formation of DOTP from PET. However, the kinetics of this reaction have not been thoroughly documented. In this work, the temperature-dependent kinetics of the reaction between PET and 2-EH, catalysed by choline chloride (ChCl)-Zn acetate (ZnAc) DES, to produce DOTP are presented.

The reactions involved PET in powder form (5 g), as well as 2-EH (17 g, 99%), ChCl (≥99%) and anhydrous ZnAc (99.9%). The experiments took place in a 100 mL glass reactor with continuous stirring at atmospheric pressure, and heating was provided by an oil bath. Reaction temperatures ranged from 150 °C to 190 °C. The yield of DOTP was determined by gas chromatography, while PET conversion was determined gravimetrically. The kinetic model developed from this study can predict the maximum yield observed at specific temperatures, aligning with findings from this and previous research.

# sciforum-124839: Micronutrient-loaded biopolymer as slow-release behavior

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Hydrogels are 3-dimensional cross networked polymeric materials that can absorb and retain a large amount of water. Nature-derived hydrogels are biodegradable, low cost, non-toxic and biocompatible. Here we developed agricultural waste-derived hydrogel in which cellulose was extracted from rice straw and Carboxymethyl Tamarind Kernel Gum (CMTKG) (made from tamarind's seed) was collected from market. CMTKG and Rice Straw Cellulose (RSC)-based superabsorbent hydrogels by in situ incorporation of Copper (Cu) were synthesized by graft copolymerization using epichlorohydrin as a crosslinker. Cu-loaded CMTKG-RSC superabsorbent hydrogel (CSH) was applied as a carrier vehicle for Cu micronutrient release for applications in the field of agriculture. The synthesized CSH was characterized using Fourier transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM), thermal gravimetric analysis (TGA), and UV–visible spectrophotometer analysis. The prepared CSH was analyzed regarding its swelling, deswelling, water retention, recyclability, and biodegradation. The synthesized CSH observed to have a water absorption capacity (663 – 832% in distilled water) with entanglement of Cu with weak physical forces. The water absorption kinetics exhibited that the rate-controlling step was Fickian diffusion, revealing a slower diffusion rate of water transport into the hydrogel network. The CSH showed a slow release of Cu with ~80% release within 184 h in distilled water. Different kinetic models were studied to observe the release kinetic parameters. The Peppas–Sahlin model was the best-fitted model among all studied models, revealing Cu release controlled by Cu diffusion with polymeric relaxations. Considering these findings, the synthesized hydrogel can be used as a water reservoir for agriculture and reducing irrigation in plants. Slow release of micronutrients (such as Cu) from CSH also enhances the plant growth.

# sciforum-138133: New Powder Polymer For 100% Bio-based Cosmetic Formulations

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This study addresses the increasing market demand for natural and environmentally friendly cosmetic formulations. Current trends favor responsible excipients derived from biosourced raw materials with eco-responsible exploitation and low-energy processing. A significant challenge exists in developing bio-based rheology modifiers with performance comparable to synthetic polymers like polyacrylates or polyacrylamides. While natural polymers such as hydrocolloids, polysaccharides, and proteins possess thickening and stabilizing properties, they often exhibit lower thickening power and formulation difficulties compared to petroleum-based polymers [1].

To bridge this gap, strategies are explored to improve the properties of natural polymers by modifying their chemical structure and therefore their properties in cosmetic formulations. Various academic studies deal with the chemical functionalization of natural polymers (cross-linking, grafting of different chemical moieties on the backbone) in order to improve some of their properties according to the final application.

The present work investigates the cross-linking of polysaccharides using environmentally friendly reactants and processes. A novel method of chemical cross-linking that enables the isolation of the functionalized biopolymer in a highly concentrated powder form (exceeding 90%) is presented, thereby enhancing its applicability for cosmetic formulations. Furthermore, the functionalized biopolymer presents good thickening properties and is readily biodegradable.

The impact of various process parameters on the final product properties is examined.

# sciforum-138929: Partially Bio-based Aliphatic Diisocyanate Crosslinker as a Reactive Diluent in 2K Polyurethane Resins

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The continuous trend towards enhancing the bio-based content of polyurethanes in parallel with balancing their properties for optimized chemical, physical and mechanical properties has lead to the exploration of various alternative components of bio-based diisocyanates, polyols and their combination. In this work, the role of a semi bio-based aliphatic diisocyanate polymer synthesized from hexamethylene diisocyanate (HDI), poly(ethylene glycol) and palmitic acid containing 32 % bio-based carbon content was investigated as a reactive diluent and crosslinker in combination with the pentamethylene diisocyanate (PDI) containing 68% bio-based carbon content, and a reference petrol-based hexamethylene diisocyanate (HDI). The diisocyanate mixtures were consequently crosslinked with a selected polyester polyol for making fast air-drying 2K solvent-free coating formulations, which were evaluated on mechanical and thermophysical properties. The addition of the synthesized aliphatic diisocyanate in combination with both PDI or HDI resulted in homogeneous mixtures up to 1:1 concentrations, with a progressive reduction in viscosity and possible formation of smooth coatings on wood. Therefore, the aliphatic diisocyanate functions as a levelling agent, enhancing flow and gloss levels of the coating, while introducing hydrophobicity through an increase in water contact angles. The mechanical properties of crosslinked polyurethanes demonstrated higher flexibility and ductility, owing to the molecular configuration of the aliphatic diisocyanate, resulting in a reduced hardness and better resistance against scratching or abrasive wear for balanced concentrations of crosslinkers. The performance was confirmed through FTIR spectroscopy, indicating the higher crosslinking densities and presence of hydrophobic moieties at the surface. The curing reactions were confirmed by DSC and DMA measurements, confirming the progressive shift in glass transition temperatures, loss modulus and dampening peak depending on aliphatic diisocyanate concentrations, confirming its role as a plasticizer.

# sciforum-144491: Performance and Migration Stability of PVC Plasticized with Poly(ethylene glycerol sebacate)

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PVC occupies a leading position among thermoplastics in terms of production and application. The main part of PVC is used in the form of plasticized products. The search for alternatives to phthalate plasticizers remains an urgent task, with priority given to materials with low toxicity and migration resistance. Saturated polyesters based on sebacic acid are a promising eco-friendly substitute. The development of PVC materials with such polyesters solves the problems of environmental safety, durability of products and compliance with international standards. Plasticization of polyvinyl chloride was carried out with DOP and polyethylene glycerol sebacinate containing terminal hydroxy and carboxyl groups, 50 wt. h. and 10 wt.h. respectively per 100 wt.h. PVC. The physico-chemical, technological and operational characteristics of plasticized PVC are determined. The tensile strength was 19.7 MPa, the elongation of PVC plastics was determined at a closing rate of 100 mm/min - 367%. The melt flow rate was determined on a plastometer (T=190 °C, P=98 H): MFI = 64.5 g/10min. The thermal stability of the Congo red (185 °C) method was 209 min. The glass transition temperature was determined by the DMA method in the stretching mode and in the temperature range from minus 100 °C to plus 100 °C at a frequency of 1 Hz in a nitrogen atmosphere: -26.5 °C. An increase in the amount of polyester (20 wt.h.) leads to increased resistance to migration to polar and nonpolar environments, increased thermal stability – 211 min, MFI – 188 g/min.

# sciforum-143063: Pine Bark as a Renewable Feedstock for the Production of Rigid Polyurethane Foam

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The use of biomass waste for polymer production is a key component of the global plastic sustainability strategy. Bark contains low molecular weight polyphenolic and carbohydrate compounds rich in hydroxyl groups, making it a potential macromonomer source for plastics. The global annual volume of bark waste is estimated at 300–400 million $m^3$, making it a cheap and highly available raw material.

This study focused on the waste-free processing of pine (*Pinus sylvestris*) bark into rigid polyurethane (PUR) foam. Extractives, obtained in a yield of 25%, enriched with low molecular weight carbohydrates, were separated via pressurized water extraction at 150 °C. Increasing the extraction temperature above 150 °C significantly reduced both the extractives yield and their hydroxyl content due to carbohydrate dehydration. Extractives were converted into liquid polyols through "green" oxypropylation with propylene carbonate (PC), varying PC/OH ratios. The residual bark was introduced into PUR foam formulation as a filler.

The resulting polyols exhibited viscosities ranging from 8.6 to 210 Pa·s, and hydroxyl values between 580 - 660 mg KOH/g were used to synthesize PUR foams with PMDI at an NCO/OH ratio of 1.1.

In the PUR foam formulations, commercial polyols (Lupranol 3300 and Lupranol 3422) were partially or fully replaced by the bark extractives-based polyols. Key material properties — apparent density, deformation, morphological, and thermal characteristics—were evaluated and compared to foams based on commercial polyols.

Polyol synthesized at a PC/OH ratio of 3 was the most promising for PUR foam production, yielding materials with properties equal to or better than those of foams based on commercial polyols. However by incorporating the residual bark after extraction as a filler led to a slight reduction in mechanical performance.

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# sciforum-139087: Polyhydroxyalkanoate Biosynthesis from Sugarcane Bagasse by *Paramecium caudatum* Isolated from Industrial Wastewater

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Polyhydroxyalkanoates (PHAs) are microbial-derived biodegradable polymers with significant potential to replace conventional synthetic plastics. This study investigates the novel biosynthesis of PHAs by *Paramecium caudatum*, a ciliated protozoan, using lignocellulosic waste sugarcane bagasse (SCB) as a low-cost carbon source. *Paramecium* sp. was isolated from industrial wastewater and identified as *P. caudatum* via 18S rRNA gene sequencing (GenBank: PQ038083). *P. caudatum* cultures were incubated separately with SCB at 4% (w/v) and glucose at 3% (w/v) for comparison, under optimal conditions (25°C, pH 7). PHA accumulation was assessed using Sudan Black B and Nile Blue A staining during the log phase. Extracted PHAs were characterized using Fourier-transform infrared spectroscopy (FTIR), gas chromatography–mass spectrometry (GC–MS), scanning electron microscopy (SEM), and thermogravimetric analysis (TGA). PHA synthase expression in total cellular protein was assessed via SDS-PAGE, and PHA film biodegradability was evaluated through a soil burial test. PHA yields reached 2.43 g/L with glucose and 2.21 g/L with SCB. FTIR and GC–MS analyses revealed predominant PHA monomers, including 3-hydroxybutyrate ethyl ester (92.6%), hexadecanoic acid ethyl ester (74.4%), and octadecanoic acid ethyl ester (65.9%). TGA showed good thermal stability, with Tmax at 280°C (glucose) and 270°C (SCB). SEM imaging displayed a porous, pseudospherical surface morphology, indicating strong polymer integrity. The PHA films exhibited favorable plasticizing properties and fully biodegraded within 30 days in soil. SDS-PAGE confirmed consistent expression of a ~63 kDa PHA synthase under both carbon source conditions. This is the first study to report *P. caudatum* as a microbial cell factory for scalable bioplastic production via lignocellulosic waste valorization, contributing to circular bioeconomy goals.

# sciforum-130945: Processing and properties of novel PBS/PVOH-based films for sustainable food packaging applications

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The use of biodegradable or biobased materials in the packaging sector represents one of the main solutions for reducing plastic pollution. Polybutylene Succinate (PBS) is among the most promising biopolymers for food packaging due to its easy processability, good thermal stability, ductility, and flexibility, which make it suitable for film production. However, it has poor barrier properties, similar to those of Polylactic Acid (PLA). Polyvinyl Alcohol (PVOH), on the other hand, is a biodegradable polymer with excellent gas, odour, and aroma barrier properties, high mechanical strength, and chemical resistance, but it is highly water-sensitive and difficult to process. Melt blending may offer a valid strategy to combine the advantages of both materials.

In this study, PBS/PVOH blends at different weight ratios (100/0, 80/20, 60/40, 40/60, 20/80, 0/100 wt%) were prepared via melt-compounding and characterized in terms of their rheological and structural properties. Subsequently, the blends were processed into blown films, which were evaluated for their mechanical, morphological, and barrier properties, as these are critical for food packaging applications. The results showed that PBS exhibited higher viscosity and more pronounced shear-thinning behavior compared to PVOH. Furthermore, incompatibility between the two polymer phases was observed. The blends demonstrated increased stiffness, evidenced by an increase in elastic modulus and a decrease in elongation at break. The incorporation of PVOH significantly improved the barrier performance of the films, with reductions in oxygen and water vapor permeability of up to 53% and 42%, respectively. These findings underscore the potential of PBS/PVOH blends as sustainable materials for food packaging applications requiring enhanced gas barrier properties.

# sciforum-138225: Protecting perishable food by using renewable and biodegradable polyester films

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The growing need to reduce food loss and environmental pollution has intensified research into sustainable packaging solutions, particularly in regions like the Mediterranean, which produce large quantities of perishable food. Biobased and compostable polymers offer a promising alternative to conventional fossil-derived plastics, supporting carbon neutrality and circular economy principles. However, their barrier properties often fall short of those required for effective food preservation. This study investigates the potential of poly(lactic acid) (PLA) and poly(butylene succinate-co-adipate) (PBSA) blends to enhance the performance of compostable films for packaging perishable liquid and semi-liquid foods. This study considers that a PLA/PBSA 60/40 blend was developed and evaluated for its mechanical and barrier properties, demonstrating improved flexibility, impact resistance, home-compostability and industrial recyclability. Then, by using a mini-extruder, various PLA/PBSA formulations, including nanostructured fillers like clay and talc, were produced and tested for their melt fluidity. Then the materials were used to prepare films that were tested for their ability to retain liquid whey over time. Infrared spectroscopy and analysis of morphology by Scanning Electron Microscopy were employed to assess surface and bulk characteristics of films. Results indicated that blend composition significantly influenced barrier performance, with certain formulations showing enhanced resistance to mass loss. This research highlights the critical role of material composition in designing effective compostable packaging systems for perishable food products. These findings have implications in preservation of perishable foods that may include Mediterranean fruits such as strawberries, dates, and tangerines. In fact, the development of such biobased films could contribute to reduce food waste and extending shelf life, aligning with environmental sustainability goals.

# sciforum-138923: Recyclable Multi-Layer Films from Virgin and Recycled Polyethylene

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Flexible multilayer films are indispensable in food packaging, but their complex composition makes recycling significantly more difficult. To support a circular packaging economy, this study investigates mono-material multilayer films based entirely on polyethylene (PE), incorporating both virgin and recycled feedstocks.

Several three-layer films were fabricated via film blowing extrusion using ultra-low-density polyethylene (ULDPE), post-consumer recycled low-density polyethylene (rLDPE), and their blends. A comprehensive set of characterizations was conducted, including differential scanning calorimetry, thermogravimetric analysis, and melt flow index to assess thermal and molecular properties, as well as mechanical testing (tensile, tear, and dart drop impact). Proxy-based migration experiments were conducted to determine contamination risks relevant to food-contact applications.

Molecular analyses revealed opposing degradation mechanisms: chain scission in ULDPE and crosslinking in rLDPE. The rLDPE showed higher crystallinity, contributing to mechanical robustness when combined with ULDPE. Mechanical tests indicated that increasing rLDPE content reduces ductility and impact strength, though moderate levels preserve acceptable performance. Migration testing confirmed no detectable proxy contaminant transfer through virgin outer layers down to 10 μm thickness, even in films with 75% recycled content.

Controlled blending of rLDPE and ULDPE enables the design of recyclable, mono-material multilayer films with tailored mechanical and barrier properties. The findings suggest that high recycled content can be safely used in packaging, provided design-for-recycling principles are applied. This work highlights a viable strategy for integrating post-consumer waste into high-performance flexible packaging.

# sciforum-147118: Recycle of PA12 Scrap: Mechanical and Structural Performance of FDM Printed Parts from SLS Waste

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Additive manufacturing is rapidly expanding across industries but generates substantial polymer waste, particularly in Selective Laser Sintering (SLS), of which considerable quantities of unfused powder and faulty prints are typically discarded. The development of sustainable recycling pathways is therefore essential to minimize losses in material and adopt circular economy strategies in polymer processing.

In the present research, a recycling process is proposed for polyamide 12 (PA12) waste retrieved from SLS 3–Dimensional (3D) printer. Faulty parts and scrap material were collected, mechanically pulverized to an average particle size of ~2 mm for ease of handling, and subsequently reprocessed with a filament extrusion system. Homogeneous continuous filament with a diameter of 1.75 ± 0.05 mm was successfully produced and used as Fused Deposition Modeling (FDM) input material. Standardized tensile (ASTM D638) and compressive (ASTM D695) test samples were printed using FDM for determination of the mechanical properties of the recycled material.

Since the PA12 would undergo three (3) consecutive thermal cycles—initial sintering in SLS, re-melting in filament extrusion, and FDM printing—this study addresses the measurement of the effects of these thermal cycles on the structural integrity and mechanical behavior of the resultant FDM prints. In addition, Differential Scanning Calorimetry (DSC) and X-ray Diffraction (XRD) analyses were performed to investigate the semi-crystalline nature of PA12 and to evaluate possible changes in crystallinity after recycling. The outcomes of mechanical testing provide information on the retention of properties and compatibility of recycled PA12 as an input for FDM. The outcomes reveal the possibility of converting SLS scrap into FDM filament and demonstrate a feasible recycling process that not only minimizes polymer waste but also enhances material usage on multiple platforms of additive manufacturing.

# sciforum-138734: Revaluation of agro-industrial waste through Biotechnology: Papaya peel waste as feedstock for PHB production by native *Bacillus* strains

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The environmental impact of synthetic plastics and agro-industrial waste has made it necessary to develop sustainable biopolymer alternatives. This research evaluated the potential of papaya peel waste, an abundant agricultural byproduct in the Santander region, as an alternative carbon source for the synthesis of bioplastics like polyhydroxyalkanoates (PHAs) by bacterial fermentation. The process was carried out in two steps. In the first stage, a central composite design based on response surface methodology was applied to optimize four process variables (carbon source concentration, temperature, pH and inoculum concentration) using *Bacillus thuringiensis* fermentation cultivated on papaya peel extract. The optimal conditions were identified as a temperature of 31.4 °C, a sugar concentration of 10 g/L, a pH of 5.5 and an inoculum concentration of 4% (v/v). In the second step, a validated fermentation process under these optimized conditions resulted in a maximum PHA accumulation of 81.0±0.85% of cell dry weight. Chemical analysis confirmed that the major biopolymer produced was the homopolymer poly(3-hydroxybutyrate) (PHB). These results demonstrate the potential of valorizing papaya peel waste as sustainable fermentative carbon source to produce high-value biopolymers, promoting the circular economy in Santander and reusing agricultural waste that is usually discarded while contributing to the sustainable management of organic waste in the region.

# sciforum-127789: Selective ABS dissolution with eutectic solvents: toward greener recycling

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Acrylonitrile-butadiene-styrene (ABS) plastics, commonly found in electronics, automotive parts, and household items, continue to pose a substantial environmental challenge, with the majority still ending up in landfills or incinerators. Dissolution-based recycling methods have emerged as effective alternatives to conventional mechanical recycling, particularly for recovering high-quality fractions. This work explores the use of eutectic solvents (ESs) as renewable, low-impact alternatives for the selective dissolution and recovery of ABS components—specifically, the styrene-acrylonitrile (SAN) copolymer. A computational solvent screening of over 30 000 potential candidates was conducted using the COnductor-like Screening Model for Realistic Solvents (COSMO-RS), followed by experimental validation to assess the solubility of SAN in selected ESs. The solubility of SAN was assessed under mild conditions (60 °C, 1 h), and three ESs systems were found to be effective, with recovery yields up to 70%. The recycled polymer and residues were characterized using Fourier-transform infrared spectroscopy (FTIR) and nuclear magnetic resonance (NMR) analyses. Notably, preliminary results suggest that effective dissolution is possible even at ambient temperature and pressure. These findings highlight the potential of ESs as sustainable and scalable solutions for the recovery of difficult-to-recycle polymeric waste such as ABS.

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# sciforum-138510: Solvolytic Depolymerization of PA6 from Marine Waste Using Structurally Diverse Deep Eutectic Solvents

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The accumulation of discarded fishing nets in coastal zones significantly contributes to marine pollution, with polyamide 6 (PA6) being the predominant polymer in these residues [1]. Chemical recycling through depolymerization offers a promising strategy to transform this waste into high-value building blocks, particularly ε-caprolactam, supporting circular economy initiatives while reducing ocean contamination.

Neoteric solvents have the potential to act as catalytic cosolvents for other purposes [2]. In this study, deep eutectic solvents (DES) were evaluated as green media for depolymerizing PA6 recovered from fishing nets. The tested DESs included choline chloride (ChCl):urea, ChCl:glycerol, ChCl:monoethanolamine (MEA), and ChCl:diethanolamine (DEA) under mild conditions (160–180°C). The catalytic effect of 4-(dimethylamino)pyridine (DMAP), solvolysis time, and the reaction system were investigated to determine their effectiveness in promoting depolymerization. After solvolysis, the crude reaction mixture was filtered to assess conversion, and attenuated total reflectance Fourier-transform infrared (ATR-FTIR) spectroscopy was used to monitor the depolymerization process by identifying the functional groups associated with PA6 chain cleavage.

Although several DES facilitate polymer dissolution, those containing MEA and DEA exhibited significantly higher depolymerization efficiencies. This enhanced performance was attributed to their dual function, acting not only as solvents but also as nucleophilic agents capable of attacking amide bonds, thereby promoting solvolysis reactions under the tested conditions. The findings of this screening enable the selection of MEA- and DEA-ChCl-based DES as the most promising candidates for subsequent optimization through experimental design. This approach will contribute to advancing chemical recycling pathways for fishing net waste by enabling the recovery of high-value building blocks for future production of new polyamides and advanced materials, thus supporting environmental sustainability while generating added value within the polymer recycling chain.

# sciforum-137784: Structural, Thermal, and Morphological Characterization of Biobased Wheat Straws as Sustainable Alternatives to Single-Use Plastics

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Plastic pollution from single-use products such as drinking straws has prompted a global shift toward sustainable, biodegradable alternatives. This study explores the potential of wheat-derived straws, produced from post-harvest agricultural residues in Central Macedonia, Greece, as eco-friendly substitutes for conventional plastic straws. Three wheat straw types (Staramaki K1, G1, and A1) were examined and compared with commercial straws made from reed, bamboo, paper, and bioplastics. Structural analysis using X-ray diffraction (XRD) revealed high crystallinity in all wheat samples, with K1 exhibiting the highest value (77.1%), indicating a more organized cellulose matrix. Water absorption tests in water, orange juice, and coca-cola showed that K1 absorbed significantly less liquid than other wheat and paper straws, suggesting enhanced barrier performance. Scanning electron microscopy (SEM) was employed to assess morphological changes before and after immersion. While all samples showed surface degradation, K1 retained its integrity better than others, both externally and internally. Thermogravimetric analysis (TGA) demonstrated that K1 also offered superior thermal stability, with delayed decomposition and reduced weight loss at elevated temperatures, confirming its suitability for hot beverage use. Additionally, impact resistance tests showed that the wheat-based straws, particularly the K1 variant, retained sufficient mechanical integrity under moderate loading, confirming their practical durability in real-use scenarios. Overall, the results confirm that Staramaki K1 straws, derived from agricultural waste, combine high crystallinity, low water uptake, and good thermal resistance, making them strong candidates for replacing synthetic and pulp-based straws. This study highlights the feasibility of converting local biowaste into high-performance, food-safe, and compostable materials, promoting circular economy principles and sustainable material design.

# sciforum-139102: Structure–Reactivity Relationships in Catalyst-Free Curing of Epoxy Resins with Carboxylic Acids

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Epoxy resins are extensively utilised across diverse applications owing to their superior chemical resistance, thermal stability, and mechanical properties. Traditionally, these resins are cured using amine or anhydride hardeners; however, increasing attention is being directed towards alternative, more sustainable curing agents, notably carboxylic acids. These acids offer environmental advantages and enable simpler processing without the need for catalysts; however, their curing efficiency is highly dependent on their chemical structure. This study examines the curing of epoxy resin using three distinct carboxylic acids—salicylic acid (a monoacid), citric acid (a triacid), and maleic acid (a diacid featuring conjugated double bonds)—in the absence of catalysts. The objective was to assess their effectiveness in facilitating epoxy ring-opening and network formation. Formulations were prepared by combining each acid with the epoxy resin in stoichiometric proportions, followed by thermal treatment. Curing progression was monitored using Fourier-transform infrared spectroscopy (FTIR), while differential scanning calorimetry (DSC) was employed to evaluate thermal behaviour and degree of cure. Furthermore, gel content analysis quantified the insoluble fraction of the cured samples, serving as a direct indicator of crosslink density. The results revealed that both salicylic and citric acids effectively promoted epoxy ring-opening, leading to the formation of crosslinked networks. Citric acid exhibited superior performance, attributed to its three carboxylic groups, resulting in higher gel content and enhanced crosslink density. In contrast, maleic acid failed to promote curing under the applied conditions, likely due to its conjugated double bonds diminishing the nucleophilicity of its carboxylic groups or causing steric hindrance in reactions with epoxy moieties. These findings highlight the critical influence of acid structure on curing efficiency, positioning multifunctional acids such as citric acid as promising sustainable alternatives for catalyst-free epoxy resin curing.

# sciforum-141343: Sustainable Bio-Based Polyester: Advancing Self-Healing and Recyclability Through Covalently Adaptable Linkages

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The rising concern over plastic pollution and its long-term environmental consequences has intensified global efforts to discover sustainable alternatives to conventional synthetic polymers. In this study, we report on the development of fully bio-based dynamic polyester covalent adaptable networks (CANs), synthesized from renewable and environmentally friendly resources. These advanced polymeric systems incorporate dynamic covalent bonds that enable reversible chemical transformations, allowing the materials to be reprocessed, recycled, and even self-healed. Such features make them particularly attractive for sustainable material applications. This approach directly addresses the escalating accumulation of plastic waste, aiming to minimize its adverse impact on both the environment and human health. The polyester CANs developed here demonstrate adequate mechanical strength and can be reprocessed multiple times under mild conditions without significant loss of performance. Comprehensive material characterization confirms their structural integrity and adaptability across repeated recycling cycles. This work represents a significant advancement in polymer science, offering a pathway to reduce plastic waste while enhancing the functionality and lifecycle of materials. The findings underscore the potential of integrating bio-based sources with dynamic bonding strategies to create smart, durable polymers that align with circular economy principles. Overall, this study offers valuable insights into developing the next generation of environmentally responsible materials.

# sciforum-145627: Sustainable bio-compounds for a circular economy: insights from the Life Restart project

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The close-to-market Life Restart project, co-financed by the European Union (LIFE Program for the Environment and Climate Action), focuses on recycling agri-food waste to produce biodegradable bio composites within a “green” and circular economy framework [1].

The project aims to recover and reuse 75% of a major beer production by-product (brewer's spent grains—BSG), while reducing the consumption of fossil-based polymers by 15% and virgin biopolymers by 35%. This approach promotes the use of bioplastics (bio-derived/biodegradable) instead of fossil-based alternatives, as well as the re-use of waste products from the agri-food chain, to contribute to the achievement of carbon neutrality and “net zero emissions” by 2050 [2].

In this study, bioplastics are mixed with agri-food waste (brewer spent grain, BSG), to create bio-compounds. We evaluated the mechanical performance of various bioplastics (bio-derived and/or biodegradable) to produce bioplastic–waste mixtures [3]. This approach transforms waste into a valuable resource within the framework of a circular economy. By incorporating BSG, the process reduces the amount of bioplastic required, lowering production costs, as bioplastics are significantly more expensive than fossil-based plastics.

As part of the project, partners and stakeholders have developed the first prototypes of different objects, with different processing technologies (such as injection molding, extrusion, melt-mixing, 3D printing) by using these bio-compound mixtures. The mechanical tensile performance of some objects made from bioplastic–waste mixtures was analyzed and compared to that of objects formed from pure bioplastic and to that of fossil-based plastics. We focused on plant pots, in particular, as an example object. The results showed that the bio-compounds made from thebioplastic–waste mixtures exhibit good mechanical tensile strength compared to commercial pots, with the additional advantage of their biodegradability ensuring a fully sustainable product life cycle.

Several other physical, mechanical, rheological, and morphological characterizations of the bioplastic–waste mixtures, before and after degradation (photo-degradation and thermo-mechanical degradation), have been studied.

# sciforum-138649: Sustainable Crop Protection with PHA-Based Active and Biodegradable Mulch Films

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Plastic mulch films are widely used in agriculture to improve moisture retention, weed suppression, and enhance yields. However, conventional films, typically made of polyethylene (PE), pose significant end-of-life challenges due to their low commercial value, contamination with soil and residues, and high transportation costs. They often leave persistent fragments in the field that contribute to microplastic pollution and soil degradation.

Although some biodegradable mulch films are commercially available, most are based on PBAT, PLA, or their blends. While compostable under industrial conditions, their degradation in soil or agro-composting environments is often too slow. Furthermore, some studies have highlighted potential ecotoxic effects from PBAT degradation intermediates. Meanwhile, active mulches described in the literature commonly rely on pesticidal or biocidal agents, raising environmental and regulatory concerns.

The ACTIBIOMULCH project proposes an alternative: multilayer mulch films based on polyhydroxyalkanoates (PHA), fully biodegradable in soil, incorporating natural compounds that activate plant defense mechanisms and enhance resilience to biotic stress without direct toxicity. A biodegradation-promoting additive is also included to modulate the disintegration rate under different conditions.

This work focuses on the polymer technology side. The structural layer was produced by extrusion of PHA-based blends, and the active layer applied by electrospinning using biodegradable matrices with functional compounds. Structure and morphology were analyzed by SEM, and thermal and mechanical properties by DSC, TGA, and tensile testing. Biodegradability was evaluated under industrial composting, soil burial (ISO 14855, ISO 17556, ISO 20200), and greenhouse conditions. In addition, a comprehensive ecotoxicological evaluation was carried out, with no adverse effects observed.

Preliminary results show that the films offer suitable mechanical properties, efficient biodegradation, and good environmental compatibility. In tomato trials, they improved pathogen resistance and increased the proportion of top-quality fruits. These findings support their potential as sustainable alternatives to conventional mulches, in line with circular economy principles.

# sciforum-139186: Sustainable Depolymerization of Marine PA6 Waste Using a Choline Chloride–Diethanolamine Deep Eutectic Solvent

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The accumulation of end-of-life polyamide 6 (PA6) fishing nets in marine environments poses a serious ecological and waste management challenge[1]. Recent advances in chemical recycling through solvolysis have opened new avenues for recovering high-value monomers such as ε-caprolactam from polyamide waste streams, thus supporting circular economy principles and the production of next-generation materials. In this investigation, a deep eutectic solvent (DES) composed of choline chloride and diethanolamine (ChCl:DEA) at different molar ratios is employed as both reaction medium and nucleophilic agent for the depolymerization of PA6 sourced from marine waste[2].

The study systematically explores the solvolysis process under moderate thermal conditions (170–210 °C), focusing on the optimization of reaction parameters such as molar composition, catalyst loading, and temperature, using a statistical experimental design. The catalytic role of 4-(dimethylamino)pyridine (DMAP) is evaluated for its potential to enhance depolymerization kinetics and product selectivity. Structural changes in the polymer matrix are monitored via attenuated total reflectance Fourier-transform infrared spectroscopy (ATR-FTIR), while depolymerization efficiency is assessed through gravimetric analysis. The ChCl:DEA DES demonstrated a robust performance, promoting extensive amide bond cleavage through its dual-function behavior and serving both as a polar solvent and as a reactive nucleophile capable of exerting an aminolytic attack on the polymer backbone.

Previous studies have shown the effectiveness of DES and related ionic media in the chemical depolymerization of polyesters and polyamides due to their unique hydrogen-bonding and catalytic properties (Badia et al., 2024; Sert et al., 2021). The present work contributes to this growing body of knowledge by demonstrating the applicability of ChCl:DEA for the efficient recycling of real-world marine PA6 waste under relatively mild and scalable conditions.

This approach highlights a promising route for upcycling problematic marine plastics into valuable chemical feedstocks, reducing the environmental impact of discarded fishing gear while enabling the development of sustainable materials from secondary raw resources.

# sciforum-138863: Sustainable formulations made of a furan-based copolyester and nisin for flexible antimicrobial packaging applications

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**Introduction**

The growing concern over environmental impact caused by fossil-based plastics has intensified the search for sustainable alternatives, in particular in the field of food packaging, which is a short life-cycle application involving high volumes of plastics. Among bio-based polyesters, those containing 2,5-furandicarboxylic acid (FDCA) have emerged as promising candidates and green alternatives to the fossil-based terephthalic polyesters. Apart from their renewable origin, their success is due to their outstanding mechanical and barrier properties. However, they lack intrinsic antimicrobial features, which is a preferable requirement aiming to extend the shelf-life of food products, enhancing at the same time their safety.

**Methods**

This work focuses on the realization of fully bio-based blends from a furan-based copolyester and a natural preservative to obtain novel solutions in the field of antimicrobial food packaging. Nisin, a polycyclic antibacterial peptide which can be isolated from *Lactococcus lactis*, was chosen as preservative, and mixed, in different weight amounts, with poly(butylene/pentamethylene furanoate), P(BPeF). The compression-moulded films where then deeply characterized.

**Results**

The incorporation of nisin allowed for a modulation of mechanical flexibility and toughness, whilst retaining the thermal stability, which is one of the main advantages of the pristine polyester, as well as the main thermal transitions. Moreover, the excellent gas barrier properties of P(BPeF) were preserved. Lastly, the implementation of antibacterial features otherwise absent in the pristine polymer was obtained, as estimated by disc diffusion assay against *L. Plantarum* and *L. Monocytogenes*.

**Conclusion**

The films investigated in this work are valuable candidates for application in the field of flexible and active food packaging, and credible substitutes of currently used unsustainable materials for the fabrication of flexible, high-barrier containers.

# sciforum-121298: Synthesis, thermal, mechanical, and hydrolysis properties of poly(hexamethylene furandicarboxylate)-based copolyesters

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To improve the hydrolysis ability of poly(hexamethylene furandicarboxylate) (PHF), novel biobased poly(hexamethylene-*co*-diethylene glycol furandicarboxylate) (PHDEGF) copolyesters were successfully synthesized by a two-step melt polycondensation method. The chemical structure and composition of the copolyesters were characterized using $^{1}$H-NMR and $^{13}$C-NMR, revealing that the PHDEGF copolyesters were random. The intrinsic viscosity of all polyesters ranged from 0.76 to 0.87 dL/g, indicative of relatively high and close molecular weights. The thermal properties and crystallinity of the copolyesters were investigated with DSC, TGA, and WAXD. With the increase in diethylene glycol 2,5-furandicarboxylate (DEGF) unit content, both the thermal stability and the glass transition temperature of the copolyesters were improved. The crystallinity and melting point of the copolyesters gradually decreased when the DEGF unit was 21.2 mol% and below, while the copolyesters were amorphous when the DEGF unit was 41.6 mol% and above. In addition, the hydrolysis and mechanical properties of the polyester were further investigated. As the DEGF segment content increased, the water contact angle (WCA) value of the copolyesters gradually decreased; consequently, the hydrolysis rate accordingly increased. After 9 d of degradation at pH=14 and 37 °C, the remaining mass decreased from 92.9% for PHF to 7.1% for poly(diglycol furandicarboxylate). The mechanical properties of PHDEGF were increased by introducing a small amount of DEGF units. In particular, the elongation at break of PHDEGF30 (DEGF unit = 21.2 mol%) was comparable to that of poly(butylene adipate-*co*-terephthalate) (PBAT); moreover, its modulus exceeded that of poly(butylene succinate) (PBS). Therefore, PHDEGF30 has the potential to replace PBAT and PBS as a promising packaging material.

# sciforum-147122: Targeted Delivery of Quercetin to the Brain via a Modified Polymeric Nanocarrier

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Polyethyleneimine (PEI), a cationic polymer, has been extensively studied by researchers for its applications in gene delivery and drug transport. However, due to its toxicity, there are some limitations, such as cytotoxicity and non-biodegradability. In this study, PEI was conjugated with polyethylene glycol (PEG) to enhance its stability and prolong its residence time in the body. To make it more suitable for brain delivery, we further modified it with the addition of an amino acid, phenylalanine, which improves its physicochemical properties for brain delivery in Alzheimer's disease (AD) and other neurodegenerative disorders. Quercetin is a flavonoid with notable pharmacological effects and promising therapeutic potential in AD. This novel polymer is utilized to prepare nanoparticles (NPs) for the effective delivery of quercetin in the brain. The synthesis of acryl PEI derivatives is the first step, followed by PEGylation of the acryl PEI derivative, and further derivatization of PEI-PEG with a disulfide linker. Lastly, the above compound is attached to the amino acid phenylalanine, as confirmed by FT-IR, mass spectroscopy, and DSC. Then, after preparation of nanoparticles, which were evaluated through particle size, zeta potential, PDI, SEM, and in vitro release, the MTT assay was performed to ensure that cell viability remained above 80%, and the ex vivo intestinal permeability of the novel polymer NPs remained at 5μg/cm. A further blood–brain barrier permeation study was carried out, in which the novel polymer showed the highest permeability. The histopathological evaluation of the brain hippocampus region, Ca1, was tested for novel polymer and formulation, and the absence of observable variations such as lesions, necrosis, and inflammation,confirmed that the synthesized polymer was non-toxic and had high permeability. Studies further demonstrated that the polymer and its NPs are safe and capable of effectively crossing the blood–brain barrier, highlighting their potential for targeted neurological therapies.

# sciforum-146850: Technologies for obtaining new biocomposites based on polylactide with natural fillers of waste origin manufactured using the injection molding method

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Every year, huge amounts of natural waste are produced by various industries. In the current raw materials crisis, particular attention should be paid to the possibility of reusing them instead of disposing of them. After appropriate processing of natural raw materials, e.g., through alkalization or the addition of modifiers, they can be successfully used as fillers for plastics. Adding them to bio-based polylactide enables the production of composites with new properties that are also environmentally friendly.

In this study, several plant-based wastes were selected as fillers: straw, grass, reed, sunflower husk, as well as raspberry, evening primrose, and milk thistle pomaces. The raw materials were subjected to grinding, alkalization, and rinsing to neutralize the pH. Before further processing, the fibers were dried to remove residual solvents and moisture.

Concentrates with 20 wt% filler content were obtained by mixing PLA with the plant-based fillers in the molten state. The resulting materials were crushed using a knife granulator, and the granules were processed via injection molding. Ultimately, samples containing 5, 10, and 20 wt% of filler were produced.

To characterize the PLA composites, melt flow index (MFI) measurements, FT-IR spectroscopy, thermal analysis, and mechanical tests (tensile and flexural strength and impact strength) were performed. The results allow the assessment of flowability, processing behavior, and the basic mechanical and structural properties of the obtained composites. In this work, particular emphasis is placed on the properties of composites containing grass filler.

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# sciforum-137824: Thermomechanical Properties of Virgin and Recycled Polymers: A Comparison

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The European Commission promotes the increase of recycled plastic in short-term applications as its strategy to introduce plastic products into a circular economy model. However, the mechanical recycling process could reduce the thermal stability and mechanical properties of plastics. In this regard, six (TGA) and tensile tests were performed and case materials assessed included two (PET), two (PP), and two (PE) in their virgin and recycled forms.

The samples were sorted, cleaned, shredded into flakes, and then extruded. So, according to the manufacturer, the samples were processed with the same conditions used for the virgin counterparts. However, additives such as plasticizers and fillers were added in order to increase the thermomechanical properties of the materials, among others.

The TGA curves obtained were similar no matter the origin of the plastic, although a residue of 5% was found in some recyclates—in all except for PET.

Relative to the mechanical properties, the elongation, Young modulus, and ultimate tensile strength for the three polymers PET, PP, and PE were analyzed. In the case of PET, the recyclates showed greater ultimate tensile strength and elongation than the virgin plastics, showing, however, the same young modulus. For the other polymers, the virgin PP material showed better properties by 10% to 15% in all the parameters. Regarding PE, the recyclate had a greater elongation by 5%, and the other properties of the virgin PP were about 35% above the recyclates.

The studies showed a good overall performance of the recycled material thermally and mechanically, which makes the recycled polymers a good replacement for the virgin polymers.

# sciforum-138569: Tin-Catalysed vs Non-Catalysed Curing of Epoxidized Soybean Oil: Insights from Isoconversional Analysis

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The pursuit of sustainable polymeric materials has driven the development of epoxy systems derived from renewable sources, such as epoxidized soybean oil (ESO). Understanding their curing kinetics is essential for process control and optimisation of final properties. In this study, the curing behaviour of ESO/MTHPA/DEH 35 (epoxidized soybean oil/methyl tetrahydrophthalic anhydride/2,4,6-tris(dimethylaminomethyl) phenol) systems—with and without a tin-based catalyst (Tin) (Tin(II) 2-ethylhexanoate)—was evaluated using the isoconversional Friedman method. Samples were analysed via Differential Scanning Calorimetry (DSC) at heating rates of 5, 10, and 20 °C/min. Data were processed using the differential form of the conversion equation (α) to obtain the apparent activation energy (Ea) as a function of conversion. Model validation was achieved by comparing experimental and calculated conversion values (αexp vs αprev), and by linear regressions of ln(dα/dt) versus 1000/T. The Friedman model adequately described the kinetic behaviour of both systems. The Tin-containing formulation started curing at higher temperatures (~140–150 °C), indicating a greater initial energy barrier. The Ea(α) curve showed high values (~80 kJ/mol) for α 0.2, attributed to the formation of high-energy catalytic complexes. For α > 0.2, a sharp decrease in Ea ( 20 kJ/mol) indicated the onset of autocatalytic propagation. In contrast, the system without Tin exhibited stable Ea values (~45–55 kJ/mol), suggesting a more homogeneous and thermally controlled process. Regression coefficients ($R^2$ > 0.98) and sigmoid fits (deviation ±10%) confirmed the model's validity. Overall, the Friedman method proved effective for describing the curing kinetics of these bio-based epoxy systems. The presence of Tin led to a multifaceted and accelerated curing mechanism, while its absence resulted in a simpler, thermally governed process with lower chemical complexity.

# sciforum-138647: Turning trash into treasure: PHB bioplastic production from agro-industrial waste by native *Bacillus* strains

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Given the growing accumulation of waste from agricultural, domestic, and industrial activities, and the continued dependence on fossil-based plastics, a sustainable alternative based on the bacterial biotransformation of waste for the production of polyhydroxyalkanoate (PHA) bioplastics is proposed. This research focuses on evaluating agro-industrial waste generated in Santander, Colombia, as a raw material for the production of PHAs, within a circular economy framework that aims to repurpose waste and give it a second useful life. A methodology was designed based on the fermentation of two native bacterial strains, *Bacillus thuringiensis* and *Bacillus cereus*, using waste such as pineapple peels and copoazú pulp. The process consisted of two stages. In the first stage, PHA production by each strain was evaluated using the waste products, with concentrations based on their reducing sugar content (10 g/L). In the second stage, fermentation parameters such as time, agitation, waste concentration, inoculum concentration, and pH, were optimized using the waste–strain combination that showed the highest yield in the initial evaluation. The preliminary results show that the highest yield of polyhydroxybutyrate (PHB), the predominant PHA produced, was obtained using pineapple peels and *Bacillus thuringiensis*, with an accumulation of 71.8 ± 4.5%. Meanwhile, *Bacillus cereus* showed a biopolymer accumulation of 68.19 ± 14.02%. This demonstrates the potential of pineapple peels as a carbon source for the production of biopolymers, highlighting their viability as an economic and environmental alternative to synthetic plastics. In addition, it contributes to the recovery of agro-industrial waste and the reduction in the environmental impact associated with its poor management.

# sciforum-146044: Valorization of Waste Fishing Nets: Mechanical Recycling and Characterization of Recycled/ Virgin Blends

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The fishery supply chain, encompassing fishing and aquaculture, processing, preservation, and marketing of fish products, relies extensively on plastic materials. Items such as fishing nets, crates, containers, mussel nets, and packaging are essential for daily operations, but their widespread use contributes significantly to marine litter and environmental pollution. Among them, discarded fishing nets are of particular concern, as they are typically produced from oil-derived polymers and represent a persistent source of plastic waste in marine ecosystems.

In recent years, the development of recycling technologies, especially mechanical recycling, has offered promising solutions to recover these materials and reintegrate them into new production cycles, supporting the transition toward a circular economy.

In this study, fishing nets made of polypropylene (PP) were collected and mechanically recycled. Post-consumer nets were blended with virgin PP to obtain formulations containing 10 wt% and 30 wt% of recycled material. These blends were processed by extrusion and subjected to rheological, morphological, and mechanical characterization in order to evaluate their processability and to assess their suitability for new applications.

The results demonstrate that recycled PP fishing nets can be effectively reprocessed and valorized as secondary raw materials, highlighting their potential for the development of sustainable polymer systems suitable for different applications, thereby reducing reliance on virgin plastics and mitigating environmental impacts.

# Session 2. Polymer Analysis and Characterisation

# sciforum-139269: Advanced Thermal Analysis of Melatonin-Loaded Alginate Hydrogels for Biofunctional Agricultural Coatings

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Hydrogels are crosslinked hydrophilic polymer networks that are capable of absorbing high levels of water without dissolving. Among naturally derived systems, alginate-based hydrogels are particularly attractive due to their biodegradability, non-toxicity, and mild gelation in the presence of calcium ions. In this study, we report the synthesis and thermal characterisation of sodium alginate hydrogels crosslinked with varying $CaCl_2$ concentrations and physically loaded with melatonin, a bioactive indoleamine with antioxidant and plant-growth regulating properties. The aim was to investigate the thermal behavior of the systems and analyze the effect of melatonin incorporation on the polymer matrix. A combination of Thermogravimetric Analysis (TGA), Differential Scanning Calorimetry (DSC), and Temperature-Modulated DSC (TMDSC) was used to assess water content, thermal transitions, and structural interactions. TGA indicated a gradual reduction in water retention with increasing $CaCl_2$ concentration, reflecting the formation of denser, more tightly crosslinked hydrogel networks. Following a seven-day swelling period in deionized water, the observed mass loss below 150 °C was attributed to the evaporation of both free and bound water. Differential Scanning Calorimetry (DSC) and Temperature-Modulated DSC (TMDSC) offered further insight into the structural integrity of the hydrogels and the interactions between melatonin and the polymer matrix. The presence of melatonin led to more distinct and slightly shifted endothermic peaks, potentially linked to the melting of crystalline melatonin or weak, non-covalent interactions with alginate chains. TMDSC enabled the separation of reversing and non-reversing events, highlighting possible reorganization of the matrix upon melatonin inclusion. This supports the hypothesis of partial structural rearrangement of the hydrogel network upon melatonin incorporation. In some cases, the typical melting peak of crystalline melatonin was absent or shifted, suggesting a degree of amorphous dispersion within the hydrogel network.

# sciforum-139366: Exploration of the Scorpion *Buthus atlantis* as a Chitinous Source: Preparation, Characterization and Comparison of Chitins and Chitosans from Different Morphological Parts and the Whole Body

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Chitin and its derivative chitosan are two biopolymers that find numerous applications in various fields. Their industrial production, carried out mainly from marine crustaceans, does not meet the demand either in quantity or quality; hence, the exploration of new chitinous sources is necessary today. In this context, we explored the scorpion Buthus atlantis as a chitinous source in order to evaluate the quality and quantity of chitin it contains. The extraction, carried out with the objective of preserving as much of the native structure of chitin as possible, was carried out solely by deproteinization without resorting to other treatments. The chitins extracted from the different morphological parts of the scorpion were transformed into chitosans by N-deacetylation reactions under the conditions of the Kurita and Broussignac processes. The characterization of chitins and chitosans was carried out using the techniques of Scanning Electron Microscopy, Energy-Dispersive X-ray Spectroscopy, X-ray Diffraction, Fourier Transform Infrared Spectroscopy, Proton Nuclear Magnetic Resonance, Capillary Viscosimetry and Acid-Base Titration. All chitins, obtained with relatively high contents (16 to 24%), are pure and have an alpha structure. As for chitosans, they are prepared with low-value degrees of acetylation (8 to 15%) and molar masses that can vary from low to high (78000 g/mol to 270000 g/mol) depending on the application for which they are intended. These results show that the scorpion Buthus atlantis is a potential source for the production of biopolymers.

# sciforum-139370: Extraction of Chitin from Desert Locust (Schistocerca Gregaria) Wings: Protocol Optimization

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This research focused on the extraction of chitin from an unconventional and underexploited biological source: the wings of the desert locust (*Schistocerca gregaria*). The primary objective was to optimize the conventional chemical extraction protocol to enhance both the yield and quality of the recovered chitin. To achieve this, an additional depigmentation step was introduced prior to the standard deproteinization phase. This modification proved to be highly effective. Notably, it reduced the number of chemical treatments required from seven baths in the classical method to only four, thus decreasing the overall processing time and chemical consumption, while simultaneously limiting the environmental footprint of the extraction process. The optimized protocol also led to substantial improvements in the extraction outcomes. The chitin yield increased markedly, rising from 10% to 29%, which reflects nearly a threefold improvement. In addition, the quality of the biopolymer was enhanced, as demonstrated by the increase in its molar mass, from 537,000 g/mol to 847,000 g/mol, suggesting better preservation of the polymer chains and reduced degradation during processing. These findings highlight the critical impact of both the biological origin and the protocol design on the final characteristics of chitin. This study underscores the necessity of tailoring extraction strategies to specific raw materials in order to obtain high-performance biopolymers suitable for advanced applications in biotechnology, agriculture, and materials science.

# sciforum-138608: Ionogels Containing EMImFSI Obtained via Photopolymerization: Tailoring Mechanical and Electrochemical Properties for Flexible Energy Storage Devices

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In recent years, the rapid advancement of electrochemical technologies—such as supercapacitors, fuel cells, and flexible energy storage—has intensified the search for new functional materials. Ionogels, hybrid systems combining ionic liquids and polymer matrices, have gained attention for their high ionic conductivity, mechanical flexibility, and chemical stability.

This study reports the synthesis and characterization of ionogels containing 1-ethyl-3-methylimidazolium bis(fluorosulfonyl)imide (EMIm FSI), aimed at evaluating their applicability as gel electrolytes in electrochemical capacitors. Various formulations were prepared using different monomer mixtures, and the most promising systems were selected based on visual inspection, conductivity, and mechanical properties.

The most notable result was the development of an ionogel based on Dymax XR-*7*71-MS resin, which exhibited high ionic conductivity, excellent flexibility, and no ionic liquid leaching. The addition of thiol T2 significantly increased conductivity but reduced mechanical strength, especially in systems containing ≥85% IL, which showed low puncture resistance.

Mechanical tests showed that increasing IL content decreased Young's modulus and tensile strength while enhancing elongation, indicating a trade-off between conductivity and durability. FTIR analysis confirmed efficient cross-linking through the disappearance of C=C bands after photopolymerization.

Electrochemical performance was evaluated in three capacitor configurations (IL+GF/A, gel+GF/A, gel+gel). Ionogel-based electrodes enabled pseudocapacitive effects associated with redox reactions, increasing capacitance. The gel+GF/A configuration offered the best performance, balancing conductivity with internal stability. Capacitance declined with increasing scan rate and current, due to ion transport and redox kinetics limitations. High capacitance values in gel systems were attributed to pseudocapacitive contributions, dependent on accessible surface area and reaction dynamics.

Overall, the results show that EMIm FSI-based ionogels can be tailored for optimal performance by adjusting their composition, offering potential as safe and flexible electrolytes in electrochemical energy storage devices.

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# sciforum-135185: Preparation of Highly Filled Metal Polymer Composites and Analysis of Their Physical Properties

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This thesis presents a comprehensive study on the preparation and characterisation of a highly filled metal–polymer composite. The aim of this thesis is to prepare highly filled metal–polymer composites and investigate the effect of filler content on their physical properties. Recycled polyvinyl butyral (PVB) recovered from windshields was used as the matrix material, and two different fillers were used: magnetite iron oxide (FeO · Fe2O3) and manganese–ferrite–zinc oxide (MnO · Fe2O3 · ZnO). The composites were prepared by melt blending using a micro-compounder with varying volume percentages of the filler (20, 30, 40, 50 and 60%). Following the preparation of composites in the micro-compounder, the composites were pressed into thin sheets with a dimension of 17mm*15mm*2mm using a heated compression moulding press (hot press). This process was performed for composites with 20, 30, and 40% volume ratios. However, for 50 and 60% volume ratios, a 40% volume ratio composite was initially prepared in the micro-compounder, and the remaining filler was manually added and mixed with the hot press. To determine the effect of the filling ratio on the mechanical properties, tensile testing was performed. Optical microscopy was used to study particle dispersion, along with an examination of the tensile fractured surface. Additionally, magnetic properties such as coercivity, permeability, losses, and maximum polarisation were measured. This study successfully demonstrated that a composite with an up to 60% filling ratio by volume can be achieved using the melt blending technique, without using any compatibilisers or processing aids. Overall, a highly filled polymer–metal composite is a promising class of composites that can find applications in various industries.

# sciforum-139163: A design-driven strategy for the development of polypropylene composites tailored for 3D printing

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Despite growing interest in additive manufacturing for polymers, its industrial application is limited by a lack of suitable materials. In particular, Fused Filament Fabrication (FFF) relies primarily on amorphous or low-crystalline thermoplastics, most of which are not specifically functionalised. Although polypropylene (PP) is a widely used commodity, it still represents a challenge for FFF applications, mainly due to its semicrystalline nature and unfavourable rheological behaviour.

In this work, an effective strategy for obtaining 3D printable PP-based materials is proposed, also considering the possibility of exploiting the FFF technology for the obtainment of items endowed with specific functionalities and for upcycling purposes.

Firstly, a detailed rheological and thermal characterization of a series of PPs (both homopolymers and heterophasic copolymers) characterized by different viscosity and presence of fillers allowed for highlighting important microstructure/processabilty relationships, providing critical features for the design and development of 3D printable PP-based materials.

In a second step of the research, several kinds of micro- and nano-fillers were introduced within PP with the aim of providing the 3D printed samples with superior mechanical properties, flame retardancy or thermal conductivity.

Finally, recycled PP (r-PP) recovered from different streams was valorized through the formulation of filaments for FFF processes. In this context, on the basis of the known-how achieved in the previous research about PP printability, the formulation of r-PP deriving from municipal solid waste, e-waste or protective single-use face masks was optimized through the introduction of different types of fillers in order to adjust the rheological and thermal characteristics of the material for achieving a successful FFF process.

The obtained results showed that a proper modification of r-PP microstructure and a close optimization of the processing parameters allow for profitably, enhancing the value-added of r-PP and contributing to sustainable manufacturing practices.

# sciforum-139194: Advances in Chemical Recycling of Polyurethane Waste: A Green Chemistry Perspective

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Abstract: Polyurethane (PU) materials are extensively employed in construction, automotive, footwear, and packaging industries due to their durability and versatile properties. However, their crosslinked thermoset structure presents significant challenges for end-of-life disposal, contributing to persistent environmental accumulation and long-term waste management issues. In recent years, chemical recycling methods,particularly glycolysis, have gained attention as promising approaches for PU waste valorization.

Glycolysis involves the cleavage of urethane linkages using a glycol (e.g., ethylene glycol) in the presence of catalysts such as organometallic compounds. This process leads to the formation of low-molecular-weight polyols, which can be reused in repolymerization or formulation of new materials. Optimization of parameters, such as temperature, catalyst concentration, and glycol-to-PU ratio, significantly influences degradation efficiency and product quality.

Analytical techniques like FTIR, NMR, and GPC are commonly used to characterize the glycolyzed products. FTIR spectra typically show the disappearance of urethane peaks and emergence of hydroxyl functionalities, indicating successful depolymerization. NMR provides detailed insight into the structure of the recovered polyols, while GPC confirms molecular weight reduction and homogeneity. During the reaction, controlled volatilization of excess reagents or by-products may occur, which can be minimized or recovered under reduced pressure conditions.

This review highlights recent developments in the glycolytic recycling of PU waste, emphasizing environmentally benign protocols aligned with green chemistry principles. The process not only reduces dependency on fossil-based raw materials but also enables a circular economy approach to polymer sustainability. Continued research is essential to scale up these methods and integrate them into industrial waste management systems.

# sciforum-129203: Crystal Clear: A Bottom-Up Strategy for Polymer Structure Determination Using Vibrational Spectroscopy

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Determining the crystal structure of semi-crystalline polymers is still quite the challenge, especially when relying on powder X-ray diffraction (PXRD) alone. The (typically) poorly resolved patterns often lead to multiple competing models with indistinguishable powder profiles. Herein, an alternative bottom-up strategy is proposed, using experimental vibrational spectra as a diagnostic tool to iteratively build crystal structures piece by piece, from 1D chain conformation to full 3D packing.

The vibrationally-guided methodology was applied to poly(trimethylene 2,5-furandicarboxylate) (PTF), a promising biobased polyester. Infrared and inelastic neutron scattering (INS) spectra collected for amorphous and semi-crystalline samples revealed conformationally sensitive bands that were matched against spectra estimated from discrete DFT models. This allowed the identification of the chain conformation (ss-tggt) present in the crystalline phase and rejection of those incompatible with spectroscopic observations. Using this conformer as a building block, a 3D crystal structure was assembled, comprising 2D sheets stabilized by C–H···O bonds and π–π interactions, and then refined using periodic DFT. This model, which greatly resembles that found for the terephthalic counterpart poly(trimethylene terephathalate) (PTT), proved able to reproduce experimental INS data.

This case study demonstrates the power of vibrational spectroscopy not only as a validation tool, but as an active guide in structure determination. By leveraging spectral sensitivity to local conformation and intermolecular contacts, this bottom-up strategy narrows the pool of viable models early in the process, reducing computational cost and ambiguity. This method complements existing techniques such as NMR crystallography and opens new avenues for understanding structure–property relationships in complex polymer systems.

# sciforum-138522: Design of Safe and Sustainable Hyperbranched Polyesters as Additives for PHAs

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## Introduction

Biopolyesters such as polyhydroxyalkanoates (PHAs) are promising biodegradable polymers for replacing conventional plastics, but their limited toughness and brittle fracture limit their industrial application. To improve these limitations, polymer additives are employed to enhance the mechanical properties. However, most of these are derived from non-renewable resources, and some of them have proven to be harmful to both the environment and human health. So, on these terms, the development of safe and sustainable alternatives is essential. Some of the most promising candidates are hyperbranched polymers (HBPs), characterized by a highly branched architecture and a high functional group density, making them candidates as biodegradable alternatives to common additives.

## Results and discussion

This study focuses on the synthesis and functionalization of hyperbranched biopolyesters supported on microcrystalline cellulose (MCC) for use as an additive to improve the mechanical properties of poly(hydroxybutyrate-co-valerate) (PHBV). These polymers were synthesized via the polycondensation of 2,2-bis(hydroxymethyl)propionic acid (bis-MPA) in the presence of MCC, followed by grafting of linear polycaprolactone chains to enhance the flexibility. The results of thermal and structural characterization (FTIR, TGA, NMR, and DSC) confirm successful synthesis and functionalization; however, they show a higher proportion of linear over branched polymers.

The mechanical properties demonstrate a significant improvement in PHBV's toughness, including the emergence of post-yield fracture behaviour and increased plastic deformation. Moreover, a slight decrease in crystallinity was also observed. This communication will present the results obtained with the newly synthesized additives, confirming their potential as sustainable additives in plastic formulations.

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# sciforum-132668: Easy surfactant-free microemulsions and drawings of their particle size distributions from light microscopy images

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Microemulsions are an effective system for administering active compounds in humans. Regarding this topic, one of the challenges is to obtain surfactant-free microemulsions using biocompatible stabilizers, such as chitosan, to avoid the use of conventional surfactants. Currently, most methods used to obtain average droplet sizes are based on techniques supported by high-cost equipment. Therefore, this study aimed to evaluate the dispersion of olive oil in an aqueous medium stabilized by chitosan, as well as to generate particle size distributions from light microscopy images and software (ImageJ and ORIGIN®). Briefly, olive oil and chitosan in acidic aqueous media were vortexed (3200 rpm); afterward, the samples were filtered through filter paper to obtain the final emulsions. Thus, microemulsions with different oil-to-polymer ratios (1:5, 1:10, and 1:15) and different chitosan concentrations (5, 10, and 15 mg/mL) were prepared. To obtain particle sizes, images of emulsion samples at different storage times (1, 24, and 168 h) were acquired using an optical microscope and processed by Digital Image Analysis (DIA) with the ImageJ software. Particle size distributions were generated from different particle sizes of each sample, and their respective graphs were designed in the ORIGIN® software. As shown in the results, 5 min under stirring was a suitable time to obtain microemulsions, and the filtration improved the homogeneity of droplet sizes. Also, it was found that the higher the concentration of chitosan or oil, the greater the number of particles. After 1 h of preparation, particle sizes increased slightly with the chitosan concentration (e.g., from 1.37 to 1.62 µm). The emulsion with 10 mg/mL of polymer (1:10 oil-to-polymer ratio) remained stable for up to one week, irrespective of the type of chitosan. It was concluded that the proposed low-energy method led to the formation of stable surfactant-free microemulsions, and particle size distributions can be generated using a free standard tool.

# sciforum-147077: Experimental, Computational and statistical Analysis of the mechanical response of 3D-Printed TPU and PLA

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With the help of experimental testing and finite element analysis (FEA), this study conducts an in-depth investigation into the mechanical action of thermoplastic polyurethane (TPU) and polylactic acid (PLA) that have been created using 3D printing technology. In order to characterize their behavior under a variety of infill densities and patterns, tests of uniaxial tensile and cyclic compression were carried out. PLA revealed stronger stiffness and yield strength, making it excellent for rigid prototypes, but TPU demonstrated superior elasticity and energy dissipation, making it suited for flexible applications. Furthermore, TPU was shown to be suitable for flexible applications.

For the purpose of developing predictive models for the mechanical qualities, the research combined statistical analysis through the use of Response Surface Methodology (RSM). This made it possible to optimize the printing parameters. The capacity of finite element analysis (FEA) simulations to accurately replicate experimental results by utilizing proper hyperelastic models is evidence that these simulations are capable of capturing the complicated material response. The purpose of this effort is to build a reliable system for evaluating and improving the mechanical performance of 3D-printed materials. This methodology will provide useful insights for the design of these materials and their application in a variety of engineering branches.

# sciforum-137436: Influence of boundary conditions and impact velocity on the ballistic behavior of aramid fabrics

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This paper explores the ballistic impact behavior of a 1/1 fabric composed of aramid yarns using numerical simulations in ANSYS Explicit Dynamics. The main objective is to analyze the influence of boundary conditions applied to the yarns and the impact velocity on the structural response of the material under the action of a 9 mm FMJ (Full Metal Jacket) projectile. The fabric is modeled at the meso scale, where the structure of the yarn fabric is represented explicitly, without detailing the individual filaments in the composition of each yarn. The yarns are defined as elastoplastic materials with bilinear isotropic behavior, using parameters obtained from the literature for Kevlar or Twaron aramid fibers. Four fastening scenarios were analyzed: four-edge fastening, two-edge fastening by blocking the transverse faces of the yarns, and fastening applied over a length of 1.5 mm at the ends of the yarns. Five impact speeds were investigated: 430 m/s (according to the NIJ standard), 330 m/s, 320 m/s, 220 m/s, and 120 m/s. The results obtained include the maximum deformation of the fabric, the distribution of stresses, and the analysis of projectile penetration. The simulations indicate a clear correlation between impact velocity, fastening type, and the fabric's ability to dissipate energy and resist penetration. The study contributes to the understanding of the protective mechanisms of ballistic textiles and supports the development of more effective configurations. The results obtained are validated with papers from the specialized literature.

# sciforum-137581: Low-density polyethylene beads integrity disruption induced by native *Fusarium oxysporum*

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Low-density polyethylene (LDPE) is a widely used thermoplastic polymer in the production of plastic bags and pipes due to its flexibility, chemical resistance, and low cost. However, its recalcitrance to degradation contributes significantly to global plastic pollution, underscoring the need for strategies to enhance its breakdown. This study assessed the physicochemical alterations in LDPE beads after 30 days of exposure to native Colombian fungal strains of *Fusarium oxysporum* (FOCIC01), under conditions where LDPE served as the sole carbon source. The experimental setup included mineral salt medium inoculated with the FOCIC01 strain. Following incubation, LDPE beads were separated from fungal biomass via sequential washing with 1% SDS, rinsing with 70% ethanol and sterile distilled water, followed by sonication to ensure thorough removal of biofilm and surface residues prior to analysis. Structural and chemical changes in the polymer were analysed through Scanning Electron Microscopy (SEM), Fourier Transform Infrared Spectroscopy (FTIR), and Matrix-Assisted Laser Desorption/Ionization Time-of-Flight Mass Spectrometry (MALDI-TOF). SEM revealed pronounced surface erosion, fissures, and pitting in LDPE beads exposed to the fungal strain, in contrast with the smooth, intact control beads. FTIR analysis showed the appearance of new absorption bands corresponding to hydroxyl (–OH) and carboxyl (–COOH) groups, indicating oxidative modification of the polymer structure. These spectral changes suggest the occurrence of oxidative degradation processes, likely facilitated by fungal enzymatic activity. MALDI-TOF mass spectrometry, performed on the supernatants of the degradation assays, revealed fragmentation patterns indicative of partial depolymerisation, with signals consistent with low-molecular-weight polyethylene oligomers. The integration of these complementary analytical approaches demonstrates the potential of native *F. oxysporum* to initiate degradation of LDPE through extracellular mechanisms. This work provides new insights into polymer–fungus interactions and supports the development of fungal-based biodegradation strategies for synthetic plastic waste.

# sciforum-128031: Mathematical Modeling, Derivation, and Analysis of Polymer Transportation in Extrusion Molding

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Extrusion molding is a widely utilized technique for processing polymers—particularly plastics and rubbers. Despite its broad industrial application, several aspects of the transport behavior of polymers during extrusion remain inadequately understood. Undesirable and unexpected phenomena such as sharkskin instabilities, turbulent flow transitions, and flow fractures frequently occur during the process. However, definitive explanations for these phenomena are still lacking. Numerous studies suggest that the transport behavior of polymers plays a crucial role in the emergence of these instabilities. To date, several empirical investigations have examined the rheological properties of conventional polymers to better understand these transport dynamics. Nonetheless, significant limitations persist, and a comprehensive theoretical model that can predict and explain these behaviors remains elusive.

To contribute toward resolving this issue, the present study employs both single- and double-concentric cylinder models to simulate the screw mechanism within an extruder. These models are used to derive and analyze the transport characteristics of polymers during extrusion molding.

This study was divided into two main sections. The first section focuses on the transport behavior of solid polymer particles, typically occurring in the feed zone (zone 1) of the screw. The second section examines the transport of polymer melts, which predominantly takes place in the melting and metering zones (zones 3 and 4). Key boundary conditions—including velocity profiles, flow rates, shear rates, and shear stresses—are systematically investigated and discussed to provide deeper insight into the mechanisms governing polymer transport in extrusion molding.

# sciforum-130134: PET glycolysis in the presence of solid $CoMnAlO_x$

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PET glycolysis corresponds to a highly efficient Chemical recycling process, which offers some advantages over physical recycling. The main product is the Bis(2-hydroxyethyl) terephthalate – BHET, the PET monomer, which provides high-quality recycled PET, such as the one used in food packaging. BHET can also be used in the production in the production of new copolymers. PET glycolysis has its efficiency improved in the presence of a catalyst. Therefore, in the present work, Co, Mn, and Al-based oxide catalysts were synthesized by coprecipitation followed by calcining at 400 °C. These catalysts are poorly crystallized, hydrotalcite-like structured, with surface areas of 114 $m^2.g^{-1}$ and 103 $m^2.g^{-1}$, for CoMnAl and CoAl, respectively. Both catalysts were applied in the conversion of PET to BHET through glycolysis. Best results were obtained in the optimized parameters of 0.5% catalyst/PET, EG/PET = 5, reacting at 200°C in 60 minutes, which resulted in PET conversion of 96.7 and 40.2% in the presence of CoMnAl.c and CoAl.c, respectively. Both catalysts were still advantageous when compared to the non-catalysed PET glycolysis, which led to 0% PET conversion in the same optimized parameters. The results show that Mn promoted the performance of CoAl.c, which led to CoMnAl.c with a higher efficiency on PET conversion.

# sciforum-142796: pH- and thermoresponsive amphiphilic terpolymers: Synthesis and formulation of drug-loaded nanomicelles

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**Introduction**

Smart polymers that change their structural conformation upon external stimuli have emerged as candidates for the formulation of multi-responsive nanocarriers. Development of such nanoplatforms is crucial for bypassing body resistance mechanisms in targeted drug or gene delivery applications.

**Methods**

In this work, reversible addition–fragmentation chain transfer (RAFT) polymerization led to the synthesis of a series of poly(2-(diisopropylamino)ethyl methacrylate-co-2-(dimethylamino)ethyl methacrylate-co-oligoethylene glycol methyl ether methacrylate), P(DIPAEMA-co-DMAEMA-co-OEGMA) terpolymers. Molecular characterization and self-assembly of polymers in various aqueous environments were carried out. The organic co-solvent protocol was followed for the drug loading of curcumin and quercetin in polymeric micelles. Physicochemical and photophysical properties of loaded nanoparticles were evaluated for a period of three weeks.

**Results**

P(DIPAEMA-co-DMAEMA-co-OEGMA) terpolymers were successfully synthesized, presenting different pH responses at pH values of 3, 7, and 10 in terms of mass and size of the self-assembled copolymer structures. Temperature-dependent dynamic light scattering (DLS) experiments revealed the thermoresponsive properties of the copolymer micellar aggregates. Curcumin and quercetin were efficiently encapsulated within the micelles, presenting colloidal stability as measured by DLS and ultraviolet–visible absorption spectroscopy (UV-Vis). Fluorescence experiments resulted in enhanced and red-shifted spectra for curcumin-loaded nanoparticles compared to pure curcumin. Quercetin-loaded ones also exhibited an enhancement in aggregation characteristics.

**Conclusions**

Multi-responsive and stable nanocarriers were fabricated, showcasing the applicability of P(DIPAEMA-co-DMAEMA-co-OEGMA) terpolymers in biomedicine.

# sciforum-129753: Preparation and characterization of carrageenan/gelatin microcapsules with the addition of essential oil

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Encapsulation consists in surrounding the encapsulated substance (core, nucleus, active substance) with walls and thus closing it in the resulting structure. Most often, this is done by coating with a thin film of polymer (single capsule) or placing the core substance in the produced polymer matrix (agglomerate) by occlusion and/or adsorption [1-3]. One of the methods of obtaining microcapsules is coacervation. In this paper, microcapsules based on κ-carrageenan and gelatin type A were prepared by coacervation. The microcapsules were enriched with essential oils such as citronella oil and cinnamon oil, which has antimicrobial properties, in order to obtain materials that inhibit the growth of microorganisms. After optimizing the microcapsule production process, they were applied to natural leather to create a new antibacterial, odorless, and environmentally safe leather material. The microcapsules containing the selected essential oil were applied to the leather material in a batch process using a padding technique using a laboratory padding machine with adjustable roller pressure. Next, the antimicrobial properties of the new leather materials were tested against two bacterial strains, E. coli and S. aureus, and two fungal strains, Aspergillus niger ATCC 6275 and Candida albicans ATCC 1023. Very good and effective microbiological and antifungal effects were achieved with just 10% of microcapsules in the bath.

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# sciforum-138953: Preparation and evaluation of Sulfadiazine loaded T908/PVP hydrogels for transdermal drug delivery through solution blow spun nanofibers. Study abstract

**Hanan Altaha**

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This study investigated the formulation, ionic conductivity, swelling properties, thermosresponsive behavior of hydrogels made of Pluronic T908 and polyvinylpyrrolidone (PVP) and their ability to enhance the solubility of the widely used antibiotic Sulfadiazine (SDZ) in aqueous solutions. To maximize the circumstances to produce a homogenous hydrogel, different concentration ratios of the two polymers were assessed. Critical transitions depending on the composition and content of polymers were identified through mapping the phase behavior under controlled heating. Ionic conductivity experiments revealed that despite both polymers are nonionic, PVP could slightly increase the ionic mobility of H2O ions, on the other hand, T908rich formulations considerably increased ionic mobility and conductivity due to micelle formation. The Arrhenius equation was used to determine the activation energy (Ea) for ion transport, and the results showed that conductivity improved at intermediate T908: PVP ratios. T908 integration improved water uptake and decreased polymer rigidity, according to swelling studies; 30 wt.%T908 pure solution showed around four times higher swelling capacity than PVP solution at the same wt.%. And the solution mixture 25% T908 5% PVP showed the maximum water uptake among the evaluated mixture formulations.

After that, SDZ was loaded into variant formulations of T908 and PVP solutions and studies proved that both pure polymer solutions and mixtures of two polymers enhanced the solubility of SDZ in comparison to H2O alone. The combined findings of this study shed light on how to modify PVP-T908 hydrogels to be used in biomedical uses and medication delivery.

# sciforum-139224: Static Tensile Loading and Its Influence on the Structural Integrity of ABS

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Plastics have become indispensable in modern life, valued for their versatility, affordability, and ease of manufacture. As their use expands across industries such as automotive, aerospace, consumer electronics, and construction, understanding their mechanical performance under various loading conditions becomes increasingly important. Despite their advantages, polymers are susceptible to damage and degradation over time, especially when subjected to sustained or repeated mechanical stresses. This study examines recent developments in fracture mechanics as applied to polymeric materials, with a focus on the need for precise design and sizing to ensure structural reliability in practical applications. A comprehensive understanding of how polymers respond to different mechanical loads, particularly in the presence of microstructural defects or environmental influences, is essential for predicting long-term performance and preventing premature failure. The research specifically investigates the mechanical behavior of ABS (Acrylonitrile Butadiene Styrene) under uniaxial tensile loading, emphasizing the role of damage accumulation in altering its mechanical properties.

To achieve this, the study employs experimental testing combined with advanced analytical techniques, including non-linear regression and damage modeling. These methods enable the identification of critical failure thresholds, providing valuable insights for maintenance planning, design optimization, and the development of more durable polymer-based components in engineering systems. Moreover, the results lay the groundwork for extending damage prediction models to other thermoplastic materials under similar loading conditions.

# sciforum-139315: Study of Cellulose nanocristals-Reinforced Polymethyl methacrylate/Polyurethane Interpenetrating Polymer Networks for Enhanced Performance in Automotive Applications

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The automotive industry aims to develop high-quality engineering materials that ensure safety and optimal performance under various conditions. A critical application example is automotive headlights, whose durability and performance can be compromised by environmental and mechanical factors. To address these challenges, an alternative is proposed through the development of interpenetrating polymer networks (IPNs) of poly(methyl methacrylate) (PMMA) and polyurethane (PU), in PMMA/PU ratios of 50/50 and 80/20 [1], reinforced with 0.1% by weight of crystalline nanocellulose (CNC) obtained from disposable cups. Using experimental techniques such as Fourier-transform infrared spectroscopy (FTIR) and X-ray diffraction (XRD), it was determined that the fiber processing for CNC extraction does not modify or degrade its main functional groups [2], and allows for a crystallinity percentage of 52.51% [3]. Additionally, to identify the characteristic morphologies of each polymer, confocal laser scanning microscopy (CLSM) analysis was employed, enabling the visualization of cellulose particles present. The observed fiber properties are also described, along with an analysis of cellulose dispersion within the polymer matrix and its fluorescence emission. Finally, durability is studied through tensile and compression mechanical tests, conducted before and after exposure to weathering. The results indicate less mechanical damage when crystalline cellulose is added to the PMMA/PU with a 50/50 ratio compared to a 80/20 ratio.

# sciforum-154427: Synchrotron X-ray Scattering as a Tool for Probing the Nanostructure of Complex Polymer Systems

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The fine-structure characterization of polymer-based materials is one of the fastest-evolving areas in polymer science. Modern synchrotron light sources, equipped with high-flux microfocus optics and advanced detectors, offer powerful capabilities for investigating morphology, crystallinity, and nanoscale organization. Over the past two decades, synchrotron wide- and small-angle X-ray scattering (WAXS and SAXS) beamlines have become increasingly accessible and very useful for studying complex polymer systems.

This lecture presents three representative case studies. First, synchrotron WAXS and SAXS reveal structural features associated with enzyme immobilization on engineered polyamide microparticles, an essential step in designing efficient biocatalytic materials. Second, microbeam WAXS scans of polyamide powders (grain sizes 20–50 μm) produced by *in situ* polymerization effectively detect micron-scale inhomogeneities caused by embedded clays or metal particles, advancing the development of smart polymer-based enzyme carriers and microdevices. Finally, in polymer microfibrillar composites (MFCs), WAXS quantifies transcrystallinity and links it directly to mechanical performance, while advanced SAXS data analysis under controlled strain demonstrates reversible, strain-induced crystallization of the matrix polymer impossible to observe by other methods.

These examples show how synchrotron-based WAXS and SAXS have become essential tools for exploring nanostructure–property relationships and guiding the design of next-generation functional and sustainable polymer materials.

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# sciforum-147257: Synthesis and Characterization of n-Butyl Vinyl Ether Copolymer

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Macromolecular chemistry profoundly shaped the twentieth century through the remarkable development of new materialsi. The ongoing expansion of polymer science is driven by the constant demand for novel materials with unique properties that can enable nnovation.

Macromolecules, polymers, and block copolymers synthesized through living polymerization are particularly well-suited to meet this challenge due to their specific synthesis methods. Poly(vinyl ethers), which can only be polymerized via cationic methods, are known for their adhesive properties and high reactivity. When copolymerized with various vinyl monomers, different types of copolymers can be obtained, which can lead to improved properties.

Maghnite-H+, a true green ecocatalyst, has been the subject of numerous studies and applications involving various vinyl and heterocyclic monomers, including vinyl ethers. The primary objective of this work is to prepare block copolymers based on n-butyl vinyl ether using Maghnite-H+ as the ecocatalyst.

The first step of this study is the synthesis of poly(n-butyl vinyl ether) catalyzed by Maghnite-H+. The resulting polymer will be fully characterized using various analytical methods, including nuclear magnetic resonance (1H NMR), infrared (IR) spectroscopy, gel permeation chromatography (GPC), viscometry, and differential scanning calorimetry (DSC).

The poly(n-butyl vinyl ether) obtained will then be used as a macrocatalyst for the cationic polymerization of styrene (in both bulk and solution). This process aims to produce a PnBVE-b-PS block copolymer. The final product will be characterized using the previously mentioned methods, in addition to thermogravimetric analysis (TGA).

# sciforum-137425: The interplay between cross-contamination, aging and reprocessing in the mechanical recycling of HDPE-based packaging

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Developing efficient mechanical recycling strategies for polyolefins is challenging due to several factors. Firstly, thermo-mechanical degradation during reprocessing and other degradation throughout their service life alters the microstructure of polyolefins, causing a gradual decline in performance. Also, minor cross-contamination in recycled polyolefins is often due to limitations in sorting technologies. These factors lead to recyclates with a complex morphology which restricts their applications. Our work aims to address these issues for high-density polyethylene (HDPE) containing low amounts of polypropylene (PP) and polyethylene terephthalate (PET) as contaminants.

Starting from the typical composition of HDPE bottles, cross-contaminated HDPE-based materials were exposed to photo- and thermo-oxidative ageing treatments. These systems were then reprocessed and analysed to evaluate modifications caused by cross-contamination and degradation, and their impact on the polymers' mechanical properties. Firstly, it was demonstrated that cross-contamination significantly reduces the formation of oxygen-containing functional groups from photo- and thermo-oxidation, particularly in photo-oxidised materials. Furthermore, the addition of polypropylene (PP) and polyethylene terephthalate (PET) led to immiscible blends, with the microstructure being influenced by the specific ageing treatment on the HDPE matrix phase. Notably, the photo-oxidised HDPE sample containing PP and PET exhibited significant morphological alterations driven by ageing and reprocessing, resulting in a more refined morphology compared to the non-aged counterpart. Finally, tensile characterisation results emphasised the critical role of cross-contamination in severely embrittling HDPE, particularly in thermo-oxidised materials. In contrast, the presence of PP and PET has a negligible impact on the ductility of HDPE under photo-oxidative ageing, which is already significantly compromised by degradation.

# sciforum-142044: Understanding changes in the microstructure of polyolefins during reactive extrusion

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Reactive extrusion is a common approach in industry to modify polymer structures and obtain and modify some of their properties. To increase the melt flow rate (MFR) in polypropylene (PP), adding peroxide during extrusion is a very common application. By adding peroxide, the molecular weight of PP is reduced by β-scission [1]. More advanced modification of the polymer structure can be performed by adding a radical initiator like a peroxide an coupling agent [2] or adding another polymer [3] or a combination of both to obtain graft polymers with the target polymer properties. This combination of different substances in conjunction with the radical process leads to variety of products and by-products, which makes the proper characterization of the various products quite challenging.

In this presentation, the characterization of two different polyolefins, LCB-PP and a HDPE-g-PP, obtained by reactive extrusion processes is presented.

To better understand the influence of chain architecture on the melt relaxation dynamics of LCB-PP, a combination of NMR spectroscopy and GPC-V-MALS was employed [2].

HDPE-g-iPP molecules were generated via reactive extrusion without the use of a coupling agent and were identified within the HDPE/iPP matrix using advanced hyphenated fractionation techniques, including cross-fractionation chromatography and two-dimensional HPLC in combination with spectroscopic techniques like IR. The effect of HDPE-g-iPP as a compatibilizer was confirmed by thermal, dynamic mechanical, and morphological analysis, as shifts in crystallization temperatures and glass transition temperatures and diffuse domain interfaces were observed [3].

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# Session 3. Recent Functional and Structural Applications of Polymer Systems

# sciforum-138404: From Wool Waste to Clean Air: A Green Sandwich Membrane Solution

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The mitigation of air pollution caused by fine particulate matter remains an urgent global concern. To address this challenge, sustainably and bio-based air filters incorporating waste-derived natural fillers offer a promising alternative to conventional synthetic materials. In this study, innovative sandwich-structured membranes were developed by integrating a hot-pressed mat of waste wool fibers (WWFs) as a structural core, flanked by two fibrous outer layers composed of polylactic acid (PLA) and finely ground waste wool powder (WWP), produced via the solution blow spinning (SBS) technique. The resulting sandwich-structured waste wool-based membrane (S-WWM) was tested under various flow conditions and environmental humidity levels. The incorporation of 10 wt% WWP into the PLA matrix enhanced the spinnability and fiber morphology due to changes in solution viscosity. The multilayer structure, characterized by a balance between pore size and low packing density, achieved outstanding $PM_1$ filtration efficiency (99.5%), with a moderate pressure drop (70 Pa) at 32 L/min. In addition, the membrane showed strong performance retention over five filtration cycles and remained stable in humid conditions. These membranes are characterized by the unique properties of wool fibers, such as excellent breathability and mechanical strength, combined with high filtration efficiency achieved by PLA composite fibers. These results demonstrate the potential of upcycled wool-based materials in fabricating high-performance, reusable, and environmentally friendly air filtration systems.

# sciforum-142085: Cellulose-driven supported liquid membranes with (choline chloride)-based deep eutectic solvents for CO2 separation from biogas

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**Introduction**. Gas separation membranes enable technologies that use selective permeation to separate gas mixtures of interest, such as biogas or flue gas, thereby reducing greenhouse gas emissions. Adding liquid additives to the polymer matrix creates supported liquid membranes (SLMs), which can improve their $CO_2$ capture performance. Neoteric additives like deep eutectic solvents (DESs) can be used for SLM production due to their highly adjustable compositions, suitable to tailor task-specific membranes. In this work, This study investigates the impact of different choline chloride (ChCl)-based DES on the stability, physicochemical properties and $CO_2/CH_4$ separation of DES-based SLMs (DSLMs) using different cellulose-based materials as a polymeric substrate, such as regenerated cellulose (RC), cellulose nitrate (CN) and cellulose acetate (CA).

**Methods**. DES used in this work were based on ChCl as a hydrogen bond acceptor and different hydrogen bond donors: urea (U), glycerol (Gly) or Malic acid (MalAc) among others. DSLMs were produced by a vacuum assisted method. Structural, morphological and thermal properties of membranes were characterized by Fourier transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM), and energy dispersive X-ray (EDX).

**Results** Single- and mixed-gas tests were conducted and permeability and selectivity of $CO_2/CH_4$ ($\alpha CO_2/CH_4$) was calculated. FTIR spectroscopy confirmed the presence of DESs within the polymeric structure. In general, $\alpha CO_2/CH_4$ of the studied membranes resulted to be competitive with those reported in specialized literature, above 100 in some cases such as ChCl:U SLMs.

**Conclusions**. DES-based SLMs developed in this work demonstrated strong potential for selective $CO_2$ separation while also presenting a greener approach within carbon capture technologies, making them promising candidates for carbon capture technologies, including environmental applications such as biogas upgrading.

# sciforum-146727: Development of poly(3,4-ethylenedioxythiophene) polystyrene sulfonate/Triton X-100-conductive hydrogels for bioelectronic applications

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Conductive hydrogels based on poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS) are widely used in bioelectronics because they combine printability with good electrical conductivity. However, their brittle nature restricts their durability, especially in implantable devices that must bend, stretch, and remain reliable over time. A key challenge is therefore to create hydrogels that are both mechanically compliant and electrochemically stable.

In this work, we describe a simple design strategy using Triton X-100, a common surfactant, as a plasticizer for lyophilized PEDOT:PSS hydrogels. Mechanical testing showed that plasticization significantly reduced stiffness and viscosity, while elongation at break more than doubled and fracture strength increased. Together, these improvements converted a fragile material into a tough, flexible, and stretchable conductor. Importantly, the electrical function of the hydrogel was largely preserved.

To evaluate device performance, the plasticized hydrogel was integrated into a polydimethylsiloxane (PDMS) encapsulation mimicking an electrode contact. Cyclic voltammetry remained stable with no significant unwanted redox reactions. Impedance spectroscopy revealed only a small increase at 1 kHz, consistent with fewer electron pathways, but this trade-off was minor compared with the substantial mechanical gains.

Overall, this study shows that simple plasticizer additives can tune the balance between mechanics and conductivity. By achieving softness, toughness, and electrochemical reliability in the same material, this strategy moves PEDOT:PSS hydrogels closer to long-term use in bioelectronic interfaces.

# sciforum-120927: A Novel Hybrid Hydrogel Cross-linked by Electron Beam for Controlled Release of 5-FU

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Multifunctional drug delivery systems incorporating 5-fluorouracil (5-FU) represent a novel therapeutic strategy in cancer target treatment while minimizing damage to healthy cells. This study aimed to develop and evaluate new hydrogel compositions based on poly(vinylpyrrolidone), carboxymethylcellulose, poly(ethylene glycol), and agar, synthesized and sterilized via e-beam irradiation using a dose of 30 kGy. The cross-linked hydrogels were evaluated in terms of swelling properties in different pH media from 4 to 8, mechanical properties, drug loading capacity, and *in vitro* drug release and biodegradation profiles. Additionally, the 5-FU release kinetics was investigated using several mathematical models. The swelling results showed that the pH of the solutions had a substantial impact on swelling, as well as on drug loading capacity. Compared to the basic medium (970%), a greater absorption capacity was seen at pH 7.4 (1385%) and in an acidic medium (1200%). In comparison to the loss modulus (G" = 1580 Pa), the hydrogels showed noticeably higher storage modulus values (G' = 36,700 Pa), indicating elastic behavior and confirming the existence of a stable macromolecular network. Notably, this hydrogel demonstrates a higher 5-FU drug-loading capacity of 5.5 mg/g at pH 6, exhibiting a cumulative release profile of 96% at pH 5 and 80% at pH 7.4 within 30 hours. The experimental kinetic data fit best to the Korsmeyer–Peppas, Peppas–Sahilin, and Makoid–Banakar kinetics models with correlation coefficients ($r^2$) above 0.99, revealing a Fickian mechanism transport of 5-FU within the hydrogel matrix. The aforementioned findings show that hydrogel has the potential to be used as an intelligent wound dressing for the treatment of local cancer.

# sciforum-139123: Advanced Multifunctional Guar Gum Hydrogel IPN: Tailored Porosity and Enhanced Gastroretentive Drug Delivery Performance

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**Introduction**

Gastroretentive drug delivery systems (GRDDSs) have emerged as a promising strategy to enhance the pharmacokinetic profile and therapeutic performance of orally administered drugs such as amoxicillin (AMOX). In the present work, innovative GRDDSs were formulated through the synthesis of super-porous guar gum (GG)-based interpenetrating polymer networks (IPNs) [1].

**Methods**

IPNs were developed via simultaneous Diels–Alder (DA) crosslinking utilizing di- and tri-functional furfuryl monomers and a dimaleimide monomer [2], within a GG solution. This one-pot procedure incorporated porogenic agents, such as polyethylene glycol (PEG) or sucrose, as well as AMOX. The physicochemical properties of the resulting systems were subsequently characterized by rheological, morphological, swelling, and floating tests.

**Results**

The incorporation of porogens was effective in generating porous structures, increasing the swelling index to 2,000%, and enhancing both the storage modulus and the complex viscosity of the hydrogels. The resulting hydrogels exhibited mucoadhesive and floating properties, making them suitable for prolonged gastric retention. PEG-based IPN offered improved drug delivery performance, including sustained release of AMOX.

**Conclusion**

In contrast to non-crosslinked control samples, all IPNs achieved uniform and mechanically resilient hydrogels. Rheological and swelling studies demonstrated that both the nature and concentration of the porogenic agents significantly influenced the structural and functional properties of the hydrogels.

These results underscore the promise of one-pot IPN biocompatible preparation, coupled with porogen modulation, as a viable strategy for the development of GRDDS, enabling sustained drug release.

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# sciforum-135520: AI-Driven Development of Carbazole-Functionalized Memristors: Unlocking Resistive Memory and Synapse-Mimicking Functionality for Next-Gen Computing

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The synthesis and characterization of a series of carbazole-based polymers are investigated, focusing on their potential application in AI-driven bistable memory devices and neuromorphic computing architectures. These polymers incorporate carbazole moieties into their sidechains, facilitating π–π interactions and enhancing charge transport. When deposited as thin films between ITO and Al or Au electrodes, these materials demonstrate clear memristive behavior through voltage-induced conductance switching. The devices exhibit bistable conductivity with a pronounced hysteresis, retaining ON/OFF states for extended periods—several hours—when subjected to electric fields above a certain threshold, as detailed in recent reports [1–3].

In addition to their non-volatile memory characteristics, these carbazole-functionalized layers mimic key features of biological synapses under low to moderate biasing. Through the repeated application of voltage pulses, the devices show short-term plasticity (STP) and long-term plasticity (LTP), paired-pulse facilitation (PPF) and depression (PPD), spike-timing-dependent plasticity (STDP), and Hebbian associative learning—traits essential for hardware-based neural networks and cognitive computing. These neuromorphic behaviors are enabled by underlying physical mechanisms such as voltage-triggered conformational transitions, charge carrier trapping and detrapping, and redox-based switching, which have been elucidated using spectroscopic and electrical measurements [1–3].

This work underscores the promise of carbazole-functionalized polymers as active materials for organic memristors. Their multifunctionality—spanning stable memory storage and dynamic synaptic emulation—makes them excellent candidates for next-generation, low-power neuromorphic systems and adaptive artificial intelligence applications. The integration of these organic materials offers a scalable and tunable approach to bridging the gap between biological computation and electronic devices.

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# sciforum-139048: Bioactive Chitosan Films via Methylimidazole Functionalization: Antimicrobial and Antioxidant Enhancement

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ICTP-CSIC

Chitosan (CS) is a biocompatible and biodegradable polysaccharide with high potential for functional material development, especially in the design of active films for biomedical or packaging applications. However, its limited solubility and moderate bioactivity restrict the applicability. In this study, a novel CS derivative was synthesized via N-acylation using 1-methylimidazole (MeIm), aiming to enhance the intrinsic antimicrobial and antioxidant properties of this native polymer. An acidic group was added into MeIm (MeImB) and then, the functionalization with the polymer was performed under aqueous conditions employing an EDC/NHS coupling, targeting the primary amino groups of CS to introduce the imidazole ring moieties covalently. Structural characterization of the modified polymer (CS-MeImB) was performed by solid state NMR and elemental analysis, confirming successful functionalization

The resulting derivative (CS-MeImB) was processed into thin CS based films by solvent casting in acidic aqueous media, and using glycerol as plasticizer. In addition, a chitin nanowhiskers (Nw) were prepared and added to reinforce these films. The characterization of these Nw and the resulting films was performed by thermogravimetric analysis (TGA) and X-ray diffraction analysis (DRX), confirming successful integration, while mechanical tests showed good flexibility and improved stability.

The incorporation of the MeIm group significantly enhanced the bioactivity of the films. Antimicrobial assays demonstrated strong inhibition against both Gram-positive (*Staphylococcus aureus, Enterococcus faecalis*) and Gram-negative (*Escherichia coli, Pseudomonas aeruginosa*) bacteria. Moreover, antioxidant activity evaluated via DPPH assay revealed a notable radical scavenging ability, which was markedly higher than that of native chitosan, reaching complete inhibition at lower concentrations.

These results suggest that the integration of 1-methylimidazole into the CS matrix is a promising strategy to create multifunctional biopolymer films with improved production for sustainable applications in food packaging requiring antimicrobial and antioxidant activity.

# sciforum-137717: Biodegradable chitosan-based nanofibers as bioabsorbable wound dressings

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## Introduction

Chitosan (CS) materials are biodegradable, biocompatible, and can exhibit antimicrobial, hemostatic, and antioxidant properties [1].

Functionalization of chitosan with quaternary ammonium groups (QCS) is beneficial for improving its properties, such as its mucoadhesiveness and bioadhesiveness, and its antimicrobial, anticoagulant, antioxidant, and immunomodulatory properties, making chitosan more suitable for tissue engineering and transdermal drug delivery [2-3].

## Methods

CS/QCS binary fibers were prepared by electrospinning using poly(ethyleneoxide) as a co-spinning agent, followed by its selective removal from the mats.

The composition, morphology, and properties of CS/QCS fibers were investigated, and biocompatible fibers with an optimal CS/QCS ratio that led to a progressive biodegradation rate were investigated in wound healing experiments.

## Results

The presence of the two biopolymers in binary fibers, CS and QCS, was confirmed by FTIR and $^{1}$H-NMR spectroscopy.

Enzymatic degradation, monitored in lysozyme solution in PBS (pH=7.4) for 7 days, showed an increase in the rate of biodegradation along with increasing QCS content.

The presence of QCS in the fibers endowed them with strong antimicrobial activity, especially against Gram-negative bacteria.

Tests on normal human fibroblasts have shown that the fibers can be safely used as medical devices.

Subcutaneous implantation of fibers in Wistar rats did not affect biochemical parameters, indicating their potential for safe in vivo use.

CS/QCS fibers in wound healing experiments proved that there was total closure and active healing of second-/third-degree burn wounds in rats.

## Conclusion

All these findings indicate their potential to function as effective bioresorbable dressings.

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# sciforum-138680: Comparative evaluation of chitosan-based hydrogels in the improvement of agronomic properties

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The urgent need for sustainable solutions in agriculture has prompted the exploration of novel materials to mitigate issues such as excessive fertilizer use, inefficient water management, and soil contamination. Addressing these challenges, this work presents innovative interpenetrated polymeric networks (IPN) based on chitosan (CTS) crosslinked with tris(cyclic carbonate) (TrisCC), engineered as controlled-release biostimulant delivery systems (BDS). The IPN synthesis employed TrisCC, prepared by means of click thiol-ene chemistry, and varying CTS concentrations (2–6% w/v) to modulate network characteristics. A fixed crosslinker-to-CTS ratio targeted 30% amino group involvement, and product properties were thoroughly characterized, including rheology, micromorphology, swelling, biodegradability, and in vitro release of biostimulants, such as melatonin (MEL) or glycine betaine (GB).

The IPN formulated with 6% CTS ($CTS_6$-$TrisCC_{30}$) demonstrated optimal mechanical strength and a highly porous architecture, achieving a remarkable swelling index of 4300%. All systems displayed soil biodegradability, with half-life values influenced by the degree of crosslinking and polymer concentration. Sustained, aqueous release profiles for MEL and GB indicated consistent attainment of bioactive concentrations.

These results highlight the considerable promise of CTS-based IPNs as sustainable, controlled-release platforms for agricultural biostimulants. The innovation lies in the integration of natural biopolymer networks with tunable degradation and release properties, potentially enabling precise nutrient and stress-mitigation strategies in crops. Future work will focus on validating these delivery systems under field conditions to confirm their agronomic efficacy in real-world environments.

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# sciforum-141345: Covalent Adaptable Networks: A New Era of Recyclable and Functional Materials

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**Introduction:**

Covalent adaptable networks (CANs) have recently emerged as a transformative class of polymeric materials that combine structural robustness with dynamic functionality. Unlike conventional thermosets, CANs incorporate reversible covalent linkages that enable reprocessability, repairability, and recyclability. In particular, the development of bio-based CANs is of significant interest, as they align with global sustainability goals while simultaneously delivering advanced performance in shape-memory and shape-shifting applications.

**Methods:**

In this work, we designed and synthesized bio-derived polyester-based CANs incorporating dynamic β-keto carboxylate linkages under catalyst-free conditions. The polymers were fabricated from carbohydrate- and renewable-based precursors, and their structural characteristics were confirmed using FTIR and NMR spectroscopy. Thermal and mechanical properties were evaluated through DSC, DMA, and UTM testing, while stress relaxation experiments were performed to probe the adaptability of the network under thermal stimuli.

**Results:**

The synthesized CANs exhibited excellent tensile strength and notable dynamic malleability, with efficient stress relaxation observed at elevated temperatures. The materials demonstrated rapid self-healing at 150 °C and could be fully reprocessed multiple times without significant loss of performance or deterioration in structural integrity.

**Conclusions:**

This study highlights the potential of fully bio-based CANs as multifunctional, recyclable, and programmable materials. Their combination of mechanical resilience, environmental sustainability, and advanced responsive behaviors provides a highly promising platform for next-generation polymer systems, including applications in self-healing coatings, recyclable plastics, smart functional devices, and sustainable material technologies.

# sciforum-139003: Design and Characterization of Hybrid Hydrogel Architectures Based on Agarose and Functional Copolymers

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## Introduction

Agarose, a marine-derived polysaccharide, is a widely used biomedicine due to its biocompatibility, gel-forming capacity, and inert nature[1]. However, its poor biodegradability and mechanical limitations restrict further clinical use[2]. To address this, we propose the synthesis of a novel biodegradable semi-IPN combining agarose with methacrylate-based polymers (DMAEMA, HEMA, OEGMA). The degradation of these networks will be enhanced by incorporating monomers like FMA and VMA, which can establish labile cross-linking points, thereby preventing the formation of microplastics.

## Methods

Copolymers were synthesized via living polymerizations —RAFT and ATRP— with reaction parameters systematically optimized. Following dialysis purification, cross-linking of copolymers was performed using Diels–Alder chemistry, thiol–ene reactions, or ionic interactions, either individually or within an agarose matrix. The resulting materials were characterized by NMR, SEC, SEM, and rheological analyses.

## Results and Discussion

Both polymerization techniques successfully yielded copolymers with the targeted monomer ratios, although RAFT provided narrower dispersity. Among the monomers tested, HEMA produced the strongest hydrogels under identical cross-linking conditions, while thiol–ene cross-linking became the most effective strategy, offering superior rheological properties—even outperforming dual-cross-linked systems (Diels–Alder + ionic). Diels–Alder cross-linked networks did not exhibit retro-Diels–Alder behavior upon heating unless equilibrium was deliberately shifted. Incorporation of agarose to form semi-IPN enhanced the rheological performance of all systems compared to blanks, with the OEGMA-based, Diels–Alder cross-linked network performing best. SEM analysis revealed well-defined microporous architectures, supporting the potential of these semi-IPNs for biomedical applications.

## Conclusions

Novel agarose-based biomaterials with enhanced mechanical strength and porous microstructures were developed for biomedical applications. RAFT and ATRP effectively yielded copolymers from HEMA, OEGMA, DMAEMA, FMA, and VMA with targeted monomer ratios. Gelation was achieved via covalent and ionic cross-linking, with Diels–Alder yielding the most robust semi-IPN.

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# sciforum-147218: Design and synthesis of tailored organic units capable of acting as mechanophores for advanced polymeric materials

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Modern polymers are evolving into multifunctional systems with highly sophisticated behavior, often termed “smart” materials due to their ability to respond to specific stimuli. Mechanophores are generally force-responsive molecules that have greater interest in the daily use of polymeric materials. Mechanoresponsive polymers are particularly attractive as they undergo molecular-level conformational changes and selective bond scission when subjected to mechanical stress. This enables productive, reversible chemical transformations rather than nonspecific degradation.

Dynamic covalent bonds, such as the furan–maleimide Diels–Alder (DA) adduct, play a crucial role in synthetic chemistry, and are now expanding into advanced polymer materials. Among various mechanophores, furan–maleimide adducts are particularly attractive due to their low reaction barrier, reversible bond scission, and efficient stress absorption. Unlike others, DA adducts enable controlled, reversible bond breaking and reforming, making them ideal for self-healing materials.

We aim to develop a novel furan–maleimide-based mechanophore by functionalizing it with different mercaptan groups under simplified reaction conditions. This newly designed mechanophore will be incorporated into polymers such as PMA (polymethyl acrylate) and SBR (styrene–butadiene rubber). After polymerization, the material will undergo vulcanization, ensuring its integration into the polymer network.

To evaluate its performance, the mechanophore will be subjected to various material tests, including tensile strength, stress, and strain under mechanical force. The goal is to confirm its ability to undergo reversible bond scission, making it a potential candidate for tire applications where durability and adaptability to mechanical stress are crucial.

# sciforum-138535: Development of PLA/PVA composite scaffolds reinforced with hydroxyapatite for bone tissue engineering applications

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Bone tissue, the second most frequently replaced tissue in the human body, requires over four million surgeries annually, often with considerable risk, driving the advancement of tissue engineering as a promising alternative to autologous grafts through the development of multifunctional, biocompatible, and bioactive 3D scaffolds that promote osteoconductivity and mimic the native bone environment. In this study, poly(lactic acid) (PLA), a bio-based, mechanically strong yet hydrophobic polymer, was blended with poly(vinyl alcohol) (PVA), a biodegradable, hydrophilic polymer with lower mechanical strength, to fabricate composite filaments. Six PLA/PVA ratios were evaluated. Scaffolds were fabricated via Fused Deposition Modeling (FDM) and subsequently freeze-dried to enhance porosity and water absorption. To improve bioactivity, scaffolds were surface-coated with hydroxyapatite (HA), a naturally occurring bone mineral synthesized via a hydrothermal method. Scaffolds were thoroughly characterized through FTIR and XRD (physicochemical analysis), SEM and EDS (morphological analysis), and micro-CT. Their performance under simulated physiological conditions was examined through water absorption and mechanical testing. The freeze-dried scaffold with a 25:75 PLA/PVA ratio showed the highest water absorption capacity of 277.7% after 210 minutes, compared to its non-freeze-dried counterpart, which reached 270.1% in 75 minutes. Compression testing further demonstrated that scaffolds possessed a Young's modulus of 12.284 MPa, closely approximating that of natural cancellous bone. The synthesized HA for coating had a meso-nanometric average particle size of 32.5 nm and a uniform spherical morphology. Its successful incorporation into the scaffold was confirmed by FTIR, while uniform dispersion across the scaffold surface was verified by SEM imaging. These findings indicate that the freeze-dried PLA/PVA (25:75) scaffold reinforced with hydroxyapatite presents an effective and sustainable approach for bone tissue engineering. Its combination of mechanical strength, high water absorption, and bioactive surface properties makes it a strong candidate for future bone regeneration applications.

# sciforum-146341: Development of technical textile with microcapsules of essential oils of cymbopogon citratus (lemongrass) and citrus aurantium (orange) via in situ polymerization.

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The increasing demand for functional textile materials has created new challenges for the sector, particularly the need to incorporate advanced manufacturing techniques and innovative finishing processes that can drive the development of next-generation sports textiles. Among the strategies available, the use of microcapsules has emerged as a particularly promising approach, as it enables the controlled incorporation of active agents into fabrics, thereby providing additional and long-lasting functionalities. In this study, an innovative textile finishing treatment was developed through the application of microcapsules containing lemongrass and orange essential oils. The microcapsules were synthesized by in situ polymerization and subsequently applied to polyamide (PA66) fabric using the pad-dry process, ensuring adequate adhesion to the textile substrate. The objective was to combine the intrinsic benefits of aromatherapy with textile performance, ultimately offering potential improvements in both the well-being and physical performance of athletes. The microcapsules obtained exhibited mean diameters of 460.08 nm for lemongrass and 1,121.43 nm for orange, with encapsulation efficiencies of 20.77% and 23.03%, respectively, confirming successful entrapment of the essential oils. Thermogravimetric analysis (TGA) demonstrated the enhanced thermal stability of the encapsulated oils, validating the effectiveness of the polymeric shell. Moreover, scanning electron microscopy (SEM) revealed the heterogeneous morphology of the microcapsules and their deposition on the fabric surface, while Fourier-transform infrared spectroscopy (FTIR) identified functional bands associated with both the oils and the polymeric matrix, evidencing molecular interactions with PA66. Taken together, these results highlight the relevance of microencapsulation as a technological pathway for textile functionalization. Furthermore, the study underscores the potential of this approach to support the development of innovative sports textiles that not only improve consumer comfort but also contribute to health and overall athletic performance.

# sciforum-120883: E-Beam Radiation Processing of Semisolid Hydrogel for Doxorubicine Drug Delivery

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Hydrogels used as local delivery systems are a viable alternative for the local administration of anti-tumor medications to overcome the side effects of oral or intravenous administration induced by chemotherapeutics. Hydrogels are considered the best alternative for cancer treatment because they allow non-invasive release, effectively support the local and gradual release of anticancer drugs, increase drug solubility and bioavailability, offer high stability and controlled drug release, and may also help reduce the total dose required. Herein, we designed and developed a novel semisolid hydrogel composed of collagen gel (calfskin), sodium carboxymethylcellulose (CMC), polyvinylpyrrolidone (PVP), and polyethylene oxide (PEO) using e-beam irradiation as the crosslinking method. According to experimental results of loading and in vitro release, the semisolid hydrogel loaded 1145±1% ng of doxorubicine (DOX) and released different amounts of DOX, such as 120 ± 0.5% ng/cm2 at pH 6.4 and 150 ± 0.2% ng/cm2 at pH 7.4, for a period of 0.5 to 60 hours. In addition to the progressive release of DOX, the hydrogel retains its structure, is transparent, allows observation of the affected tissue, and has elastic properties unique to hydrogel-type systems. The semisolid hydrogel can be used as an absorbent material with regenerative properties and as a biocompatible polymeric matrix for the progressive delivery of DOX, a broad-spectrum anticancer drug.

# sciforum-138657: Exploring and Refining Synthetic Pathways for Efficient 2-Isopropenyl-2-Oxazoline Synthesis

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**Introduction.** 2-Isopropenyl-2-oxazoline (iPOx) is a monomer belonging to the 2-oxazolines class. Unlike typical 2-oxazolines that undergo ring-opening polymerization, iPOx polymerizes via its vinyl group, retaining the 2-oxazoline functionality which offers valuable sites for post-polymerization modifications, especially with carboxylic compunds. Thus, iPOx serves as a versatile building block for the design of functional (co)polymers. Conventional synthesis routes for iPOx often involve harsh conditions, limiting their practicality and scalability. This study explores multiple synthetic routes for the preparation of iPOx, aiming to establish a more accessible and practical method.

**Methods.** The synthesis followed well-established protocols, starting from methacrylic acid or its derivatives, which are reacted with aminoalcohols or haloalkylamines in various solvents. The resulting hydroxyamides or haloamides were then cyclized to obtain the final product, iPOx.

**Results.** Several synthetic routes were evaluated for the preparation of iPOx, varying the starting methacrylate derivatives, nucleophiles, and solvents. Reactions using methacrylic anhydride and 2-chloroethylamine yielded the highest purity intermediates, which were efficiently cyclized to iPOx under basic conditions. Hydroxyamide-based routes also produced good yields although they required harsher conditions during the cyclization step. Overall, the optimized pathway demonstrated improved scalability, reduced reaction times, and minimized byproduct formation compared to conventional methods. FTIR and NMR spectroscopy was used for structural confirmation of intermediates.

**Conclusions.** This study systematically evaluated various synthetic routes for the preparation of iPOx. The influence of the starting materials and reaction conditions on the reaction yield and purity of the final compound was also assessed. The optimized synthesis protocol provided a more practical and scalable route to iPOx, with improved efficiency and reduced byproduct formation.

# sciforum-139104: Exploring the Potential of Alpha-Glucan-Enriched Mushroom Extracts as Functional Natural Polymers for Wound-Healing Applications

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Despite the extensive research focused on the immunomodulatory properties of beta-glucans, alpha-glucans have received comparatively less attention. These molecules exhibit reduced immunogenicity compared to beta-glucans, a characteristic that could present valuable advantages in specific therapeutic contexts. This study evaluates the potential of three distinct extracted fractions ($S_B$, $S_C$, and $R_D$) obtained through different extraction methodologies from *Coriolus versicolor*, *Pleurotus ostreatus*, and *Hericium erinaceus* to enhance skin repair by promoting cellular proliferation, migration, and modulating immune responses. These fractions were previously characterized using several chemical and structural characterization methods that revealed significant content in bioactive molecules, particularly alpha glucans, exceeding 80% of total polysaccharide content. Cell viability was assessed using PrestoBlue and MTT assays in the HaCat cell line, revealing the non-toxicity of the compounds at the tested concentrations. Furthermore, proliferation assays (BrdU incorporation) and migration assays (scratch assay) in HaCaT cells were conducted at optimized concentrations (0.6 and 0.3 mg/mL). *C. versicolor* extracts ($S_C$ and $R_D$) promoted the highest wound closure of the injured monolayer by 95% after 48 h (at 0.6 mg/mL) compared to 66% in the non-treated control, although BrdU incorporation revealed no significant changes in proliferation. In contrast, *H. erinaceus* extracts promoted increased cellular proliferation (>120% for $S_B$ extracts at 0.6 mg/mL) with less impact in cell migration, suggesting selective enhancement of proliferation pathways. These differences may be attributed to variations in alpha-glucan structure and receptor interactions among the three species, leading to diverging effects on proliferation and migration. Additionally, immunomodulatory effects are being assessed by measuring key pro-inflammatory cytokines (TNF-α, IL1β, IL-8, and IL-6) and anti-inflammatory (IL 10) to elucidate how these polysaccharides regulate inflammation during healing and skin repair. These findings highlight the potential of alpha-glucans as multifunctional agents in dermatological applications, supporting their role in developing innovative, natural based therapies for skin regeneration.

# sciforum-138728: High-Performance Thermoplastic/Thermoset Blends: Strategies, Challenges, and Perspectives for Advanced Structural Applications

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The blending of thermosetting polymers (TS) with high performance thermoplastics (HTP) is an effective pathway to design new advanced materials that meet the requirements of demanding sectors such as aerospace, electronics, or high performance structural applications requiring durability under thermal and mechanical stress. Although offering high mechanical properties, thermal stability and chemical resistance, TS resins often suffer from brittleness, that can be improved with the addition of a tougher HTP material, such as polyetherimides, polysulfones or polyetherketones. This study will firstly provide an overview of recent developments in the formulation, processing, and characterization of TS/HTPs blends. It highlights the fundamental challenges induced by the chemical and physical differences between TS and HTPs systems, especially their low miscibility and limited interfacial adhesion, which often lead to unstable morphologies and poor mechanical synergy. Various processing methods such as melt blending, solution casting, in situ polymerization or co-curing are analyzed, with particular focus on their impact on phase morphology and distribution. Compatibilization strategies, including the use of reactive copolymers, functional additives, or chemical modifications, have proven effective in improving interfacial interactions and promoting the formation of stable microstructures. Thereafter, special attention is given to systems displaying co-continuous morphologies or forming interpenetrating polymer networks (IPNs), as they often offer an optimal balance between stiffness, toughness, and long-term thermal resistance. Despite promising pioneering reports, the relationships between processing conditions, interfacial phenomena, and final material properties remain complex and not yet fully understood. Therefore advances in interfacial engineering, molecular-level modeling, and specific characterization techniques of these hybrid systems are necessary to unlock their full potential and enable their broader implementation in high-performance applications.

# sciforum-129979: Investigating the effects of mechanical recycling on the flame retardancy properties of polypropylene-based composites

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When dealing with applications where plastics could be subjected to combustion and fire, the addition of flame-retardant (FR) additives into the polymers becomes a mandatory requirement. While FR systems are designed on purpose depending on several aspects, such as the specific application, the type of polymer, and the various fire risk scenario, their effectiveness in recycled polymers has not yet been systematically elucidated. On the other hand, considering that FR additives are abundantly present in numerous plastic waste streams, their presence can interfere with the mechanical recycling processes, posing significant challenges for the management of end-of-life FR-plastic parts.

In this study, two different approaches were followed in order to assess *(i)* the effectiveness of an intumescent FR system as flame-retardant for recycled polypropylene (PP); *(ii)* the possible modification of the combustion behavior of PP/FR during the reprocessing.

To this aim, virgin and reprocessed PP were melt compounded with an intumescent FR composed of piperazine pyrophosphate (PPAP) and melamine pyrophosphate (MPP) and characterised in terms of combustion, thermal and rheological behaviour. Furthermore, PP/FR was subjected to five reprocessing cycles in a twin-screw extruder (trying to simulate a mechanical recycling process) and characterised after each cycle.

Despite the different combustion behavior of reprocessed PP/FR as compared to the virgin one, the intumescent FR still provided satisfactory flame retardancy properties. In fact, the flame retardancy properties remain largely unaffected by repeated processing cycles, resulting in no change in UL94 classification even if the material is reprocessed up to five times.

These results would pave the way for a greater variety of applications for recycled PP, reducing the reliance on virgin plastic and advancing the circular economy of PP-based waste.

# sciforum-139136: Leveraging the "Grafting-Through" Approach for the Synthesis of "Rod-*graft*-Coil" Conducting Polymers Suitable as Biomedical Materials: Polythiophene grafted with Oligo-(D,L-Lactide)

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The development and industrial application of synthetic polymers has had a great impact on society as these materials are used virtually everywhere. Synthetic polymers in particular are widely used as biomaterials, but in recent decades, advanced bioapplications, which require subtle responses, need numerous innovative, increasingly diverse materials that promise high added value. In this context, the polymer architecture—one physical attribute that is central to polymer science—can be used for tuning the properties of next-generation functional biomaterials. Conjugated, electroconducting polymers (CPs), designed for electronic applications, are also endowed with a multitude of well-suited properties to function as intelligent, specialized biomaterials.

In this communication, it is demonstrated that by combining polythiophene—a typical CP—with the bioresourced, biocompatible, and biodegradable oligo-(D,L-lactide), in a "rod-*g*-coil"-type architecture, a multifunctional material can be obtained by polymerizing a thiophene-containing macromonomer. The study focuses on the investigation of the resultant copolymer enzymatic bioerosion (evaluated using different methods—FT-IR, GPC, and AFM)) and the manipulation of films' surface morphology and properties by changing the specificity of the solvents from which they are deposited on supports of different rigidity (glass or PLA sheets), of the dispersion concentrations, or viacopolymer doping with $LiClO_4$.

In addition, the undoped and doped films' surface interaction with BSA protein was followed by the Quartz Crystal Microbalance with Dissipation (QCM-D) technique, which revealed that the protein binding process might be "switch on–off" by the doping state of the conjugated oligomer. Moreover, the good biocompatibility and non-cytotoxic effect of the copolymer over normal human gingival fibroblasts (NHGFs) were shown, highlighting its potential functionality as a suitable biointerfacing material for different related bioapplications.

# sciforum-139335: Microencapsulation of *Moringa oleifera* leaf extract using food-grade biopolymers: A study on structure, stability and functionality

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The encapsulation of phenolic compounds is a promising strategy to improve the stability and bioactivity of plant-based extracts for application in functional foods. This study aimed to encapsulate bioactive compounds extracted from *Moringa oleifera* leaves using gum arabic (GA) and maltodextrin (MDX), both food-grade carriers, via freeze-drying technique. These biopolymers were selected due to their non-toxic nature, emulsifying properties, and thermal resistance. The encapsulation performance was evaluated in terms of process yield, encapsulation efficiency, total phenolic compounds (TPC) and total flavonoid content (TFC), antioxidant activity, and physicochemical characteristics such as microscopical, FTIR and thermal analysis. The freeze-drying process resulted in a high yield (83 ± 3%) and encapsulation efficiency for TPC (78 ± 2%). The resulting microcapsules exhibited fine particle size ($D_{50}$ = 1.6 ± 0.1 µm). TPC and TFC were 21 ± 4 GAE mg/g and 12 ± 2 CE mg/g (dry basis), respectively. Antioxidant activity, assessed through DPPH and ABTS assays, showed $IC_{50}$ values of 171 ± 9 µg/mL and 102 ± 5 µg/mL, respectively, indicating strong radical scavenging potential. Microscopic analysis revealed irregular but compact particle morphology. FTIR spectra confirmed the presence of phenolic compounds, with characteristic O–H and C=O stretching bands, as well as evidence of hydrogen bonding interactions between the core and wall materials. Thermogravimetric analysis demonstrated good thermal stability, with major decomposition events above 220°C and structural integrity maintained below 180°C. In conclusion, freeze-drying with GA and MDX proved effective in preserving the chemical and thermal stability of *M. oleifera* leaf phenolics, supporting their potential use in thermosensitive functional food formulations.

# sciforum-139178: MOF-based Cellulose Acetate MMMs For an Advanced Propene/Propane Separation

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**Introduction.**

The separation of propene/propane is among the most energy-intensive industrial processes because of the massive scale and the high energy demanded by the traditional cryogenic distillation method [1]. In this work, we report the preparation of MMMs consisting of cellulose acetate, 30% wt. $[BMIM]^+[Tf_2N]^-$, and 20% wt. of a series of ZIFs (ZIF-8, ZIF-67, and ZIF-8-67). The aim is to surpass the current state-of-the-art by incorporating bimetallic ZIF-8-67, supported by an ionic liquid as both a compatibiliser and a promoter of permeability.

**Experimental/methodology.**

Thin film composites were fabricated by spin-coating on PAN support. X-Ray diffraction, FT-IR, and SEM were performed. Single-gas and mixed-gas permeation measurements were applied [2].

**Results and discussion.**

The addition of 30%$[BMIM]^+[Tf_2N]^-$, by showing the trade-off behaviour, led to an increase in Propene permeability, compared to the neat CA membrane. The contribution of a series of ZIFs in ZIF/IL-CA MMMs increased the $C_3H_6/C_3H_8$ selectivity as well as the $C_3H_6$ permeability, with ZIF-8-67 outperforming its parent ZIFs. $C_3H_6/C_3H_8$ Mixed-gas measurements confirmed a selective performance of ZIF-8-67/IL-CA MMM.

**Conclusion**

Overall, this study highlights the significant role of bimetallic ZIF-8-67 in enhancing gas separation performance when incorporated into IL-CA membranes. The synergistic properties of $Zn^{2+}$ and $Co^{2+}$ in ZIF-8-67, combined with the role of $[BMIM]^+[Tf_2N]^-$ in addressing interfacial inconsistency, contributed to its superior gas transport properties and selectivity.

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# sciforum-133404: Muicle (*Justicia spicigera)* Flower Extract-Loaded PVA Films as Biobased Antimicrobial Packaging Materials

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The development of biobased and biodegradable materials for food packaging is a critical step toward reducing environmental impact and replacing petroleum-derived plastics. In this work, the fabrication and characterization of polyvinyl alcohol (PVA) films incorporating extracts from Muicle (*Justicia spicigera*) flowers are presented as a green approach to active packaging. Flower extracts were obtained using water and ethanol as solvents, employing decoction and sonication as green extraction methods. The resulting extracts, rich in phenolic and anthocyanin compounds, were mixed with PVA and processed into films through solvent casting. Physicochemical characterization confirmed the successful incorporation of bioactives and showed good film integrity. Antioxidant activity was evaluated using DPPH assays, which revealed an enhanced radical scavenging capacity in films containing ethanolic extracts. To assess antimicrobial potential, the bioactive films were used to package fresh fruit samples, which were placed in sealed glass beakers. Over time, microbiological growth on the fruit surface was monitored and compared to unprotected controls. The results demonstrated a significant reduction in microbial proliferation in the presence of muicle-enriched films, supporting their potential as biobased antimicrobial packaging. These findings demonstrate a viable pathway for integrating botanical bioactives into biodegradable polymer systems, contributing to sustainable material development in food technology and packaging.

# sciforum-135868: Multiple Recycling Cycle Analysis of 3D-printed Recycled Polycarbonate Using Fused Granulate Fabrication

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This study explores degradation behaviours and mechanical performance of 3D-printed recycled polycarbonate (rPC) over multiple recycling cycles using fused granulate fabrication (FGF), a sustainable and scalable 3D printing technique. rPC flakes were subjected to ten recycling cycles, and their thermal, chemical, and mechanical properties were characterised using DSC, TGA, FTIR, and mechanical testing. The results reveal that thermal stability gradually decreases with repeated processing: the glass transition temperature dropped from 110.2 °C to 96.4 °C after ten cycles, while the degradation onset temperature reduced slightly, indicating progressive thermal degradation. FTIR analysis showed transient structural improvements in early cycles, followed by loss of key functional groups due to chain scission and oxidative degradation. Mechanical testing demonstrated a temporary enhancement in tensile strength and flexural strength—peaking at 68.59 MPa and 76.4 MPa respectively—linked to improved chain alignment. However, these gains were reversed after the fifth cycle, with significant declines in strength, modulus, and impact strength. Fractography confirmed a transition from ductile to brittle failure beyond five cycles. FGF printing also reduced manufacturing time by up to 84% compared to fused filament fabrication, emphasising its viability for circular manufacturing. The findings offer critical insights into the recyclability feasibility of engineering polymers and support broader application of FGF in polymer sustainability.

# sciforum-137408: Next-Generation Polymer Systems for Advanced Biomimetic Nanofibers: Smart, Responsive, and Adaptive

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***Introduction:***

Nature has long been a source of inspiration for material scientists, offering intricate designs and multifunctional properties. In recent years, biomimetic nanofibers have emerged as a promising class of materials for applications in healthcare, environmental sensing, and soft robotics. However, the limitations of conventional polymers in mimicking dynamic biological behavior have driven the search for next-generation materials that can adapt, respond, and evolve under varying stimuli.

***Methods:***

This study explores the literature about a novel family of stimuli-responsive copolymers synthesized through controlled radical polymerization, incorporating dynamic covalent cross-links and supramolecular motifs. Electrospinning techniques were employed to fabricate ultrafine fibers, simulating extracellular matrix architectures. A suite of characterization methods, including scanning electron microscopy (SEM), differential scanning calorimetry (DSC), and dynamic mechanical analysis (DMA), were used to assess structural fidelity, thermal behavior, and viscoelastic performance.

***Results:***

Relevant literature points out that the developed nanofibers exhibit significant responsiveness to pH, temperature, and ionic strength, enabling reversible shape transformations and tunable mechanical properties. Notably, fibers embedded with thermoresponsive domains demonstrate up to 60% contraction at mild physiological temperatures (37–42°C), while pH-sensitive segments showed self-healing capabilities under acidic conditions. Comparative analysis revealed a threefold increase in adaptability compared to conventional electrospun scaffolds.

***Conclusions:***

The integration of intelligent polymer architectures into nanofibrous formats paves the way for highly adaptive materials that closely emulate natural tissue behavior. These findings suggest strong potential for applications in regenerative medicine, wearable electronics, and responsive filtration systems. Future works are expected explore in vivo biocompatibility and long-term stability to advance toward translational applications.

# sciforum-141517: One-dimensional coordination polymers constructed from bimetallic vanadium(v) complex: Synthesis, crystal structure and catalytic activity

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Coordination polymers containing different metal ions and ligands have been widely studied in materials science and synthetic chemistry. For constructing a coordination polymer, the most useful method is to employ an appropriate bridging ligand. Many multidentate ligands bind to two metal ions in two different directions, which shows bridging capability via simultaneous ligations. In our study, we have selected N'1-((E)-2-hydroxybenzylidene)-N'2-(2-hydroxybenzylidene)oxalohydrazide (L), which is a multidentate ligand that can bind to metal ions from more than one donor's atom. In the first step, the coordination polymers were prepared by reacting the ligand with vanadium acetylacetonate, which yielded a dioxidovanadium(V) complex. In the second step, dioxidovanadium(V) complex was then reacted with sodium carbonate in ethanol solution, resulting in the formation of the one-dimensional vanadium(V) coordination polymer. A novel one-dimensional metal-based coordination polymer of the composition $[VNaO_6C_{11}H_{14}N_3]_{-n}$ was characterized by IR and NMR and the structure was established by single-crystal X-ray crystallography. The coordination sphere of the vanadium atom is square pyramidal and chelates to a tridentate (-ONO-) ligand, while the square pyramidal conformation of the sodium atom consists of one bridging oxygen atom link to the vanadium atom and the ligand which coordinates in a bidentate fashion. The coordination polymer showed very selective homogeneous catalytic activity with 80-96% conversion in oxidative bromination of the organic substrate under mild conditions.

# sciforum-147265: Preliminary results of green chemistry screening from *Nicotiana glauca* Graham with biological sensor system based on Sephadex G-10

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**Introduction.**

Size-exclusion chromatographic separation with Sephadex gels is a widely used technique for dereplication and screening methodologies of natural products. Sephadex G-10 resin is a polymeric network composed of dextran units cross-linked by epichlorohydrin and allows using physiological solutions as mobile phases for the direct coupling chromatographic separation to study living tissues or organs. Thus, this type of system enables real-time monitoring of active compounds, an application of significant importance in organic chemistry and pharmacology.

**Methods.**

Medium-pressure liquid chromatography separation (MPLC) with Sephadex G-10 coupled directly to biological detection using perfused organs was carried out for bio-guided study of hydro-ethanolic extracts from *Nicotiana glauca* Graham (Solanaceae). Sephadex G-10 provides the lowest fractionation range of gels type Sephadex, allowing the separation of substances with molecular weights below 700 Da, typically within the range of 100–1000 Da. Furthermore, this resin enabled the use of Krebs-HEPES as an elution medium, a medium that kept the studied organs in optimal conditions.

Perfused rat organs were used: Rings of aorta artery and trachea, and portions from the deferent conduct and ileum.

**Results.**

Two natural alkaloids, anabasine and nornicotine, were readily isolated and identified as the compounds responsible for the contractile activity observed in the smooth muscle of rat ileum and trachea.

The coupling of this chromatographic system with Sephadex G-10 to biological detection in living organs simplified the bioassay-guided: it carried out by a single person, with a physiological and non-contaminating medium, minimizing the number of animals slaughtered, with chemical characterization by mass spectrometry analysis, and reducing the study time.

**Conclusions.**

This application of Sephadex G-10 chromatography rationalizes the bio-guided identification of isolated natural products and advances its use toward green chemistry dereplication methodologies as well as in future automated or robotic approaches.

# sciforum-137993: Rheological and textural studies of a hydrogel with *Perovskia atriplicifolia* extract

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**Introduction**

*Perovskia atriplicifolia* Benth.is an ornamental plant with a strong, pleasant scent, belonging to the family Lamiaceae. In traditional medicine, it has been used to prevent and cure various skin diseases. In this study, the chemical components and antioxidant activity of *P. atriplicifolia* extract were analyzed and a rheological and textural characterization of the extract-based hydrogel was performed.

**Methods**

Spectrophotometric and HPLC methods were used to determine the phytochemical components and the antioxidant activity of *P. atriplicifolia* herb extract.

The rheological properties of the extract-based hydrogel were determined using a rotational rheometry method in a plate-to-plate arrangement at 25 °C. The hydrogel was also analyzed using a TX-700 texture analyzer, in the Compression/Relaxation/Tension (CRT) and Texture Profile Analysis (TPA) modes.

**Results**

The total contents of polyphenols, flavonoids, phenolic acids, and condensed tannins in the extract were 64.46 mg/mL, 17.39 mg/mL, 4.92 mg/mL, and 4.12 mg/mL, respectively. Among phenolic compounds, hesperidin (0.16 mg/mL), caffeic (0.04 mg/mL), and rosmarinic (1.32 mg/mL) acid are identified. Additionally, it was found that the course of the flow curves was non-linear. In the range of shear rates tested, the apparent viscosity decreased, indicating that the formulations are non-Newtonian fluids, diluted by shear force. The results of the CRT and TPA tests showed that the hydrogel had high adhesiveness, supporting effective skin retention and bioadhesiveness. It also exhibited high elasticity (1.32), indicating good flexibility in regaining its shape, and cohesiveness above 1, confirming strong structural integrity and good skin adherence.

**Conclusions**

A hydrogel based on *P. atriplicifolia* extract containing compounds with antioxidant activity has beneficial rheological and textural properties, ensuring optimal application of the preparation on the skin.

# sciforum-135233: Selective Removal of Direct Green-6 from Textile Wastewater Using Molecularly Imprinted Polymers

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The textile industry is one of the main sectors contributing to water pollution, with dyes being among the most significant pollutants in wastewater. In this study, molecularly imprinted polymers (MIPs) were used for the removal of Direct Green-6 (DG-6), a dye commonly found in textile wastewater. MIPs are artificially synthesized polymers that contain specific binding sites for target molecules. Due to this property, they stand out as an effective method for the selective removal of environmental pollutants.

In this study, DG-6-specific MIPs were synthesized using the bulk polymerization method and optimized with different ratios of MAA (methacrylic acid), EGDMA (ethylene glycol dimethacrylate), and the initiator AIBN (azobisisobutyronitrile). After polymerization, DG-6 was removed from the polymers through washing steps using various methanol/acetic acid solutions. The efficiency of template molecule removal was evaluated using spectrophotometric methods, and the obtained MIP and NIP (non-imprinted polymer) samples were characterized by FT-IR spectroscopy.

As a result of adsorption studies, the most efficient removal was achieved by the polymer synthesized at a 1:50:150 ratio, referred to as "β MIP." This polymer achieved 46% dye removal after 20 hours of adsorption. The results indicate that MIPs can effectively recognize and remove complex pollutants such as DG-6 dye.

This study demonstrates that molecularly imprinted polymers offer a cost-effective, selective, and environmentally friendly alternative for dye removal from textile wastewater and lays the groundwork for their use in advanced treatment processes.

# sciforum-137537: Self-assembled polysaccharide-based multilayer nanofilms of xanthan gum and diethylaminoethyl dextran on gold substrate and their interaction with model biomacromolecules

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In this study, we investigate the formation of electrostatically self-assembled multilayer films (MLFs) of the anionic xanthan gum (XG) and the cationic diethylaminoethyl dextran (DD) polysaccharides. XG/DD MLFs are formed on a gold (Au) surface by implementing the layer-by-layer (LbL) method. The MLFs are comprised of 10 alternating single layers (5 double layers) of the two oppositely charged polysaccharides. The constructed MLFs are studied by using the surface plasmon resonance (SPR) and the quartz crystal microbalance with dissipation (QCM-D) methods. The reported adsorbed masses $\Gamma$ of the layers are within the range of 8-14 mg/m$^2$. Bovine serum albumin (BSA) showcases satisfactory adsorption and interaction with the MLFs both in neutral and acidic environments with increment $\Gamma$ values of ~3 mg/m$^2$, while porcine gastric mucin (PGM) exhibits similar behavior in neutral environments. The XG/DD MLFs show decent stability against the increase of ionic strength and the rinsing with water between successive biopolymer deposition cycles. MLFs with adsorbed BSA and PGM show minimal mass losses due to pH changes and increased ionic strength, respectively. In general, the XG/DD MLFs are considered as promising options for use in drug delivery systems, wound-healing scaffolds, and biosensors, as well as for combating microbial growth due to the charges of the uncomplexed segments of the polysaccharides.

# sciforum-147107: Solution-Blow-Spun D,L-PLA Nanofibrous Materials for Biomedical and Agrifood Applications

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Nanofibrous materials have gained increasing attention for biomedical and agrifood applications owing to their high surface-to-volume ratio, tunable porosity, and ability to incorporate functional agents. Among biodegradable polymers, poly(D,L-lactic acid) (D,L-PLA) offers distinct advantages, including biocompatibility, processability, and controlled degradation kinetics, making it a versatile candidate for multifunctional nanofibrous systems.

In this work, we investigated the preparation of D,L-PLA-based nanofibrous materials using solution blow spinning (SBS), a scalable and cost-effective technique that enables the rapid fabrication of fibers without the need for high voltage or complex equipment. Processing conditions were optimized to obtain uniform fibers with controlled morphology and diameter distribution. The effects of solution properties and processing parameters on fiber morphology and distribution were systematically evaluated. Additionally, the incorporation of bioactive agents was explored to tailor the fibers for targeted applications.

The resulting materials were characterized from their structural, thermal, mechanical, and morphological properties. FTIR analyses confirmed the polymeric structure, while SEM micrographs revealed uniform and continuous fibers in the submicrometric range, with an average fiber diameter distribution of approximately 300 nm. The resulting materials exhibited favorable mechanical stability and degradation behavior. Preliminary assessments demonstrated their suitability as scaffolds in biomedical applications, where the fibrous network supports cell adhesion and growth. In parallel, the fibers showed promise for agrifood applications such as active packaging, benefiting from their barrier properties and potential to act as carriers for active agents.

Overall, this study highlights the versatility of D,L-PLA nanofibers produced by SBS and underscores their dual applicability in health-related and sustainable food systems. The findings contribute to the development of biodegradable nanostructures with multifunctional performance and scalable production pathways, reaffirming their potential as a sustainable alternative to conventional plastics and as a versatile platform for biomedical and industrial applications.

**Acknowledgments:** Project TED2021-129945B-I00

# sciforum-146535: Stimuli-responsive semi-IPN PNIPAAm/PVA hydrogels: structural, mechanical and bioadhesive properties

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Hydrogels are three-dimensional (3D) polymeric networks capable of absorbing large amounts of water, aqueous solutions, or physiological fluids, while remaining insoluble due to physical and/or chemical interactions [1,2]. Over the last decades, these materials have attracted significant interest due to their ability to respond to external stimuli such as pH, temperature, light, electric fields, or ionic strength. Owing to this stimulus-responsive behavior, so-called smart hydrogels have emerged as versatile platforms for biomedical and materials science applications [2,3]. In this study, semi-interpenetrating polymer network (semi-IPN) hydrogels were synthesized by radical polymerization of poly(N-isopropylacrylamide) (PNIPAAm) in the presence of poly(vinyl alcohol) (PVA), with the aim of evaluating their structural, mechanical, swelling, and bioadhesive properties. PNIPAAm formed a chemically crosslinked thermo-responsive network, while PVA acted as the interpenetrated linear polymer, improving biocompatibility and reinforcing the hydrogel structure. Fourier-Transform Infrared Spectroscopy (FTIR) confirmed the incorporation of PVA into the PNIPAAm matrix, as evidenced by characteristic band modifications. Scanning Electron Microscopy (SEM) revealed the influence of PVA content on the hydrogel morphology. Swelling kinetics demonstrated a temperature-dependent behavior; at 37 °C, a volume contraction was observed due to the phase transition of PNIPAAm. Overall, the results suggest that semi-IPN PNIPAAm/PVA hydrogels are promising materials for biomedical applications requiring tunable mechanical performance, thermo-responsiveness, and enhanced bioadhesion.

# sciforum-147146: Synthesis and formulation of novel polymer-based drug-eluting stents coating for extended-release.

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Percutaneous coronary intervention (PCI) is a minimally invasive technique used to reopen narrowed or blocked coronary arteries caused by atherosclerosis. In which stent is implanted to reopen arteries, but after some time, it gets narrowed again, called restenosis, which is a reduction in lumen diameter after PCI. Drug-eluting stents (DES) were developed to specifically address the problems of restenosis encountered with BMS ISR. Drug-eluting stent was found to be better than other types of stents. These stents are coated with drugs like paclitaxel, sirolimus, zotarolimus, or everolimus. Primarily, PLGA or PLA polymers are used to increase the release of the drug for a longer duration. Most drug-eluting stent manufacturers use PLGA or PLA to load the medicine and coating of the stent. The required course of release of sirolimus or everolimus for transplant success will be 90 days or more. However, the PLGA-coated Genex stents loaded with sirolimus provided the release of 30 days (Purple Micro Port Pvt. Ltd.). Chitosan is known for its extended release of drugs. Further, the drug sirolimus was analyzed to have 14 hydrogen bond acceptors. Thus, chitosan rich in hydrogen bond donors will be used for the modification. Moreover, the sulphonamide-containing linkers are reported to be pH sensitive (pH 7.2-7.4). Thus, a novel modified polymer contains PLGA and chitosan linked with a pH-sensitive sulphonamide linkage. The novel polymer rich in Hydrogen bond donors will improve drug loading and release. Thus, the pH sensitivity and enhanced drug loading may increase the release from 30 to 90 days.

# sciforum-138460: Systematic review of the use of Photosensitive Polymers in hard tissue regeneration

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Introduction: Photosensitive polymers are emerging as a new method of tissue engineering with great prospects for hard tissue in terms of bone, and cartilage, and dental tissue regeneration. Such materials experience property transformations upon light exposure, which allows us to control biocompatibility and direct cell differentiation with a high degree of precision and allows us to gett rid of the limitations of traditional methods.

Materials and Methods: Systematic searches of databases were performed in PubMed, Google Scholar, Scopus, and Web of science (2010-2024) according to the following combinations of keywords: photosensitive polymers and tissue engineering; photosensitive polymers and hard tissue regeneration; and photosensitive polymers and bone tissue engineering. English-language peer-reviewed research articles concerning photosensitive polymer sections in hard tissue regeneration were included.

Results: There were a total of 89 studies included out of 1,247 identified articles. Important polymers were poly(ethylene glycol) diacrylate (PEGDA), gelatin methacryloyl (GelMA), and hyaluronic acid methacrylate (HAMA). These materials showed the ability to form 3D scaffolds with adjustable mechanical properties, biocompatibility and growth factor release. 3D bioprinting using photosensitive polymers gave us the potential to fabricate complex bone structures.

Discussion: In this analysis, there was high potential concerning photosensitive polymers in dentistry as far as hard tissue regeneration is concerned. They have the benefits of tunable mechanical properties, excellent control of polymerization and the ability to make complex structures. Ongoing issues are the cytotoxicity of photosensitive polymers and low transparency of light through thick constructs.

Conclusion: Photosensitive polymers can be considered an optimistic approach for hard tissue regeneration. The recent developments of 3D bioprinting and the development of new polymers point towards their high clinical application potential. Future research must provide answers to the existing difficulties, develop optimal formulations, and carry out a single clinical research study.

# sciforum-138725: Thin films based on poly(*N*,*N*-dimethylaminoethyl methacrylate) and glucose oxidase: formation, properties and application as biosensor coatings

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Poly(*N*,*N*-dimethylaminoethyl methacrylate) (PDMAEMA) is a stimuli-sensitive (pH- and temperature-sensitive) polymer. Its macromolecules readily change hydrophilic–hydrophobic balance in response to external stimuli (temperature, pH, solvent composition). This feature makes PDMAEMA adaptive to surfaces of different nature and very promising for their functionalization. In particular, its tertiary amino groups, when protonated, enable the non-destructive binding of (bio)molecules bearing the opposite charge. Hence, PDMAEMA can be exploited for the surface modification and further electrostatic immobilization of (bio)molecules, thereby paving a way towards (bio)sensor coatings, which are in demand in medicine, biotechnology, ecology and related fields.

In this work, the formation and properties of polymer and polymer–enzyme coatings on model conductive surfaces (gold, graphite) were examined by means of quartz crystal microbalance with dissipation monitoring (QCM-D) and atomic force microscopy (AFM). PDMAEMA was proven to form nano-sized, stable and rigid films if adsorbed in a non-charged state (pH 10). After being brought to a charged state (pH 7), PDMAEMA films were shown to bind significant amounts of glucose oxidase (GOx). The efficiency of surface modification and amount of the immobilized enzyme were demonstrated to increase with the temperature of the polymer adsorption, changing from 25 up to 40°C.

Next, an electrochemical polymer-enzyme biosensor system was fabricated via subsequent adsorption of PDMAEMA and GOx on screen-printed graphite-based electrodes (SPE). An amperometric assay of the obtained biosensor constructs exhibited remarkable performance (i.e., a submicromolar limit of detection, a wide linear range of 3 orders of magnitude) toward glucose quantification as well as a good operational stability of enzymatic responses.

The experimental results (QCM-D and AFM) were obtained with the use of the equipment purchased within the M.V. Lomonosov Moscow State University Program of Development.

# sciforum-149286: Topology-Optimized PLA Test Fixture for Cyclic Testing of Lattice-Based Hysteretic Dampers

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**Introduction**

Reliable experimental characterization of architected lattice materials requires specialized fixture systems that ensure accurate load transfer. Traditional metallic fixtures are often prohibitively expensive and slow to produce, hindering rapid, iterative material research. This study addresses this challenge by presenting the design, finite element validation, and topological optimization of a cost-effective test fixture made from Fused Filament Fabrication (FFF) Polylactic Acid (PLA). The fixture is designed to enable the cyclic mechanical characterization of LPBF-manufactured Kelvin-type lattices.

**Methods**

The fixture's design process was iterative, combining CAD modeling and Finite Element Analysis (FEA) to refine its geometry and performance. The supports were designed for axial load transfer compatible with an Instron 8801 testing machine. The loading protocol was proportionally scaled from a recognized standard for Steel Plate Shear Yielding Dampers (SPSYDs). A density-based topology optimization was performed to minimize mass while maintaining structural rigidity, targeting a mass reduction constraint of 60%.

**Results**

The iterative design and optimization process successfully improved the safety factor from an initial 2.08 to a final value of 4.25, confirming its structural integrity under the maximum load of 5.3 kN. The topology optimization achieved a mass reduction of 40% compared to the initial design. Preliminary experimental analysis and numerical simulations confirmed that the optimized PLA supports exhibited minimal deformation, with displacements around 0.73 mm, which was significantly lower than the machine clamps.

**Conclusions**

This research demonstrated that combining numerical analysis and topological optimization can produce cost-effective, FFF-manufactured PLA components that are capable of replacing traditional metal devices in cyclic mechanical testing applications. The developed methodology can be extended to other test devices where stiffness and precision are crucial. The validated fixture provides a reliable platform for future experimental tests of lattice-based hysteretic dampers.

# sciforum-138032: Towards Green Conductive Nanocomposites Based on Epoxidized Soybean Oil (ESO) for Electromagnetic Shielding and Antistatic Application: Effect of Hybridization of Carbon Nanotubes and Graphene

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The use of resins derived from epoxidized soybean oil (ESO) promotes advances in sustainable materials and reduces carbon footprint. There is technological potential for the development of nanocomposites with viable technical performance, aligning functional properties with environmental impact mitigation. However, ESO acts as an electrical insulator, limiting applications as a material for static charge dissipation and electromagnetic interference shielding. Therefore, electrical and hybrid nanocomposites based on ESO were prepared with fumaric acid as the curing agent, using carbon nanotubes (MWCNT) and graphene (G) as conductive nanofillers. The ESO/MWCNT/G nanocomposites were evaluated through electrical conductivity (σ), electromagnetic interference shielding (EMI SE), and reflection loss (RL), adopting hybridization between MWCNT/G with 5/0, 4/1, 3/2, 2/3, 1/4, and 0/5 parts per hundred resin (phr). The pure ESO exhibited insulating behavior, with a conductivity of 1.61 x $10^{-11}$ S/cm, which resulted in low electromagnetic shielding performance (~1 dB) between 8.2-18 GHz. The ESO nanocomposite with MWCNT/G (5/0 phr) showed the highest electrical conductivity value of 5.81 x $10^{-5}$ S/cm, leading to the highest magnetic shielding performance between 12-15 dB. Among the hybrid nanocomposites, the MWCNT/G (3/2 phr) formulation demonstrated synergy in magnetic shielding effectiveness, although still lower than that of MWCNT/G (5/0 phr). The shielding mechanism of the ESO/MWCNT/G nanocomposites was primarily due to reflection, except for MWCNT/G (5/0 phr), which, in the Ku band, showed nearly identical values of energy shielded by reflection and absorption. In terms of RL, the best results were observed for MWCNT/G (3/2 and 2/3 phr) in the Ku band, reaching -10 dB (corresponding to 90% attenuation), which is the minimum standard value for a material with good absorptivity. The results suggest potential for application as a coating for static charge dissipation.

# sciforum-138356: Unlocking the potential of waste: eggshell-based $CaCO_3$ nanoparticles for functional applications of polymeric materials

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Due to the increasing environmental pollution caused by synthetic plastics, particularly in Mexico, there has been growing interest in the development of sustainable materials derived from biopolymers and agri-food waste. This research evaluated the use of eggshell nanoparticles (ENPs), which are rich in calcium carbonate, as functional reinforcements in various polymeric matrices. ENPs were obtained through high-energy milling for periods of 1–3 h, reaching an average size of 84 ± 40 nm after 2 h, with 91 % of the particles  100 nm. These nanoparticles were incorporated at concentrations of 1–3 wt.% into gellan gum (GG) films intended for the manufacture of compostable utensils and were also blended with polylactic acid (PLA) to produce filaments processed by extrusion. Additionally, superhydrophobic coatings inspired by the lotus leaf effect were developed by applying ENP and ZnO micro- and nanoparticles onto glass substrates. The materials were characterized using optical, confocal, and electron microscopy, as well as FTIR, XRD, and texture image analysis. The results for the films showed that the incorporation of 3 % ENPs into GG significantly improved their mechanical, thermal, and hydrophobic properties; in the filaments, it was observed that 2 % ENP supports flexibility. On the other hand, the coatings with the highest surface roughness were those in which ENP was used with ZnO nanoparticles with contact angles > 150°, confirming its superhydrophobic character. Overall, these results demonstrate that the use of waste materials such as eggshells enables the development of biodegradable materials with enhanced functional properties and potential applications in packaging, utensils, and surface treatments, contributing to a circular economy and reducing the environmental impact of conventional plastics.

# sciforum-138475: Using Self-Healing Polymers in the Making of Prosthetics and Orthotics: Systematic Review

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Background: Self-healing polymers are an innovative break through in material science, where autonomous repair and prolonging service life functionality in biomedical applications is possible. In prosthetics and orthotics, the materials take care of challenges such as mechanical breakdown, degradation upon wear and tear, and frequent replacement.

Materials and Methods: PubMed, Google Scholar, Scopus, and Web of Science were used to conduct a systematic search of studies up until December 2024. The inclusion criteria involved article types, including peer-reviewed articles, conference proceedings, and patents concerned with self-healing polymer use in prosthetic and orthotic applications.

Results: 34 studies were included among 1,247 identified articles. These self-healing materials were divided into intrinsic (shape memory, dynamic covalent bond) and extrinsic (microcapsule-based, vascular networks). The systems based on polyurethane possessed better mechanical behavior and healing performance (85-95% of recovery). Research indicated a major increase in fatigue resistance of 2-5 fold and an improvement of service life by 40-70 percent.

Discussion: It is observed that presently, significant benefits of self-healing polymers are associated with possible use in prosthetics and orthotics. Nonetheless, there are still issues to be dealt with, such as efficiency in healing at physiological levels and regulatory approval systems.

Conclusion: Self-healing polymers have high potential to transform prosthetic and orthotic device production with high durability, less maintenance, and satisfaction from people using the devices.

# Session 4. Polymer Composites and Nanocomposites

# sciforum-147184: Manufacturing Hybrid Jute/Glass Fiber Laminates by Leveraging Prepreg Resin Bleed

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There is a growing shift toward a circular economy, aiming to maximize recycling, minimize waste streams, and favor renewable over fossil-based materials. In this context, the composites industry—particularly in sectors such as automotive, marine, and aeronautics, where composition control is critical to mechanical performance and structural integrity—relies on semi-products with tightly controlled material properties.

Most thermoset-based prepregs used in these sectors show minimal variation in resin content. However, some commercial prepregs exhibit significant resin bleed during curing under heat and pressure (e.g., in an autoclave or hot press).

This work explores the manufacture of a hybrid jute/glass-fiber laminate using a commercial glass-fiber prepreg and plain-weave jute fabric, with no additional resin, thereby maximizing resin utilization and minimizing waste. By leveraging resin bleed and strategic lamina placement, the goal is to achieve effective impregnation of the jute layers.

The resulting laminate's composition was evaluated using a modified calcination method. Physical and mechanical properties—including density, tensile, and flexural behavior—were estimated via micromechanics and classical laminate theory and compared with experimental results.

Further characterization included Charpy impact strength and Mode I interlaminar fracture toughness via double-cantilever beam (DCB) testing. These results establish baseline values for comparison in future developments of this research.

# sciforum-138205: Three-Dimensional Printing of Acrylate Epoxidized Soybean Oil (AESO)-Based Composites Containing Bamboo

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**Introduction**

The shift from a linear to a circular economy is essential for reducing global resource consumption, minimizing waste, and promoting sustainable materials. This transition supports the development of bio-based thermoset polymers, the upcycling of industrial waste-derived fillers, and the use of environmentally friendly manufacturing technologies. Vat photopolymerization (VPP) has emerged as a highly versatile method with great potential. As a light-driven process, it enables high-resolution printing and the fabrication of complex geometries.

**Materials and Methods**

The resin formulation consisted of acrylate epoxidized soybean oil (AESO) and isobornyl methacrylate (IBOMA) in a 1:1 weight ratio, with 2 wt.% of phenyl bis(2,4,6-trimethylbenzoyl) phosphine oxide (BAPO) as a radical photoinitiator. Bamboo filler was added at 3, 5, and 10 phr to produce bio-based composites. Both neat and filled formulations were processed using a Phrozen Sonic Mini 8K LCD printer equipped with a 50 W linear projection LED module operating at a UV wavelength of 405 nm.

**Results and Discussion**

The addition of bamboo enhanced the mechanical and viscoelastic properties. The Young's modulus increased from 1189 MPa (A-IB) to 1397 MPa (A-IB+B10), corresponding to an enhancement of approximately 17%. The storage modulus (E') improved from 1140 MPa to 3324 MPa. The glass transition temperature shifted from 92°C to 95°C. Thermogravimetric analysis confirmed that thermal stability was not negatively affected. Although bamboo increased viscosity, it remained within the optimal range for VPP, ensuring processability.

**Conclusions**

This study demonstrates that bio-based photocurable formulations can be efficiently used in VPP to produce high-performance composites. Bamboo filler provides sustainable reinforcement, improving mechanical and viscoelastic performance without compromising printability or thermal stability. These findings highlight the potential of combining bio-based resins with natural fillers to develop sustainable, high-performance materials for AM applications, contributing to the broader goals of the circular economy and green manufacturing.

# sciforum-142581: Biopolymer blends containing modified metal oxide particles: performance and durability

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Blending biopolymers is a valuable method with industrial applications for tuning and improving their properties and performance, as single biopolymers often do not exhibit the appropriate properties for numerous durable applications. Furthermore, the properties of biopolymers can be modified by introducing unmodified and modified metal oxides, such as zinc oxide, titanium oxide, copper oxide and silver oxide.

This work involves adding two different blends of biopolymers, either compatible (such as polylactic acid (PLA) and polybutylene adipate terephthalate (PBAT)) or incompatible (such as PLA and polyamide 11 (PA11)), with unmodified and modified zinc oxide and titanium oxide, via melt mixing. The zinc oxide has undergone chemical modification involving the introduction of stearic acid molecules (f-ZnO). Titanium oxide particles were treated with ultrasound to modify them (us-TiO2). Additionally, an acrylate copolymer (EVA-g-AA) has been added in small amounts to improve system compatibility. All the materials have been characterised for their rheological (oscillatory test), morphological (SEM), mechanical (tensile test) and thermal (DSC) behaviour, as well as for their photoxidation resistance (UVB exposure).

Unmodified metal oxides have a reinforcing effect on compatible PLA/PBAT blends, but a less pronounced beneficial effect on incompatible PLA/PA11 blends. The presence of particles significantly influences the blends' rheological and morphological behaviour, acting as a physical compatibiliser. Chemical modification of ZnO and ultrasound treatment of $TiO_2$ favour the formulation of more compatible blends due to their pronounced compatibilising action. Compatibility is further improved by the presence of the acrylate copolymer. Both unmodified and modified metal oxides promote the photooxidative degradation of blends, as do the more modified oxides.

# sciforum-133919: A Comparative Study of Polyolefin-Based and Biodegradable Composites containing Metal Hydroxides

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The present work proposes the use of metal hydroxides, specifically aluminium and magnesium hydroxides, as halogen-free flame-retardant additives in polymer matrices. The present study focuses on comparing their performance in polyolefin-based polymers and bio-polymer composite formulations. This approach is motivated by sustainability considerations and the growing market demand for environmentally friendly flame-retardant materials.

The incorporation of metal hydroxides occurred within two different composite materials: firstly, an EVA/LLDPE blend and secondly, a PBS matrix. Two types of metal hydroxide were evaluated for use in the formulation of flame-retardant composites (FRCs): precipitated aluminium hydroxide (p-ATH) and naturally milled magnesium hydroxide (nm-MDH). The p-ATH displays a crystalline composition, whereas nm-MDH manifests a brucite crystalline form. The presence of this dolomite phase is advantageous, as it decomposes at higher temperatures than the metal hydroxides and releases inert gases such as carbon dioxide, thereby enhancing flame resistance.

The characterisation of both metal hydroxides was accomplished through a multifaceted approach encompassing X-ray powder diffraction (XRD), thermogravimetric analysis (TGA), meticulous morphological observation, and a comprehensive application of spectroscopic methodologies. It has been established that upon exposure to heat or flame, the metal hydroxides undergo endothermic decomposition, forming metal oxides and releasing water molecules. This reaction has been shown to result in an intumescent effect.

Through our investigation, we found that all of the examined FRCs displayed remarkable flame retardancy, fire resistance, and thermal stability—that is to say, resistance to static heat. These results underscore the potential of these metal hydroxides as effective halogen-free flame-retardant additives. Furthermore, while to a lesser extent, the presence of hydroxides of metals was found to reduce the accumulation of groups containing carbonyl and hydroxyl functionality during UVB weathering exposure. This finding suggests a protective effect on the polymer matrix.

# sciforum-147453: Characterization of copper oxide (CuO) nanoparticle-reinforced Bionanocomposite films from taro (Colocasia esculenta (L.) Schott) starch and Aloe Vera (Aloe barbadensis (L.) Burm.f.) gel blend

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The current study investigated the effects of increasing the concentration of CuO NPs on the performance of biocomposite films derived from taro starch and Aloe vera gel. The CuO NPs synthesized through chemical co-precipitation and calcification were mixed with taro starch and aloe vera gel to obtain biodegradable bio-nanocomposites films. The glycerol, biopolymers and the CuO NPs were mixed and cast and dried in the oven to create uniform films. The bionanocomposite film was characterized by optical, mechanical, physical, chemical, morphological analysis, antimicrobial and antioxidant properties. Results show that as the concentration of CuO NP increases, the film's opacity also increases as the film absorbs more light. Although the optimum percentage of CuO NPs enhanced the film thickness, the tensile strength decreased at higher concentrations (1. 5% and 2. 0%)

because of agglomeration. Moreover, adding the CuO NPs to the biopolymer matrix had no new chemical interaction. However, the agglomeration was caused by physical factors. The glass transition temperature (Tg) and melting point temperature (Tm) rise with increasing CuO NPs, indicating a significant relationship between CuO NPs and the biopolymer film. The antibacterial activity of the film raised with increasing CuO concentration against all bacterial strains due to the leaching of copper ions. There was no considerable impact on the antioxidant property of the bio-nanocomposite film. Therefore, Copper Oxide nanoparticles (CuO NPs) have benefits such as a high light barrier effect, possible antibacterial properties, and possibly enhanced thermal stability, making them suitable for active food packaging applications.

# sciforum-138921: Interface engineering between poly(lactic acid) and graphitic carbon nitride

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Poly(lactic acid) (PLA) is a biodegradable, bio-based polymer with promising applications in sustainable materials. However, its inherent brittleness, poor UV resistance, and limited thermal stability hinder broader use in advanced applications such as packaging and biomedical devices. Interface engineering through the incorporation of functional inorganic nanomaterials offers a potential route to overcome these limitations while maintaining the environmental advantages of PLA. In this study, we report on the design, synthesis, and characterization of PLA nanocomposites reinforced with surface-modified graphitic carbon nitride (g-$C_3N_4$, CN), a metal-free, 2D nanomaterial with unique optical and structural properties. CN was synthesized from melamine and subsequently functionalized using mild acid oxidation and silanization to improve dispersion and compatibility with the PLA matrix. These modifications introduced reactive –OH, –NH, and alkoxysilane groups on the CN surface, enabling hydrogen bonding and covalent interactions with PLA during melt blending. Mechanical testing showed that with only 1 wt% silanized CN, the elongation at break of PLA increased sevenfold, from 6% to 42%, without sacrificing tensile strength. Optical analysis demonstrated a dramatic reduction in UV transmittance below 400 nm, while visible-light transparency remained above 80%. These enhancements were attributed to improved interfacial adhesion and uniform nanofiller dispersion, as confirmed by means of FTIR, TEM, XRD, and XPS. This work demonstrates that interface engineering via surface-functionalized inorganic nanofillers can effectively enhance the mechanical flexibility, UV barrier, and thermal stability of PLA with minimal filler content. Our approach provides a scalable and environmentally conscious strategy for developing multifunctional PLA-based nanocomposites tailored for advanced material applications.

# sciforum-136460: MXene/polymer composites in food packaging: A patent overview

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MXenes are a class of two-dimensional (2D) nanostructured materials with the general formula $M_{n+1}X_nT_x$, where M is a transition metal, X is a carbon and/or nitrogen atom, and T is a functional group, such as O, F, OH, or Cl. MXenes have the capacity to be mixed with a variety of polymers, thereby imparting certain properties to the polymer. For instance, MXenes can enhance the barrier properties of plastics, suggesting a potential application as gas barrier films. Additionally, MXenes can improve flexibility, toughness, and tensile and compressive strengths. Furthermore, MXenes have been shown to possess antimicrobial and anti-fogging properties. These properties render them promising materials for use in food packaging.

The present study is focused on patent retrieval information regarding MXenes/polymer composites employed in the domain of food packaging.

A patent search was conducted on Espacenet, the EPO's free patent database, using precise keywords in the title, abstract, and claims search fields, as well as a set of classification codes, such as C08K 3/14 (use of carbides as compounding ingredients), C01B 32/921 (titanium carbide), and C08K 2201/011 (nanostructured additives).

After reading the full text of the patents/patent applications, we narrowed our initial 43 results down to 38.

Approximately 80% of patent priority filings were submitted in 2022. China is the most prolific country, with 34 results, but only one Chinese application was extended at the international level as a PCT application. The other four PCT applications derived from two EP applications, one U.S. provisional, and one application from the Czech Republic.

In most cases, $Ti_3C_2T_x$ is claimed. However, in one patent application (CN115651245A), $Ta_4C_3T_x$ is mixed with chitosan and N-hydroxyethyl acrylamide to create a chitosan-based film coating solution.

The most frequently used film matrixes are cellulose, chitosan, polyethylene, polypropylene, and polyurethane.

# sciforum-137440: Nanostructured Flame Retardant Coatings Containing Layered Double Hydroxides

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In this work, a coating approach for obtaining flame retardant EVA (Ethylene - Vinyl Acetate) and EBA (Ethylene - Butyl Acrylate) copolymers-based materials is proposed. To this aim, firstly nanocomposite films of EVA and EBA were produced by cast extrusion, by using as nanofillers two types of layered double hydroxides (introduced at 5 wt.%), having the same chemical nature (Magnesium-Aluminium with intercalated oleate anions) but differing for the aspect ratio. The morphology of the nanocomposites films, as well as their thermal characteristics were preliminary assessed through rheological, thermal, and morphological analyses.

The films were then applied as coating to the corresponding neat copolymer substrate by compression molding, and the so-obtained samples were tested through cone calorimeter. Despite the small amount of nanofiller (0.5 wt.% considering the whole specimen), the application of the coating films significantly improved the Time to Ignition as compared to the pristine copolymers, while maintaining quite unchanged the shape of the HRR curves and the HRR peak values.

In all, the obtained results demonstrated the effectiveness of the coating approach, since it allows to concentrate the flame retardant action on the surface of a polymer system, where combustion specifically takes place; consequently, the required amount of flame retardant is minimized. This last has a beneficial effect on the final mechanical properties of the material, since the tensile characteristics of the bulk polymer are preserved. Furthermore, introducing such a small amount of flame retardant does not affect the future recyclability of the polymer, that can be treated as its pristine (non-flame retardant) counterpart.

# sciforum-147096: A new approach for the development of antimicrobial coatings based on functionalized polysulfone

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## Introduction

Polysulfone is a high-performance polymer used in the biomedical field due to its thermal, mechanical, and chemical stability and biocompatibility [1]. Its performance is significantly enhanced through quaternization, which imparts antimicrobial activity, hemocompatibility, and hydrophilicity [2]. The present study aims to obtain and characterize coatings based on quaternized polysulfone (QPSF) for medical instruments with broad-spectrum antimicrobial activity by incorporating an antifungal agent, amphotericin B (AmB), and/or an antibiotic, norfloxacin (NFX), into the material's structure.

## Methods

Drug-containing coatings were prepared by mixing QPSF, AmB, and/or NFX in different mass ratios, casting the polymer–drug solutions, and drying at 70 °C for 48 h. The obtained materials were characterized from a structural, supramolecular, and morphological point of view and their surface properties, as well as antioxidant and antimicrobial activities, were also investigated.

## Results

$^{1}$H-NMR and FTIR spectra of the coatings highlighted the successful incorporation of the drugs into the QPSF matrix, as well as strong physical interactions between the components.

The absence of a specific drug's reflection in the formulations' XRD diffractograms suggested their uniform dispersion within the material's structure, and the polarized optical microscopy images revealed an interface-coupled ordering, attributed to the electrostatic interactions between the positively charged amino groups of the polymer and the electron-rich groups of the drugs.

The surface of the coatings presented a smooth morphology and moderate wettability, with contact angle values ranging from 72 to 93°.

The incorporation of the two drugs into the material structure had a beneficial effect on antioxidant activity, increasing the capacity to inhibit free radicals up to 67 %, improving antibacterial activity, and conferring antifungal activity to the materials.

## Conclusion

All these data indicate the application potential of these materials as antimicrobial coatings for surgical instruments.

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# sciforum-144635: A study of Silicate-Reinforced Polyvinyl Butyral Composites

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**Introduction**

Polyvinyl butyral (PVB) is a thermoplastic terpolymer known for its excellent optical clarity and strong adhesion to glass, which is due to its vinyl alcohol monomer units. Due to the latter characteristics, PVB is used as interlayer between two silicate glass sheets in laminated safety glass. Other interesting combinations of PVB and silicates correspond to composites based on PVB matrices and silicate dispersions [1]; we consider herein a range of properties for silicate dispersions in the form of fibers, flakes, or powders.

**Methods**

Silicate particles of varying sizes and morphology (flakes, fibers, nanoparticles), silane functionalization, and different loading levels (5%, 10%, 15% w/w) were incorporated into the PVB matrix using a Brabender internal mixer (150°C, 40 rpm, 5 min). The effects of each reinforcement were evaluated via optical microscopy, TGA, mechanical testing (tensile and impact resistance), light transmittance, and water absorption tests.

**Results**

All silicate reinforcements enhanced the thermal stability of PVB. Fumed silica nanoparticles not only increased tensile strength and maintained optical transparency but also reduced water absorption. In contrast, glass fibers primarily contributed to enhanced impact resistance.

**Conclusions**

Low-aspect-ratio silicate particles are appropriate fillers/modifiers for PVB. In addition, PVB is a good polymeric matrix material for composites with high aspect ratio silicate particles.

**Conflict of interest:** The authors declare no conflicts of interest.

**Acknowledgments:** We thank GlassFlakes Co., Ltd (UK) and NEOTEX S.A. (Greece) for supplying samples and Mr. Christophoros Razos for his assistance in the experimental work.

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# sciforum-133255: A sustainable path for composite tooling: novel materials, design, and technologies through FEM and LCA

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*Intro:* Production of composite parts requires the presence of proper tools, often made of polyurethane boards, which imply the use of harmful substances, such as isocyanates. Moreover, the standard approach for tooling manufacturing is subtractive, generating a massive amount of waste: as a thermosetting material, PU boards are not easily recycled nor re-used; hence, they are often landfilled, increasing the burdens associated with composite manufacturing.

*Methods:* TOOL4LIFE, an EU-Life project, aims to introduce additive manufacturing and design optimization in composite tooling for the automotive industry, combined with the use of thermoplastic materials. The innovations simplify the tooling (i.e. no need of master models), reduce waste scrap (i.e. direct 3-D printing), and allow for tool recycling at the EoL, in a sustainable perspective.

*Results:* Finite Element (FE) topology optimization analyses supported the definition of a proper design shape for specific tool application, reducing the amount of material mass required and optimizing the 3D printing process. Life Cycle Assessment (LCA) applied to the selected shape confirmed the reduction in associated environmental impacts with respect to the baseline PU tool.

*Conclusions:* The combination of FE analysis and LCA, along with the selection of thermoplastic polymers (i.e. PC, ABS), supported a transition towards sustainable materials and processing in composite tooling. The application in the automobile sector, whose design and requirements are challenging, is proficient and suggests a potential wider application in other hi-tech industries. This approach proves that sustainability in composites can be achieved without sacrificing technological performance and feasibility.

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# sciforum-138941: Additive Manufacturing of Wood-Based Polymer Composites Fabricated Using Vat Photopolymerization for Design Applications

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**Introduction**

In the present research work, wood-based composites were prepared by adding different poplar powders within a soybean-oil-based resin, choosing liquid crystal display (LCD) as vat photopolymerization (VP) among the additive manufacturing (AM) technologies used for polymer processing. The aim was to combine the advantages of AM with the valorization of poplar wood powder waste from the plywood industry to obtain innovative and more sustainable composite materials as alternatives to classic fossil-based materials for interior design applications.

**Materials and Methods**

Several photocurable formulations were prepared using an acrylate epoxidized soybean oil (AESO) resin as the polymer matrix and isobornyl methacrylate (IBOMA) as reactive diluent, in the presence of 2 wt.% of phenyl bis(2,4,6-trimethylbenzoyl), with phosphine oxide (BAPO) as the photoinitiator. Bio-based composites were obtained by adding 3 wt.% of different wood poplar powders ($P_I$ and $P_{IV}$), two by-products from plywood panel production, to the AESO formulations and 3D printing different parts in an LCD 3D printer.

**Results and Discussion**

A comprehensive characterization of the composites fabricated by VP was carried out. Rheological, thermal, morphological, and mechanical measurements were performed to investigate the final properties of the 3D-printed wood-based composites. Several 3D-printed components were fabricated, showing different levels of detail and complexity. The specimens showed enhanced final properties in terms of elastic modulus, glass transition temperature, and storage modulus due to the reinforcing effect induced by the presence of the fillers.

**Conclusions**

This research demonstrates that bio-based components can be successfully 3D-printed via LCD, including objects with potential application in interior design, such as joints and connections, highlighting the material's suitability to realize customized and more sustainable elements for design-oriented applications.

# sciforum-127812: Advancements in Nanofibrillar PVA Materials: Exploring Preparation of PVA-Based Materials by Solution Blow Spinning and Electrospinning Techniques

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In this work, a prospective study on the current uses and applications of polyvinyl alcohol (PVA) nanofibrillar materials is presented. Polyvinyl alcohol is a synthetic polymer that has gained attention for its biodegradability and sustainable qualities under certain conditions. It has become a valuable material in various fields, including innovative food packaging, advanced hydrogen fuel cells, and sophisticated medical applications such as wound dressings and tissue engineering scaffolds. First, the theoretical background is studied in detail to understand the structure–property relationships that govern PVA performance, examining its essential properties intrinsically linked to its structural features, such as crystallinity, mechanical properties, and bio-sustainability. Then, the main processing parameters dictating nanofibrillar morphology and the factors and parameters that may control the morphological characteristics of PVA-based materials to favor the formation of nanofibers are focused on, with particular emphasis on the electrospinning (ES) and solution blow spinning (SBS) techniques. Finally, to give consistency on the practical feasibility of both approaches, PVA nanofibers were experimentally fabricated under the optimized ES and SBS conditions established herein. Morphological, structural, and thermal characterization of the resulting materials was carried out to elucidate the differences between the two processing techniques. Ultimately, this article discusses the future research directions to address the current challenges and prospective ways to fabricate PVA nanofibrous materials for potential biomedical applications.

# sciforum-136525: Aging of Poly(3-Hydroxybutyrate-Co-3-Hydroxyhexanoate)-Based Biocomposites under Accelerated Photo-Oxidation

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In recent decades, the use of polyhydroxyalkanoate biopolymers has drawn increasing attention. Still, one of the biggest challenges that hinders their wide applications is the fine-tuning of their photooxidative aging. Therefore, the objective of this study is to investigate the effect of Agave Americana fibers (AFs) before and after surface treatment with sodium bicarbonate ($NaHCO_3$) on the accelerated photooxidation of PHBHHx using a SEPAP 24-48 enclosure. Biocomposite samples are prepared by melt compounding at a filler content of 30 wt.%. Colorimetric analysis reveals a yellowing effect of neat PHBHHx after 216h of exposure to UV rays, which is attributed to the formation of carbonyl groups. For the untreated biocomposites (PAF), they show a browning in color, while the PHBHHx-treated AF (PAFB) shows a lighter surface. The former process is attributed to the presence of lignin, whereas the latter is owing to the successful removal of lignin and hemicellulose by $NaHCO_3$. Changes in the chemical structure are assessed via FTIR-ATR spectroscopy, which shows a decrease in the 1741 $cm^{-1}$ band intensity for PHBHHx and PAF (after photooxidation) due to chain scission. However, no noticeable change is observed considering the same peak in the PAFB spectra. Furthermore, the evaluation of the hydroxyhexanoate (HHx) content in the different formulations is evaluated by $^1H$ NMR spectroscopy. The results show a slight decrease in HHx molar % after exposure to 216 h under accelerated photooxidation. Nevertheless, the decrease seems to level off after the addition of AF, particularly the treated ones. The overall findings highlight the beneficial effect of the incorporation of AF into the PHBHHx matrix, especially when treated with $NaHCO_3$ which confers a better photostability.

# sciforum-128419: Analysis of electro-conductive network formation in multilayer graphene sheet/epoxy nanocomposites

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The development of polymer nanocomposites with enhanced electrical conductivity is of considerable interest for advanced technological applications such as sensing, electromagnetic shielding, and printed electronics. In this context, the formation of electrically conductive networks is critical to the functional performance of these materials. Incorporation of multilayer graphene sheets (MLGs) into polymeric matrices enables the formation of three-dimensional conductive networks, characterized by significant increases in electrical conductivity and associated with percolation phenomena. However, a detailed understanding of the factors governing the morphology and connectivity of these networks is still incipient. Previous studies have suggested that mesoscale network connectivity is one of the key factors influencing the conductivity of composite material. This work investigates the formation of electrical percolation networks in MLG/epoxy nanocomposites through an experimental study of the electric domains based on the analysis of images acquired via optical microscopy and electrostatic force microscopy (EFM). Specimens with several MLG concentrations were prepared using a three-roll mill calender. Electrical characterization was performed through direct current conductivity measurements. The electrical domains were evaluated at the microscale (optical) and nanoscale (EFM), providing insights into the local conductive behavior and network formation. The analysis of network connectivity was evaluated using a custom-developed software tool for image processing and quantification of structural network metrics. The results indicate that network conductivity and electrical conductivity are strongly influenced by the density of agglomerates and their degree of interconnection. Topological parameters used to characterize the networks were found to correlate directly with the electrical conductivity of the nanocomposites. Such a correlation highlights the potential of quantitative multiscale analyses to characterize and predict the behavior of electrically conductive networks in graphene-based composites.

# sciforum-129335: Antimicrobial $Bi_2O_3$-Chitosan Nanocomposite Films for Sustainable Food Packaging: Enhanced Barrier Properties and Preservation Performance

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Demand for sustainable packaging in the global market has led to the development of environmentally friendly alternatives to conventional plastic materials. This study investigates the synthesis and characterization of $Bi_2O_3$-loaded chitosan nanocomposite films as advanced eco-friendly packaging materials with enhanced antimicrobial and barrier properties.

$Bi_2O_3$ nanoparticles (20-50 nm) were produced using controlled precipitation and then embedded in high molecular weight chitosan matrix at 1, 3, 5, and 7 wt% using solution casting coupled with probe sonication. Plasticization of films was achieved using glycerol (30% w/w).

Detailed characterization confirmed $\alpha$-$Bi_2O_3$ crystalline phase with homogeneous nanoparticle dispersion throughout the chitosan matrix. The nanocomposite films demonstrated excellent broad-spectrum antimicrobial activity, achieving 99.9% elimination of E. coli and S. aureus within 4 h and complete elimination within 8 h. Growth of A. niger was completely inhibited after 7 days, with reasonable antibacterial activity retained after 30 days under ambient conditions.

Practical food preservation trials using fresh strawberries showed superior performance compared to conventional polyethylene packaging, with 60% less weight loss (8.2% vs. 20.5%), reduced firmness loss (15% vs. 45%), and extended shelf life by 8 days. Microbial counts were significantly reduced, and nutritional quality was better preserved with 23% higher ascorbic acid retention.

Biodegradation studies demonstrated complete degradation within 45 days under composting conditions, with life cycle assessment indicating 65% lower carbon footprint than conventional plastic packaging. The synergistic action of $Bi_2O_3$ nanoparticles and chitosan matrix exhibits improved mechanical strength, enhanced barrier properties, and sustained antimicrobial activities, demonstrating excellent potential for food packaging applications.

# sciforum-147129: Application of spectroscopic methods in the in-line analysis of gradient polymeric materials

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The integration of spectroscopic methods into in-line analysis systems presents a new approach to real-time monitoring and control of polymeric materials processing, bridging the gap between materials science, analytical chemistry, and advanced manufacturing. This study explores the potential of spectroscopic methods for dynamic, non-destructive analysis of functionally graded polymeric materials (FGMs), in the form of filaments designed for fused filament fabrication (FFF) 3D printing. FGMs are a class of advanced engineered materials characterized by a smooth change of properties, composition, structure, or functional additives across their volume. This gradient architecture enables the optimization of local properties such as stiffness, thermal conductivity, or chemical resistance, enhancing mechanical performance, durability, and interfacial adhesion in multimaterial systems.

To tackle the challenges of FGM filament production, this research develops a controlled extrusion protocol and implements an in-line spectroscopic monitoring system capable of detecting real-time changes in chemical composition and additive distribution. By integrating this analytical data into a closed-loop control system, process parameters are dynamically adjusted to maintain consistent material quality. Initial results highlight difficulties in achieving uniform modifier distribution, particularly with viscous blends. Ongoing work focuses on optimizing processing conditions and formulations. The ultimate goal is to create a closed loop for the production and control of new polymeric filaments for 3D printing.

# sciforum-138034: Ballistic ion transport through hierarchically-ordered-structure polymer binder

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All-solid-state batteries (ASSBs) have emerged as a promising solution to enhance battery safety by employing solid electrolytes in place of flammable organic electrolytes. However, ASSBs encounter several challenges that limit their practical applications. Silicon (Si) is among the potential negative electrode materials for high-energy-density ASSBs, owing to its specific capacity of approximately 3700 mAh/g. Employing polymer binders is an effective strategy to accommodate the significant volume changes of Si during electrochemical lithiation and delithiation.

Unlike liquid electrolytes, solid electrolytes exhibit a less effective contact interface with active materials. Mixed electronic-ionic conductive (MEIC) polymer binders appear to be a promising solution to mitigate interface issues and the challenge of poor ionic conductivity within electrodes. Cutting-edge approaches to engineering mixed electronic-ionic conductive polymer binders include mixing conjugated polymers with ion-conductive polymers or modifying conjugated polymer backbones by grafting ion-conductive side chains. However, nearly all of these ion-conductive polymers, such as poly(ethylene oxide) (PEO), rely on polymer segmental motions to drive ion diffusion. This ion transport mechanism faces a trade-off between ionic conductivity and mechanical strength. Specifically, it must compromise mechanical strength to enhance ionic conductivity, or vice versa. In addition, the ion transport based on polymer dynamics features low ionic conductivity at room temperature and is highly dependent on temperature. Here, we report a ballistic ion transport mechanism in a MEIC polymer binder, where its hierarchically ordered structure facilitates ion diffusion and achieves solid-state lithium-ion conductivity in the range of $10^{-4}$ to $10^{-3}$ S $cm^{-1}$ from -20 to 70 °C. This mechanically robust MEIC polymer is a versatile ionic conductor, allowing $Li^+$, $Na^+$, or $K^+$ to diffuse through polymer matrix, with their cationic charges counterbalanced by electrons on conjugated polymer backbones. Additionally, this ballistic ion transport mechanism results in enhanced cycling performance in ASSBs.

# sciforum-138006: Biocomposites of Polylactic Acid (PLA)/Cellulose to Generate Value-Added Products

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The consideration of sustainability in the plastic industry encompasses three aspects through to reduce the environmental impacts generated: migration from the use of raw fossil polymers to biopolymers from renewable sources, efficient energy consumption and greener options for final waste disposal. Therefore, biocomposites could be an option to generate impact in the three aspects.The use of polilactic acid (PLA) as a polymer matrix has the potential to enable a great number of final disposal options, since PLA is considered biodegradable and compostable, but also to reduce energy consumption in processing and assure the migration to the use of biopolymers. Although this polymer is relatively fragile, this could be interpreted as an opportunity for improvement by using cellulose as a reinforcement agent and a way to utilize by-products such as sawdust, a typical waste that is not currently taken advantage of, to generate valued-added products that have the biodegradable characteristics whilst simultaneously displaying improved mechanical properties. In this study, a biocomposite generated by reactive extrusion, combining PLA, maleic anhydride as the coupling agent, and cellulose isolated from sawdust, is created. The composite's mechanical properties were evaluated through RSM and the energy consumption of the process was monitored in real time, with the biodegradability of the product measured according to ISO 14855-2. Finally, as a final product, a reusable plate was created, which was then tested according to temperature and mechanical assays in order to evaluate its possible uses.

# sciforum-139265: Biosorbent nanocomposites as an innovative strategy for solving water pollution problems

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Environmental pollution is one of the most challenging problems worldwide, and water is one of the most vulnerable environmental matrices, being an essential resource for life. The exponential increase in industrial manufacturing processes, technological development, urbanization, natural climatic events, and agricultural practices, among others, have generated environmental exposure to numerous chemical compounds that cause the contamination of aqueous matrices. This challenge has led to the development of hybrid nanocomposite biosorbents as an innovative strategy for the aqueous removal of relevant pollutants. These nanocomposites, created from biopolymeric hydrogels and nanoclays, are an effective, sustainable, and scalable strategy for the removal of these pollutants. Our work seeks to provide concrete solutions to the complex problems of water pollution, using the potential of nanocomposite biosorbents. The present work aims to develop materials with biosorbent capacities, based on natural and innocuous raw materials such as the biopolymers chitosan (Q) and sodium alginate (Alg), as well as natural and organomodified bentonite (B) and organomodified (OB) nanoclays. These starting materials are abundant, inexpensive, and environmentally friendly. Nanocomposite biosorbent hydrogels of Q/OB, Alg/B, and Alg/OB were developed using simple and low-cost techniques. The biosorbents were physicochemically and morphologically characterized. These tests revealed internal structures with large porosity, favorable for the diffusion and adsorption of the pollutant. Preliminary atrazine, ciprofloxacin, and arsenic removal tests were performed under batch conditions. The results showed promising biosorptions for all the pollutants studied. These results show the potential of the developed biohydrogels as efficient systems for the aqueous remediation of contaminants of relevance to mitigate a real problem of global concern.

# sciforum-138957: Boosting Biobased Content in PVOH Films: Comparative Thermo-Mechanical Performance of Lignin and Nanocelluloses as Reinforcements

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The transition to a circular economy in packaging has become a strategic priority due to increasing regulatory pressure and environmental awareness. The use of bio-based and degradable, and/or recycled materials contributes to the development of sustainable, circular material flows. This has driven research into incorporating renewable components into polymer systems. Poly(vinyl alcohol) (PVOH), a water-soluble synthetic polymer with excellent film-forming properties, is particularly suitable for such enhancements due to its compatibility with natural additives.

In this study, we investigate the thermo-mechanical performance of PVOH films reinforced separately with lignin and nanocelluloses to assess their effectiveness in improving thermo-mechanical properties and increasing overall bio-based content.

PVOH composite films were prepared by solvent casting with varying loadings (5%, 10%, 20%) of lignin and nanocellulose. Hydropol™ PVOH was provided by Aquapack Polymers. Organosolv lignin was extracted from Jartropha Curcas L. seed coats, while enzymatic cellulose nanofibrils were obtained from bleached kraft pulp. Mechanical and thermal properties were evaluated using tensile testing and thermal analysis (DSC, TGA).

Results showed that 5% loading of both reinforcements improved the mechanical strength and thermal stability of PVOH films. Nanocellulose provided greater increase in tensile strength and modulus due to its high aspect ratio and strong hydrogen bonding with the PVOH. In contrast, lignin improved thermal stability while preserving the film's flexibility, likely due to its aromatic, amorphous structure.

These findings reveal distinct reinforcement mechanisms, highlighting the potential for tailored material design based on specific performance needs. Overall, lignin and nanocellulose are promising sustainable reinforcements for PVOH films, advancing the development of high-performance, bio-based polymer composites.

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# sciforum-147149: Chitosan/starch-based films modified with alginate dialdehyde

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Biopolymers are macromolecular organic compounds derived from living organisms. They can be classified into polysaccharides, proteins, and nucleic acids. Chitosan and starch belong to the group of polysaccharides and are widely investigated for applications in tissue engineering, including wound healing. However, materials based on single biopolymers or their blends often exhibit insufficient physicochemical properties. Therefore, modification strategies, such as chemical cross-linking, are required. Dialdehydes are increasingly explored as natural, non-toxic cross-linking agents. Starch dialdehyde, chitosan dialdehyde, alginate dialdehyde, and other modified polysaccharides have been used for the modification of biopolymer materials.

The aim of this study was to obtain and characterize thin films based on chitosan and starch, modified with alginate dialdehyde. Alginate dialdehyde was synthesized by means of sodium periodate oxidation. The films were prepared using the solvent evaporation method. Structural characterization was performed by means of Fourier Transform Infrared Spectroscopy, while moisture content, hydrophilicity, and antioxidant activity of the obtained materials were also evaluated.

The results demonstrated that the addition of alginate dialdehyde significantly influenced the physicochemical properties of the films. It can be concluded that the properties of biopolymeric materials strongly depend on their weight ratio composition and the applied cross-linking agent. Novel biopolymeric composites based on chitosan and starch, chemically cross-linked with alginate dialdehyde, show promising potential for biomedical applications, particularly in wound healing.

# sciforum-138613: Coaxial fibers based on polycaprolactone and collagen: effects of active component concentrations (CuO NPs and aloe vera extract) on the antibacterial properties of the material

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The main task of modern biomedical engineering is to prevent and control infections during the healing of skin wounds. Conventional antibacterial therapies frequently prove ineffective due to the emergence of antibiotic-resistant bacterial strains and their ability to form biofilms. Consequently, the development of antibacterial non-woven wound dressings that promote tissue regeneration, combat infections, and combine biocompatibility, mechanical strength, and potential for bioactive functionalization is regarded as a promising direction.

The aim of this study is to evaluate the antibacterial activity of coaxial nonwoven materials based on polycaprolactone (PCL) and collagen (Col), modified with varying concentrations of aloe vera (AV) extract and copper oxide (CuO) nanoparticles (NPs). The materials, with an average fiber diameter of 110–120 nm, were fabricated using electrospinning. The successful incorporation of AV extract and CuO NPs was confirmed using scanning electron microscopy with energy-dispersive X-ray spectroscopy, Fourier-transform infrared spectroscopy, and contact angle measurements. The antibacterial activity of the resulting materials was assessed by the colony-forming unit counting method. The tested strains included both Gram-positive and Gram-negative bacteria, as well as *Candida* species.

The resulting coaxial PCL/Col-based materials modified with CuO NPs and AV extract exhibited strong antibacterial properties. The most effective formulation, containing 2 wt.% CuO NPs, achieved complete inhibition of eight Gram-negative, five Gram-positive bacterial, and three fungal strains within the first 6 hours of incubation. Materials containing 15% AV extract also showed significant antibacterial activity within 24 hours against strains including *E. coli* ATCC25922, *E. coli* S176, *E. coli* ATCC35218, *P. aeruginosa* S246, *S. aureus* ATCC29213, and *S. aureus* ATCC700699. The combined use of CuO NPs and AV extract represents a promising strategy for developing biocompatible materials with prolonged antibacterial activity.

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# sciforum-114979: Comparative study on different coating strategies in organically synthesized iron-oxide nanocubes by microwave-assisted method

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The microwave (MW)-assisted method for the synthesis of nanoparticles has been studied for a long time due to its rapid synthesis and lower consumption of energy, ultimately reducing cost. In this study, we synthesized for the first time, monodisperse iron-oxide nanocubes (IONCs) by MW-assisted method using an environmentally friendly precursor and organic solvents [1]. The cubic shape of iron-oxide nanoparticles provides superior magnetic properties over the spherical counterparts and, due to this, can be exploited in magnetic hyperthermia (MHT) applications to generate local heating effects under the influence of alternating magnetic fields (AMF) to kill cancer cells. However, IONCs synthesized in organic solvents must be transferred to water using polymers or ligands for solubility, dispersity, and to prevent agglomeration in biological fluids. Therefore, this study explored different coating strategies to transfer organic synthesized IONCs into water. This was done by coating the IONCs with different polymers and ligands, including dopamine-poly(isobutylene-*alt*-maleic anhydride)-poly(ethylene glycol), poly(maleic anhydride-*alt*-1-octadecene), gallol-derived ligands, and cetyltrimethylammonium bromide. The coated IONCs in water were further characterized via transmission electron microscopy (TEM), dynamic light scattering (DLS), and agarose gel electrophoresis. The magnetic properties of the coated IONCs were also evaluated by conducting specific absorption rate (SAR) measurements. By comparing the SAR values of the differently coated IONCs, it emerges the critical role of the coatings on the magnetic heating efficiencies of the resulting nanoparticles, therefore suggesting the choice of the hydrophilic coating as a critical parameter to further optimize the magnetic hyperthermia treatment.

## Reference

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# sciforum-139211: Composite Microgels Based on Polyelectrolyte Complexes for Hemostatic Applications

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**Introduction**

Uncontrolled hemorrhage is a major cause of death in civilian and military settings (30 and 80%, respectively), often complicated by infection. This underscores the critical need for rapid, effective hemostatic materials. Natural polysaccharides are promising for this purpose. This study aimed to synthesize a novel powdered hemostatic material using a scalable spray-drying technique for rapid hemorrhage control, leveraging the polyelectrolyte properties of chitosan **(CHI)** and carboxymethylcellulose **(CMC)**.

**Methods**

Polyelectrolyte complexes (PECs) were formed by dropwise mixing of CHI (1.5% w/v) and CMC solutions (0.5, 1, and 1.5% w/v). These PECs were then spray-dried (inlet temperature 160°C, outlet temperature 80°C, aspirator 70°C) to yield powdered microgels (1.5Q/1.5CMC; 1.5Q/1.0CMC; and 1.5Q/0.5CMC). The resulting microgels were evaluated for their morphological, physical, thermal, swelling, and hemostatic properties.

**Results**

ATR-FTIR spectra confirmed electrostatic interactions between amino and carboxyl groups of CHI and CMC in all microgels. The SEM technique revealed an irregular spherical morphology with an average size of 2–3 μm for all microgels. The gel fraction test (GF) showed that 1.5Q/1.5CMC samples had higher crosslinking between CHI and CMC (64.2±1.7%) compared to 1.5Q/1.0CMC (49.9±2.5%) and 1.5Q/0.5CMC (42.9±3.8%). Additionally, 1.5Q/1.5CMC microgels exhibited higher swelling percentages (up to 900%) in PBS solution (pH 7.4) than 1.5Q/1.0CMC and 1.5Q/0.5CMC (up to 600%). TGA analysis indicated similar thermal behavior across all microgels, with three or four degradation stages and a degradation temperature (Tp) around 240°C. Hemolysis testing (ASTM-F756-00) showed all microgels had a hemolysis percentage below 5%, confirming their hemocompatibility. Furthermore, all microgels reduced the coagulation time by 20% in comparison with whole blood without microgels.

**Conclusions**

Three powdered microgels were successfully obtained using CHI and CMC via spray drying. Among them, 1.5Q/1.5CMC microgels demonstrated superior physicochemical properties, including higher gel fraction and swelling percentages, making them particularly promising for use as hemostatic materials.

# sciforum-127838: Cost-effective eco-friendly synthesis of iron oxide nanoparticles from waste cans as a precursor for magnetic polymer fabrication

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Municipal solid waste (MSW) poses significant risks to both environmental health and human well-being. Therefore, devising innovative and sustainable solutions for transforming MSW into valuable resources is crucial. MSW composition exhibits marked differences between developed and developing nations. While MSW in developing countries largely comprises organic matter such as food waste, wood, foliage, and agricultural residues, developed countries produce MSW dominated by inorganic materials like plastics, paper, metals, and electronic devices. Globally, MSW encompasses a diverse array of materials including household refuse, agricultural remnants, metals, paper, glass, plastics, electronics, inert substances, and miscellaneous debris. Current waste management strategies worldwide heavily favor landfilling, which accounts for approximately 70% of generated MSW. Alternative treatment methods include classified recycling, incineration, pyrolysis, gasification, composting, and anaerobic digestion.

This research investigates a cost-effective chemical process for converting waste cans, a major component of MSW, into active iron oxide nanoparticles. The synthesized nanoparticles were characterized using techniques such as X-ray diffraction (XRD) and Fourier transform infrared spectroscopy (FTIR). To highlight the potential applications of these nanoparticles, they were incorporated into the fabrication of a magnetic polymer, utilizing magnetite nanoparticles as stabilizers in an emulsion template. This novel material holds promise for use in various fields, including diagnostic devices and smart systems.

# sciforum-146052: Cu(I) oxide- decorated Polypyrrole nanocomposite: Multifunctional versatility towards Ammonia gas sensing and regioselective synthesis of 1,4-disubstituted 1,2,3-triazoles and 2-Phenylquinazolin-4(3H)-ones.

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In this work, Cu(I) oxide –decorated Polypyrrole nanocomposite (PPy-$Cu_2O$) was synthesized by in-situ polymerization, and a high- performance $NH_3$ gas sensing activity was studied along with regioselective synthesis of 1,4-disubstituted-1,2,3- triazoles and 2- (Phenyl)-quinazolin-4(3H)-ones. $Cu_2O$ nanoparticles were synthesized via a green synthesis approach employing *Ocimum tenuiflorum* leaf extract as a biogenic reducing agent and $CuCl_2{\cdot}2H_2O$ as the copper precursor. The morphology, composition and chemical state and morphology of the PPy-$Cu_2O$ nanocomposite was characterized by XRD, FTIR, SEM-EDX, TEM and XPS. The UV–Vis optical band gaps of PPy, $Cu_2O$, and the PPy–$Cu_2O$ nanocomposite were determined to be 3.1 eV, 3.0 eV, and 2.9 eV, respectively. Notably, the PPy–$Cu_2O$ nanocomposite exhibited enhanced $NH_3$ gas sensing performance, achieving a maximum sensitivity of 52.9% at 500 ppm, compared to 17.3% for pristine PPy. Response times for the nanocomposite at 100, 300, and 500 ppm $NH_3$ concentrations were 85 s, 70 s, and 60 s, respectively, with corresponding recovery times of 100 s, 120 s, and 135 s. In addition to its sensing capability, PPy–$Cu_2O$ demonstrated catalytic efficiency in the regioselective synthesis of 1,4-disubstituted-1,2,3-triazoles in aqueous medium at room temperature, using both terminal and internal alkynes—without the need for any base, ligand, or reducing agent. Furthermore, the nanocomposite was successfully employed in the synthesis of 2-phenylquinazolin-4(3H)-ones via the condensation of anthranilamide (1 mmol) and 4-methylbenzaldehyde (1.2 mmol) under varied reaction conditions. This work introduces a novel, multifunctional nanocatalyst that offers cost-effective and high-performance $NH_3$ sensing alongside green synthetic protocols for value-added heterocycles. The study underscores the potential of PPy–$Cu_2O$ as a sustainable platform for both sensing and catalytic applications, demonstrating strong potential for environmental and pharmaceutical applications.

# sciforum-147108: Design of CMC/g-$C_3N_4$ Beads Crosslinked with Metal Ions for Enhanced Wastewater Treatment

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## Introduction

Graphitic carbon nitride (gCN) exhibits a unique combination of visible-light responsiveness, suitable band structure, chemical stability, and low cost, making it a highly promising photocatalyst. In photocatalysis, one of the major challenges lies in the difficult separation of the photocatalyst from the reaction medium and its reuse over multiple cycles. This problem can be addressed by immobilizing gCN onto solid support. Therefore, developing reliable immobilization strategies is essential to ensure the long-term stability, reusability, and ecological safety of gCN-based photocatalysts. One of the solutions presented in this research involve the formation of carboxymethylcellulose/gCN (CMC/g-$C_3N_4$) beads supported by metal ions.

## Methods

Beads were synthesized from urea-derived gCN, CMC, $CuSO_4$ and $FeCl_3$. The preparation involved the dropwise addition of CMC solution (1 and 2wt%) into a 10wt% aqueous solution of $Fe^{3+}$ or $Cu^{2+}$ ions with dispersed gCN. The resulting beads were characterized by FTIR spectroscopy and compression testing. Stability and reusability of obtained beads as photocatalyst carriers were evaluated and compared through three successive photodegradation cycles using azo-dye Acid Orange 7 as model compound.

## Results

In this study, CMC/gCN beads were designed and fabricated. CMC served as a supporting anionic polymer matrix, capable of reacting with cationic crosslinkers such as $Cu^{2+}$ and $Fe^{3+}$ through its –COOH groups, thereby promoting the formation of a dense and stable network with enhanced mechanical strength. The successful formation of the composite structures was confirmed by FTIR analysis, while compression testing and photocatalytic evaluation demonstrated superior durability and efficiency of the beads crosslinked with $Cu^{2+}$-ions.

## Conclusion

The study provides insights into how the choice of metal ion crosslinker and synthesis strategy affects the physicochemical properties, structural integrity, and photocatalytic efficiency of the beads. These findings highlight the potential of synthesized beads for their use in sustainable and efficient wastewater treatment.

# sciforum-138425: Designing bio-based photocatalytic platforms: from cellulose hybrids to aerogel-supported systems

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Water pollution remains a critical global environmental challenge. According to UNESCO, approximately 80% of wastewater is discharged without adequate treatment, while nearly half the world's population resides in water-stressed regions. Photocatalysis has emerged as a promising green technology for combating water pollution due to its efficiency, cost-effectiveness, and environmental compatibility. In particular, photocatalytic degradation of organic pollutants, such as dyes, has garnered significant attention.

Our research focuses on the development of novel, sustainable cellulose-supported photocatalysts designed for efficient sunlight-driven degradation of organic contaminants. Cellulose, with its high surface area, reactive functional groups, and compatibility with metal oxides, serves as an effective support material. Additionally, its capacity to mediate electron transfer contributes to reduced charge recombination and enhanced photocatalytic activity. We engineered a range of cellulose-based platforms for the immobilization of metal oxide nanoparticles ($CeO_2$, ZnO), to create hybrid nanocomposites with improved photocatalytic performance under both UV and visible light. These materials demonstrated effective degradation of a range of hazardous dyes (methyl orange, Congo red, rhodamine B, methylene blue), alongside excellent reusability and operational stability.

Currently, we are designing aerogel-based macroporous matrices as advanced supports for photocatalyst immobilization. These structures aim to increase catalyst loading, improve mass transfer, and prevent leaching. Unlike dense films or submerged polymeric composites, our approach employs floatable substrates positioned at the air–water interface. This configuration maximizes solar light exposure, enhances oxygen availability for radical generation, and significantly boosts overall photocatalytic efficiency.

Our work contributes to the advancement of sustainable water treatment technologies and highlights the potential of biopolymer-based photocatalytic systems for practical environmental remediation applications.

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# sciforum-138518: Development of an advanced biopolymer patch for skin tissue regeneration

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Traditional passive wound dressings present significant limitations, including poor biocompatibility, inadequate mechanical strength, and uneven material distribution. This study addresses these challenges by enhancing hydrogel strength through UV-induced thiol-ene click chemistry, incorporating biocompatible polymers, chitosan (CS), hyaluronic acid (HA), and polyvinyl alcohol (PVA), and leveraging 3D printing for uniform porous scaffold architecture. Hydrogels composed of CS, HA, and PVA were prepared in various ratios. Chemical cross-linking was achieved using thiolated HA or PVA blended with allyl-modified CS, resulting in OAL-CS/PVA-SH/HA and OAL-CS/PVA/HA-SH formulations. The degree of cross-linking was evaluated through printability parameters (extrudability, uniformity, pore integrity) and physicochemical characterizations, including FTIR, XRD, water sorption, and hydrolytic degradation studies. FTIR analysis confirmed successful UV cross-linking via the disappearance of the alkene ($CH_2$=$CH_2$) peak at 1637 $cm^{-1}$. XRD patterns revealed that UV-cross-linked scaffolds exhibited reduced crystallinity, indicating a more amorphous structure—contributing to enhanced water absorption and permeability. Among all tested formulations, the OAL-CS/PVA-SH/3HA scaffold demonstrated the most favorable properties, including controlled degradation over 30 days, with minimal mass loss and exceptionally high water absorption (2412%), attributed to its amorphous network. Furthermore, 3D printing evaluations showed that this scaffold maintained a stable, uniform porous structure during multilayer deposition, supporting better cell distribution and facilitating uniform tissue formation. In conclusion, the OAL-CS/PVA-SH/3HA scaffold emerges as a promising candidate for tissue engineering, outperforming physically cross-linked variants in terms of mechanical stability, print fidelity, and biocompatibility.

# sciforum-136536: Development of Exfoliated Graphene-PEDOT:PSS Nanocomposites for High-Performance Supercapacitor Electrodes

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Supercapacitors, also commonly known as 'ultracapacitors', represent a promising alternative for meeting the escalating power demands of energy storage systems, particularly within the realm of portable electronic devices and batteries in the automotive sector. Their capacity to store and release energy at notably elevated rates, exceeding the capabilities of conventional batteries, stems from the fundamental charge-separation mechanism similar to that observed in traditional capacitors. In this scenario, the present study focuses on the development of environmentally friendly nanocomposites based on Poly(3,4-ethylene-dioxythiophene): polystyrene sulfonate (PEDOT:PSS) and Exfoliated Graphene (ExG) to produce electrodes for supercapacitor applications. The ExG-PEDOT:PSS nanocomposites were characterized via X-ray diffraction (XRD) and Raman analysis, revealing a uniform dispersion of ExG within the PEDOT:PSS matrix and providing evidence of electronic interactions between the two materials.

Subsequently, a morphological investigation combining XRD and TEM led to a comprehensive understanding of the structure of the inks. It was revealed that the materials combine perfectly into a homogenous mix with the polymer coating the graphene nanosheets. The interplay of the two materials leads to a boost of the performance when used in a capacitor. Thermogravimetric analysis (TGA) revealed an enhancement in thermal stability upon the incorporation of ExG, as evidenced by a higher residual mass for the ExG-PEDOT:PSS nanocomposite compared to pristine PEDOT:PSS. Moreover, scan rate-dependent cyclic voltammetry measurements were performed in phosphate buffer (PB) electrolyte; the incorporation of a small amount of ExG (1.4% wt/V) led to a 20 % increase in specific capacitance compared to pure PEDOT:PSS. Additionally, by repeating the CV tests for 1000 cycles under the same conditions, a higher capacitance retained ratio (96%) was observed for the ExG(1.4%)-PEDOT:PSS nanocomposite relative to pure PEDOT:PSS (90%). This advancement highlights the promising capabilities of these nanocomposites in developing electrodes for supercapacitors.

# sciforum-146879: Development of Non-Antibiotic-based Formulations and Materials for the Treatment of recurrent vaginal infections

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**Introduction**

Vaginal infections remain a prevalent global health concern among women, often resulting in symptoms such as pain, itchiness, and dysuria (1). Despite available treatments, recurrence and persistence of infections are common. This study explores a novel therapeutic approach using bioactive films composed of curcumin and Myrtus communis to manage recurrent vaginal infections. Importantly, the goal is to identify a natural solution that avoids the use of antibiotics, addressing concerns related to antibiotic resistance and the side effects associated with conventional treatments.

**Methodology**

Films were formulated using 2% sodium alginate and 10% polyvinyl alcohol (PVA), embedded separately with either pure curcumin or Myrtus communis extract to assess their individual contributions to the film's performance. The swelling behavior of each film type was assessed using standardized 1×1 cm samples, providing a reliable measure of their capacity to absorb moisture, which is critical for their functionality in a vaginal environment.

**Preliminary Results**

Both types of circular film samples exhibited swelling behavior. Notably, the curcumin-based films demonstrated superior swelling capacity compared to the Myrtus communis films; this difference might enhance the retention of moisture, which is beneficial for maintaining prolonged contact with the mucosal surface.

**Conclusion and Future Work**

The curcumin-based films showed promising swelling characteristics, suggesting potential for improved mucosal adherence and drug delivery in the vaginal environment. Further research is underway to enhance the swelling properties of the Myrtus communis films and evaluate the antimicrobial efficacy of both formulations.

# sciforum-138654: Development of plasticized PLA and reprocessed PLA films with eggshell waste-based fillers for sustainable packaging

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Chicken eggshells are an abundant waste from the food industry, composed mainly of calcium carbonate (~96%) along with proteins, and have demonstrated potential as reinforcing agents in biodegradable polymeric matrices. Their rigid mineral structure, biodegradability, and high surface area after milling make them suitable candidates for use in sustainable packaging development. In this study, eggshell powder (ESP) was valorized as inorganic fillers for the development of poly(lactic acid) (PLA) and reprocessed PLA (rPLA) biocomposites plasticized with acetyl tributyl citrate (ATBC). ESP was obtained from post-consumer eggshells by a process involving washing, sterilization, shredding, grinding and sieving to achieve particle sizes below 45 µm. ESP microparticles were incorporated into PLA-rPLA-ATBC matrices at 1, 3 and 5 wt.%, and further processed by melt extrusion (170-190 °C) into filaments for subsequent thermoforming by hot-pressing. The mechanical, morphological and thermal properties of the resulting biocomposites were analyzed. Homogeneous and transparent ESP-loaded films were successfully obtained. The results indicate that increasing the ESP content improves the stiffness of the material, while the addition of ATBC improved processability and the flexibility of the final biocomposites. This work contributes to the circular economy by valorizing agro-industrial waste as functional additives in biodegradable polymers. This first step shows that eggshell particles as mechanical reinforcements and potential carriers of active compounds within matrices, such as active food packaging, are an attractive alternative for the development of next generation sustainable packaging materials.

# sciforum-124804: Electrical sensing of vibrations using smart carbon-based polymer composites

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Vibration monitoring is critical in several disciplines, such as machine and civil engineering, structural health monitoring, biomedical diagnostics, and interactive technology. Mechanical vibrations can cause structural deterioration in engineering systems, or manifest as symptoms in neurodegenerative diseases. As an alternative approach to accelerometers for vibration sensing, carbon-based polymer composites with piezoresistive responses show great potential for detecting and monitoring vibrations. This study investigates the vibration sensing capabilities of polymer composites incorporating carbon black and carbon nanotubes embedded in polyurethane and polylactic acid matrices, and processed via additive manufacturing. Vibratory response tests were conducted on thin rectangular cantilever specimens using a custom-built vibrometer. In a typical free vibration test, a single air pulse is applied to induce oscillation, while the electrical resistance of the specimen is continuously recorded. The oscillatory changes in electrical resistance are correlated with the mechanical vibrations of the specimens, which are also independently measured by optical methods. The natural frequency and vibration amplitude are extracted from the electrical response of the material and validated with independent optical measurements of vibration. The measured natural frequencies are compared to vibratory analytical models. Carbon-based polymer composites demonstrated excellent capabilities to monitor vibratory stimuli and measure natural frequencies through their electrical responses, supporting their great potential for vibration-sensitive applications. These applications range from structural health monitoring to tremor detection in patients with neurodegenerative diseases. Additional advantages are offered by additive manufacturing in terms of fabrication simplicity and design flexibility.

# sciforum-139392: Extraction of lignin from pecan nutshell using the Organosolv process: characterization and potential applications as biomaterials

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Lignin is the second most abundant biopolymer in nature, after cellulose, and is found in the cell walls of various plant species (particularly in wood), agricultural residues, fruit peels, and other biopolymeric sources. This biopolymer has antioxidant and biodegradable properties, making it a valuable raw material for the development of highly functional bio-based materials. Therefore, this study focuses on the extraction of lignin from pecan nutshell (*Carya illinoinensis*) using the Organosolv technique. Additionally, its potential applications in the development of superhydrophobic surfaces are explored. The extracted lignin was characterized using UV-Vis spectrophotometry and scanning electron microscopy (SEM), which allowed the analysis of both its spectral composition and morphology. For the characterization of the superhydrophobic surfaces, optical microscopy and contact angle measurement techniques were employed to assess their surface structure and water repellency. The results showed that the extracted lignin presented well-defined bands in the wavelength range of 280 to 312 nm, similar to those of reference lignin. Furthermore, this lignin exhibited a morphology with poorly defined shapes and varying sizes. On the other hand, the superhydrophobic surfaces presented a heterogeneous structure and high contact angle values (> 150.10 ± 0.21), indicating high water repellency. Based on these results, it can be concluded that the extraction of lignin from agroindustrial residues, such as nutshells, is a sustainable and efficient strategy that not only enables the valorization of agroindustrial waste but also the production of a versatile biopolymer with potential applications in various fields. This approach promotes the use of more eco-friendly materials and contributes to the development of functional products, advancing towards a circular economy and reducing dependence on non-renewable resources.

# sciforum-139371: Functionalization of pectin hydrogels with in situ synthesized magnetite nanoparticles for hyperthermia treatments against cancer

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Cancer remains one of the leading causes of mortality worldwide. Despite the availability of various treatments, most of them cause adverse side effects that affect the health and well-being of patients. This has driven the search for innovative, less invasive, and more body-friendly therapies, such as hyperthermia, which involves raising the temperature of tumors to between 40 and 45°C to induce cellular damage without compromising healthy tissue. With the goal of developing a localized treatment that targets tumor tissue without affecting surrounding tissue, the use of magnetite ($Fe_3O_4$) nanoparticles has been proposed. These nanoparticles have generated significant interest due to their ability to generate heat when exposed to an alternating magnetic field. However, their stability in biological systems represents a challenge; therefore, the present project proposes the functionalization of pectin hydrogels with magnetite nanoparticles, taking advantage of the biocompatibility and encapsulation capacity of pectin together with the magnetic properties of magnetite. The hydrogel was synthesized in situ by mixing a pectin solution with iron salt precursors and stabilizing agents ($FeSO_4$, urea, and glycine). The pH was adjusted to 9-11 to favor magnetite formation over the other oxide phases, using NaOH and $NaHCO_3$. Subsequently, the hydrogel was crosslinked with $CaCl_2$, and once the polymeric three-dimensional network was stabilized, it was analyzed using various characterization techniques. Among these techniques, Fourier Transform Infrared Spectroscopy was employed to assess chemical structural changes resulting from the synthesis process. The analysis confirmed the crosslinking of pectin chains by $CaCl_2$ addition and the interaction of magnetite nanoparticles with the polymer matrix. Additionally, X-Ray Powder Diffraction analysis confirmed the formation of pure magnetite, distinguishing it from the other iron oxide phases. The preliminary results suggest that pectin–magnetite hydrogels may offer a promising platform for magnetic field response in biomedical applications.

# sciforum-138378: Green Composites from Recycled Polypropylene and Hazelnut Shell Flour for Irrigation Systems Application

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The use of recycled polymers and agricultural waste could be an important tool to reduce the environment impact of plastic manufacts and to valorize the agricultural waste. In this work recycled PP and hazelnuts shells were used in order to produce green composites to be applied for the production of fittings for irrigation systems. In order to improve the poor adhesion between matrix and filler an adhesion promoter was also used. The adhesion improves in particular for the composites with the recycled polymer probably because of the presence of polar groups in the recycled sample. The rheological properties clearly indicate that the composites show a processability similar to that of the pure polypropylene and this feature has been corroborated by industrial preliminary injection molded tests where the fitting was easily produced. The deformability of the composites is reduced with respect to the pure matrix although slightly improved by the presence of the adhesion promoter. The composite with RPP as matrix and 5% of hazelnut shells with and without adhesion promoter were also used to produce a fitting by injection molding and all the fittings were resistant to the water pressure of 3.50 bar according to the internal test used by the company

# sciforum-138291: Green Fabrication of Hydrophobically Functionalized Cellulose Nanomaterials via Citric Acid-Assisted Wet Ball Milling with N-Alkanals

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The development of cellulose-based nanomaterials with tailored surface properties is essential for advancing their integration into high-performance polymer nanocomposite systems. In this work, a mechanochemical strategy for the simultaneous production and surface functionalization of cellulose nanofibrils (CNFs) via wet ball milling, employing citric acid as a green crosslinking catalyst and N-alkanals (octanal, heptanal, and their binary mixture) as hydrophobizing agents, is presented. This one-pot process enables in situ surface modification while preserving the nanofibrillar structure of cellulose, providing a scalable, environmentally friendly method for the fabrication of functional nanofillers. Commercial microcrystalline cellulose was milled in an aqueous medium using high-energy planetary ball milling for an optimized time of 20 minutes. The resulting nanofibrils exhibited diameters below 100 nm and improved surface hydrophobicity, confirmed by increased static contact angle measurements. The modified CNFs also displayed stable dispersion behavior and were fabricated into thin films using vacuum-assisted self-assembly. Optical microscopy in reflected light mode revealed morphological differences linked to the specific N-alkanal used, indicating tunable surface texturing. This dual-function approach not only simplifies nanocellulose processing but also enables the engineering of interface-active nanomaterials suitable for reinforcing biodegradable polymer matrices. The resulting nanocellulose systems demonstrate strong potential for use in advanced nanocomposite applications, including sustainable packaging, coatings, and barrier materials.

# sciforum-138231: Humidity-Responsive Conductive Hydrogels: A Bio-Based Material for Flexible Electronics

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**Introduction:** The increasing demand for biocompatible and flexible electronic materials has stimulated the research into conductive hydrogels, particularly for biosensors and wearable device applications. Gelatin methacryloyl (GelMA), derived from cold-water fish skin, offers a renewable and biocompatible matrix. This study investigates the synthesis and characterization of GelMA hydrogels loaded with silver nanoparticles (AgNPs) to achieve conductivity, exploring the impact of formulation and environmental factors on material properties.

**Methods:** GelMA was synthesized and crosslinked using a visible light-activated photoinitiator (BAPO-PEG). AgNPs were incorporated via *in situ* reduction during crosslinking and by post-crosslinking immersion in silver nitrate solutions. Hydrogel properties were assessed using Fourier-transform infrared spectroscopy (FTIR), photorheology, thermogravimetric analysis (TGA), swelling tests, and electrical conductivity measurements under varying humidity conditions. Piezoresistive behavior was evaluated by measuring current changes under applied compressive strain.

**Results:** FTIR confirmed successful GelMA synthesis. Photorheology optimized BAPO-PEG concentration for rapid curing. TGA demonstrated thermal stability up to 260-270°C. High water absorption (300%) was observed. *In situ* AgNP formation delayed gelation, favoring immersion for AgNP incorporation. Electrical conductivity was highly dependent on humidity, with dried samples exhibiting insulating behavior. Conductivity significantly increased with hydration, reaching 6.84 S/m for samples with the highest silver content (GelMA/Ag-50) at 100% relative humidity. Compressive strain enhanced conductivity, indicating piezoresistive properties suitable for sensing applications.

**Conclusion:** This study demonstrates the successful synthesis of conductive bio-based hydrogels by incorporating AgNPs into a GelMA matrix derived from fish skin gelatin. The resulting materials exhibit tunable electrical properties responsive to humidity and mechanical strain, making them promising candidates for biosensors, humidity sensors, and flexible electronic devices. Further research will focus on optimizing AgNP dispersion and long-term stability for real-world application.

# sciforum-139086: Hybrid nanocomposite beads of Areca husk-derived cellulose fibre, sodium alginate and green-synthesized $TiO_2$ for controlled release of bioactive agents

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Towards the development of sustainable and multifunctional materials, a hybrid polymer composite system composed of cellulose fiber, sodium alginate and titanium oxide ($TiO_2$) nanoparticles has been made in the form of beads. The cellulose fiber was extracted from Areca husk, an agricultural waste material. $TiO_2$ was made in nanosize by the green synthesis method using *Azadirachta indica* (neem) leaf extract. Hydrogel beads were fabricated from a mixture of sodium alginate, cellulose fiber, and $TiO_2$ nanoparticles by an ionic gelation process achieved using calcium chloride. The physicochemical characterization of the gel beads was carried out using FTIR, SEM, XRD, TGA, and TEM techniques. The pH-responsive swelling of the gel beads was demonstrated from the swelling studies carried out in aqueous medium under different pH conditions. The beads were evaluated for the slow release of bioactive agents, namely neem seed oil (NSO), a biopesticide and urea, and a fertilizer molecule. The loading and release of these agents were studied in an aqueous medium. The results indicated percentage loadings of 93.96% and 90.55% for neem seed oil and urea, respectively. The slow release of NSO and urea was observed to occur from the gel beads in a sustained manner during a 3-day period. The kinetic analysis of the release data indicated the release of both agents, following the Korsmeyer–Peppas model. The release exponent ‘n’ obtained from this model was less than 0.5 in both cases, indicating the release to be a Fickian process. The NSO- and urea-loaded gel beads were also evaluated for antibacterial characteristics against *E. coli* and *S. aureus,* and the results indicated the role of NSO in enhancing the antibacterial activity of the gel. Thus, this study exemplifies a sustainable approach to valorize agricultural waste for the development of smart materials in agricultural use.

# sciforum-137738: Hydrothermal Aging of SAPO-34/Nexar Composite Coatings for Thermal Energy Storage

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Efficient Thermal Energy Storage (TES) systems are vital for advancing energy efficiency and integrating renewable sources. Within this context, innovative composite coatings offer a promising avenue to enhance TES system effectiveness and longevity. This study focuses on developing and characterizing novel composite coatings, specifically tailored for TES applications, consisting of a sulfonated pentablock terpolymer (Nexar) matrix, known for its excellent water vapor permeability, filled with SAPO-34 zeolite filler, a microporous substance with high heat exchange capabilities at lower temperatures. A significant challenge for adsorbent coatings and composite materials lies in their susceptibility to aging, particularly when the polymeric matrix is crucial for maintaining structural and functional integrity. Prolonged exposure to adsorbates like water vapor can severely degrade the coating's performance. Therefore, assessing the composite's aging response is crucial for confirming its practical viability.

In this work, we subjected SAPO-34/Nexar composite coatings, with varying zeolite concentrations, to hydrothermal aging to verify their stability. The aging protocol involved hundreds of wet (30°C, 80% RH) and dry (40°C, 20% RH) cycles within a controlled climatic chamber. We evaluated the coatings' mechanical properties (including pull-off strength and scratch resistance) and adsorption/desorption capacity (by means of DVS analysis), both before aging and after specific aging durations. The mechanical properties of the coatings decrease with an increasing number of cycles: a decline that is most pronounced at lower zeolite concentrations. The 90 wt% zeolite composition offers superior mechanical stability over cycles, while exceeding this percentage leads to a degradation of properties due to the reduced amount of polymer binder. DVS analysis indicated only a minimal reduction (between 2.9% and 3.5%) in adsorption capacity. These findings highlight that a balanced composition is crucial for the practical viability of high-filler content SAPO-34/Nexar coatings in long-term TES applications.

# sciforum-144666: Improvement of Thermal Characteristics of Plasticized PVC via a Complex of Eco-Friendly Additives

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Enhancing the thermal stability of plasticized PVC is a critically important task for expanding its practical application areas. The development of eco-friendly modifying additives is a promising direction in this field. Titanium phosphates meet the requirements of green chemistry, and their use in the form of hierarchical microstructured materials contributes to improving material characteristics. Complex esters of adipic acid are widely used as alternative PVC plasticizers that promote increased thermal stability. This study investigates the combined effect of titanium phosphates and diphenoxyethyladipinate on the thermal characteristics of PVC. The thermal stability of PVC compositions was studied using Thermogravimetric Analysis (TGA) and Differential Scanning Calorimetry (DSC) in an oxidative environment (air). The obtained results show an improvement in the thermal characteristics of the compositions compared to the base PVC compound plasticized with dioctyl phthalate (DOP). The key evaluation parameters for the composition are as follows: initial mass loss temperature ($T_{on}$); coke residue; temperature of maximum decomposition rate (Tmax DTG); and temperature of maximum heat flow (Tmax DSC) during the main stage of thermolysis. Increasing the DFEA (diphenoxyethyladipinate) content in the PVC composition from 16 to 49 parts by weight demonstrated improved thermal characteristics. The initial temperature of the sample mass loss indicated a shift of the degradation process towards higher temperatures. The shift in the maximum of the first stage of PVC composition degradation—dehydrochlorination—confirmed a reduction in the rate of thermal degradation of the material. Analysis of DSC data confirmed an increase in the thermal stability of the composition, expressed in an increase in the Tmax DSC value. A PVC composition with improved thermoanalytical characteristics using eco-friendly additives was developed.

# sciforum-137874: Influence of Poly(sodium 4-styrenesulfonate) on the Optical Response of Reduced Graphene Oxide Thin Films

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Graphene-based nanocomposites stabilized with polymers are emerging as promising materials for optoelectronic applications due to their tunable optical and structural properties. In this study, we investigate and compare the optical behavior of graphene oxide (GO), thermally reduced graphene oxide (RGO), and RGO films functionalized with poly(sodium 4-styrenesulfonate) (PSS). Thin films were deposited by dip-coating aqueous dispersions onto $SiO_2$/Si substrates and characterized using Variable Angle Spectroscopic Ellipsometry (VASE) in the 0.38–4.1 eV photon energy range. The dielectric response of GO and RGO films was modeled using three Lorentz oscillators, reflecting transitions associated with oxygenated functional groups and partial restoration of $sp^2$ hybridization. Conversely, the optical properties of PSS-RGO films are described by a single Lorentz oscillator at approximately 2.8 eV and a pole, indicating the formation of new electronic states likely arising from the improved ordering of $sp^2$ carbon domains during reduction in the presence of the polymer. Scanning Electron Microscopy (SEM) analysis reveals that PSS enhances the homogeneity and compactness of the films, preventing aggregation and promoting uniform coverage. These findings highlight the critical role of PSS as a functional matrix capable of modulating both the morphology and optical response of RGO, particularly in the extended near- and mid-infrared spectral range.

# sciforum-138046: Interfacially Engineered Chitosan-Imide Functionalized $Fe_3O_4$ Nanozymes for Dual Peroxidase-Mimetic and Visible-Light Photocatalytic Applications

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Artificial nanozymes are gaining prominence as robust alternatives to natural enzymes for catalytic and sensing applications, yet their use is often hindered by poor colloidal stability, inefficient electron transfer, and low catalytic activity under harsh conditions. To address these limitations, we developed a chitosan-imide-functionalized $Fe_3O_4$ nanocomposite (FeNp-CSNI) via sequential hydrothermal synthesis, polymer grafting, and interfacial assembly. Comprehensive material characterization was carried out using XRD, FTIR, BET, TEM, EIS, and DFT analyses. FeNp-CSNI exhibited a worm-like mesoporous morphology with high surface area, reduced bandgap, and significantly lower charge transfer resistance, suggesting improved electron mobility and catalytic efficiency. The peroxidase-like catalytic activity was assessed by OPD oxidation in the presence of $H_2O_2$, where hydroxyl radicals were confirmed as the dominant reactive species. Under visible-light irradiation, FeNp-CSNI achieved >95% degradation of crystal violet, demonstrating strong photocatalytic activity. The nanozyme retained ~97% of its catalytic performance over five reuse cycles, indicating high stability. Furthermore, real-sample testing showed accurate and efficient detection of $H_2O_2$ in milk, with excellent recovery rates, highlighting the nanozyme's practical potential in biosensing. This work establishes that interfacial engineering of $Fe_3O_4$ nanoparticles with chitosan-imide substantially enhances both catalytic performance and environmental durability. The FeNp-CSNI nanozyme offers a multifunctional and sustainable platform for biosensing, environmental remediation, and photocatalytic applications, paving the way for future nanozyme-based technologies.

# sciforum-147173: Intranasal Mucoadhesive Chitosan-Coated SNEDDS of Apocynin for Nose-to-Brain Delivery in Glioblastoma: Minimizing Dose Dumping

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Glioblastoma multiforme (GBM) is one of the most aggressive brain malignancies, with treatment failure often resulting from the restrictive blood–brain barrier (BBB) and the poor solubility of therapeutic agents. Apocynin, a NADPH oxidase inhibitor with anticancer and neuroprotective potential, suffers from low aqueous solubility, limited permeability, and poor bioavailability. To address these challenges, mucoadhesive chitosan-coated self-nanoemulsifying drug delivery systems (SNEDDS) of apocynin were developed and optimized for intranasal delivery. SNEDDS were prepared using Capryol 90 (oil), Tween 20 (surfactant), and Transcutol HP (co-surfactant) and optimized via a Box–Behnken design. The optimized formulation exhibited a mean droplet size of 112.4 ± 3.2 nm, a polydispersity index of 0.21 ± 0.04, and a zeta potential of −18.7 ± 2.1 mV, confirming nanoscale uniformity and stability. After chitosan coating, the zeta potential shifted to +24.6 ± 1.9 mV, indicating successful surface modification and improved mucoadhesive properties. Both uncoated and chitosan-coated SNEDDS demonstrated more than 90% drug release; however, the chitosan-coated system reduced burst release, providing controlled release and minimizing dose dumping. Dissolution studies showed an approximately 4.5-fold enhancement in release compared with pure apocynin. Stability evaluation under temperature variation and freeze–thaw cycles confirmed formulation robustness. SEM, DSC, and PXRD analyses revealed conversion of apocynin from crystalline to amorphous form, correlating with enhanced solubility and dissolution. Collectively, chitosan-coated SNEDDS present a promising mucoadhesive and controlled intranasal delivery platform for apocynin in glioblastoma therapy.

# sciforum-113933: Iron-Modified Illite-Chitosan Composite as an Efficient Catalyst for Environmental Pollutant Degradation

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Illite, a naturally abundant clay, was modified with iron to enhance its catalytic efficiency and incorporated into a chitosan matrix to create a composite catalyst for environmental remediation. The synthesis involved impregnating illite with 10% (w/w) iron, followed by integration into a chitosan polymer using ionotropic gelation. The resulting composite was characterized using X-ray Diffraction (XRD), Fourier Transform Infrared Spectroscopy (FTIR), Scanning Electron Microscopy (SEM), and Brunauer–Emmett–Teller (BET) surface area analysis. Characterization confirmed the successful incorporation of iron into the illite structure and its homogeneous dispersion in the chitosan matrix, yielding a porous material with a surface area of 85 $m^2/g$.

The composite's catalytic activity was tested on the degradation of a model organic pollutant (50 mg/L concentration) under optimized conditions of pH 4.5, temperature 50°C, and a catalyst dosage of 1 g/L. The results showed an exceptional degradation rate of 98.5% within 90 minutes of reaction time. Reusability tests demonstrated that the composite retained 92% of its initial catalytic activity after five cycles, indicating excellent stability and reusability.

These findings establish the iron-modified illite-chitosan composite as a highly efficient and sustainable catalyst for environmental applications. Its high degradation efficiency, coupled with economic and environmental benefits, makes it a promising candidate for large-scale pollutant degradation and wastewater treatment processes.

# sciforum-147152: Janus-structured amphiphilic nanofibers by conjugate bubble electrospinning for effective wound healing

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Wound healing remains a major biomedical challenge, requiring the design of advanced multifunctional dressings that can simultaneously manage exudates, prevent microbial infection, and provide controlled drug release. In this study, amphiphilic Janus nanofibers were fabricated via a conjugate bubble electrospinning technique, integrating hydrophilic and hydrophobic domains within a single fibrous structure. The hydrophilic side was composed of polyvinyl alcohol (PVA) blended with chitosan (CS) or sodium alginate (SA), while the hydrophobic side consisted of poly(ε-caprolactone) (PCL) or polyvinylidene fluoride (PVDF) loaded with curcumin (Cur) or rutin (Ru).

Comprehensive characterization, including fiber diameter, air permeability, tensile strength, and water contact angle, was performed to evaluate physicochemical properties. Biological performance was assessed through in vitro drug release, antibacterial activity against Vibrio vulnificus and E. coli, cell viability using L929 fibroblasts, and in vivo wound healing in a murine full-thickness excisional wound model. Results demonstrated that the incorporation of CS and SA significantly enhanced hydrophilicity and exudate absorption, while rutin-loaded PCL facilitated efficient drug release compared to PVDF-based systems. Antibacterial studies confirmed strong inhibitory activity in Janus scaffolds containing SA, and cell viability assays indicated high biocompatibility, particularly in SA-based nanofibers.

Among the various formulations, Janus nanofibers composed of SA-PVA on the hydrophilic side and PCL–rutin on the hydrophobic side (PSA/PCRu) achieved the best overall performance, with superior in vitro drug release, minimal cytotoxicity, and the highest wound closure rate (95.2% at day 15) in vivo. Degradation and thermal analyses further confirmed the structural stability and tunability of the scaffolds.

This work highlights conjugate bubble electrospinning as a scalable platform for fabricating multifunctional Janus nanofibers. The resulting chitosan- and alginate-based wound dressings offer synergistic benefits in exudate management, antimicrobial defense, and sustained therapeutic delivery, positioning them as promising candidates for next-generation wound care applications.

# sciforum-138219: Kinetic study of thermo-oxidative degradation of Poly(3-Hydroxybutyrate-Co-3-Hydroxyhexanoate) (PHBHHx)-Agave Americana Fiber Biocomposites

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Thermo-oxidation of natural fibers and their biocomposites has attracted considerable interest from researchers due to their wide-ranging applications in the fields of textile fabrics, construction materials, insulation, and automotive components. This makes the comprehension of their thermal degradation mechanisms, especially in the presence of oxygen, a matter of critical interest. Therefore, this study aims to investigate the effect of untreated and alkali-treated Agave Americana Fibers (AAF) on the kinetics of thermo-oxidation of PHBHHx biocomposites at 30 wt.% filler content. The experimental approach consists of subjecting neat polymer and its biocomposites to different heating rates, i.e., 5, 10, and 20 °C/min, under oxygen using thermogravimetric analysis, while applying the Coats–Redfern model-fitting method. The results reveal that TGA/DTG thermograms exhibit a single-step degradation process for PHBHHx, whereas the biocomposites show multi-step degradation phenomena attributed mainly to the cellulose and PHBHHx matrix. Kinetic analysis of the samples indicates that PHBHHx degrades via a diffusion-controlled mechanism, showing the best model fitting to the D2 Model. However, both untreated and treated biocomposite samples exhibit two degradation steps related to the base components, occurring via the P2 Model. This suggests that degradation is governed by the reactions occurring at the filler–matrix interfaces. Moreover, it has been demonstrated that alkali treatment of the fibers results in an increase of activation energy and onset temperature of the biocomposites (P-AAF-B) compared to those of untreated ones (P-AAF). Indeed, at a heating rate of 5°C/min, the activation energy values increase from nearly 178 and 537 KJ/mol for P-AAF relative to phases 1 and 2 to 426 and 623 KJ/mol for P-AAF-B, respectively. Moreover, at the same heating rate, the onset temperature increases from 221.70°C for P-AAF to 236.51°C for P-AAF-B. These results show that the addition of natural fibers, especially with surface treatment, is beneficial for enhancing the material's overall thermo-oxidative stability.

# sciforum-138331: Lead-Free 2D $MA_3Bi_2I_9$-Polymer composite for Nanogenerator and Energy Storage Applications

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With the rise of wearable electronics, the need for sustainable, portable power is increasing. To overcome battery limitations, energy harvesters converting solar, thermal, and mechanical energy into electricity have been developed. Mechanical energy, abundant but underused, can be captured via piezoelectric and triboelectric nanogenerators (PENGs and TENGs). TENGs offer high output and low-cost fabrication, with performance influenced by material properties and surface treatments. Halide perovskites (HPs) show strong potential for energy harvesting and storage due to their dielectric and piezoelectric properties. A recent $MA_2SnCl_6$-based self-charging unit combines a PENG with a lithium-ion battery. Lead-free, efficient HPs are vital for self-powered wearable devices.

Herein, we present the utilization of air-stable, 2D-layered, lead-free $MA_3Bi_2I_9$ for stretchable $MA_3Bi_2I_9$-SEBS (Styrene Ethylene Butylene Styrene) composite-based hybrid nanogenerators and as an electrode material in LIBs. Initially, high-performance, stretchable hybrid nanogenerators based on $MA_3Bi_2I_9$ (MBI; MA = $CH_3NH_3$) perovskite were developed by compositing with SEBS polymer to harvest mechanical energy in both PENG and TENG modes, achieving the highest output at 12 wt% film loading. Specifically, the 12 wt% TENG demonstrated an output voltage of 537 V and a power density of 3.04 $mW/cm^2$. Furthermore, the electrochemical performance of $MA_3Bi_2I_9$ as a cathode material was investigated, revealing high specific capacity and long-term cycling stability. Finally, we demonstrate the practical application of the developed hybrid nanogenerator by using it to charge the $MA_3Bi_2I_9$-based LIB. The charged LIB, powered by the TENG, is capable of operating small-scale electronic devices, including a smartwatch and a calculator.

# sciforum-138454: Mechanical and thermal properties of liquid crystalline epoxy thermosets

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Liquid crystalline epoxy resins containing mesogenic groups were cured under controlled temperature conditions to suppress the molecular mobility and promote crosslinking while maintaining an ordered alignment structure. The resulting alignment of polymer network chains in the cured materials was thoroughly characterized using polarized optical microscopy (POM) and X-ray diffraction (XRD). By varying the curing temperature, significant changes were observed in the domain size of the aligned liquid crystalline phases. These phases were identified as either nematic or smectic liquid crystal structures, which were found to be retained and fixed within the polymer network. The mechanical and thermal properties of the cured liquid crystalline epoxy thermosets were evaluated, and their relationship with the alignment structure of the network chains was discussed. In particular, fracture toughness was found to increase markedly with the enlargement of the liquid crystalline domains, indicating that the anisotropic order contributes to enhanced energy dissipation during the crack propagation.

Furthermore, the incorporation of cellulose nanofibers (CNFs) into the curing system led to an increased proportion of smectic liquid crystalline alignment. This enhancement is attributed to the hydroxyl groups present on the surface of the CNFs, which likely induced alignment of the liquid crystalline epoxy matrix through polar interactions.

# sciforum-138908: Monofilament melt spinning of PET-based antimicrobial composite fibers with hybrid fillers

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Antibacterial fibers play a crucial role in enhancing hygiene, safety, and comfort in textiles. This study explores the monofilament melt spinning of polyethylene terephthalate (PET) composite fibers incorporating hybrid fillers of copper (Cu) and a low-melting-point alloy ($In_{51}Bi_{32.5}Sn_{16.5}$). The research evaluates the impact of these fillers on spinnability, morphology, thermal degradation, and electrical resistance of the melt spun fibers across various loading levels. A key motivation for this approach is the incorporation of copper as an embedded antimicrobial agent. Unlike surface-coated treatments, copper dispersed within the fiber matrix has the potential to deliver durable antimicrobial functionality, making these fibers particularly attractive for medical, hygienic, and performance textile applications. Additionally, the use of low melting alloy, which is significantly more cost-effective than copper, provides a low-cost pathway to functional fiber production without compromising melt processability. The study identifies some challenges but successful translation of polymer-metal composites from extrusion to continuous, spinnable monofilament fibers of good strength and well dispersed metal particles inside the polymer matrix. This work stands out as one of the few efforts to scale up lab-formulated composites into melt-spinnable and post-drawable monofilaments. Overall, the research lays a foundation for affordable, scalable antimicrobial fibers with potential applications in advanced textile systems.

# sciforum-145806: Multifunctional Nanocomposite Fibrous Architectures for Oil/Water Separation and Sorption

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Fibrous nanocomposites have become key enablers for advanced separation technologies due to their tunable structure, high surface area, and ability to integrate multiple functions. I highlight our work on electrospun fibrous nanocomposite membranes, developed through Pickering emulsion templating and bio-inspired design strategies, for efficient oil/water separation and pollutant remediation. Using a Pickering emulsion approach, silica nanoparticles were uniformly distributed within electrospun fibers, creating hierarchical porosity and tailored wettability. The silica nanoparticles acted as a Pickering stabilizer as well as surface modifier. The resulting nanocomposite membranes exhibited superhydrophilic and underwater superoleophobic behavior, achieving oil/water separation with excellent fluxes and rejection efficiency over 99%. The templated nanocomposite structure also enhanced mechanical stability and anti-fouling performance, ensuring reusability across multiple cycles.

In parallel, inspired by fish-gill morphology, we fabricated multifunctional nanofibrous membranes capable of both demulsification of stable oil-in-water emulsions and sorption of dissolved pollutants. This dual functionality was achieved through careful control of the fiber architecture and surface chemistry, enabling membranes to address complex separation challenges in a single platform. Together, these studies demonstrate the transformative potential of combining nanocomposites with rational structural design in fibrous membranes. By bridging Pickering emulsion templating with bio-inspired architectures, we provide versatile pathways for developing next-generation, sustainable membranes for oil/water separation and broader water purification applications.

# sciforum-135422: Nanoemulgels: nanoemulsion and hydrogel hybrids as polymeric nanocomposites for improved drug delivery

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Brain drug delivery poses a significant challenge due to the blood-brain barrier's extremely reduced permeability to most molecules, making it a considerable obstacle for the effective treatment of neurological and psychiatric diseases. Furthermore, conventional pharmaceutical formulations tend to lead to low drug targeting, leave drugs susceptible to enzymatic and chemical degradation, and do not easily reach high drug strength in liquid and semisolid preparations. To tackle these issues, intranasal nanoemulgels were developed, for direct nose-to-brain drug delivery, and overall improved therapeutic efficacy and safety. Nanoemulgels containing antiepileptic drug molecules phenytoin and fosphenytoin, and nanoemulgels loaded with a repurposed anti-inflammatory drug for brain cancer treatment, were produced through spontaneous emulsification, using a mixture of pre-selected oils, surfactants, co-surfactants, co-solvents and aqueous solutions of a thermosensitive gelling polymer, Poloxamer 407. Formulations were optimized and characterized in what concerned their droplet size, polydispersity index, zeta potential, pH, osmolality, stability, viscosity and rheologic behavior, *in vitro* drug release, and *in vitro* therapeutic efficacy and safety. Results showed that low droplet sizes (between 20 and 200 nm) and reduced PDI values ( 0.3) were obtained, as well as high drug strengths. The nanoemulgels depicted a pseudoplastic non-Newtonian rheological behavior, with gelling temperatures adequate for intranasal delivery (bellow the mean nasal temperature, 32 °C). An overall high controlled cumulative drug release was also obtained (around 80% or higher after 24 hours), and *in vitro* therapeutic efficacy in glioblastoma cell lines proved that the developed nanoplatforms had improved anticancer effects. Hence, intranasal nanoemulgels with ideal physicochemical characteristics and preliminarily proven therapeutic effects for the treatment of different brain diseases were successfully developed. Assays in *in vivo* models might further confirm their potential, and their simple and cost-effective production method might catapult these nanocomposites into easing their way to industrial production.

# sciforum-138515: Near-infrared-responsive dual cross-linked chitosan/hyaluronic acid/graphene oxide hydrogel microneedles for controlled transdermal curcumin delivery in cancer therapy

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Microneedle-based systems are gaining significant attention in cancer therapeutics as a promising alternative to conventional drug delivery methods, primarily due to their capacity for localized, minimally invasive target drug delivery, effectively bypassing metabolism and reducing systemic toxicity. Among these, hydrogel microneedles demonstrate more notable advantages, including biocompatibility, non-immunogenicity, and tunable drug release profiles. In this study, a fully biocompatible microneedle patch was developed using a Chitosan/Hyaluronic Acid/Graphene Oxide (CS/HA/GO) composite hydrogel, which was double-crosslinked via thiol-ene "click" chemistry and physical interactions to enhance mechanical strength and control drug delivery. A custom-designed polydimethylsiloxane (PDMS) negative mold was fabricated using a 3D-printed positive resin mold to ensure structural precision. The resulting dual-crosslinked hydrogel, CSOAL-GOSH/HA, was thoroughly characterized using Attenuated Total Reflectance Fourier Transform Infrared Spectroscopy (ATR-FTIR), X-ray Diffraction (XRD), and Scanning Electron Microscopy (SEM). Additional evaluations included water sorption analysis, drug loading efficiency, and in vitro release of curcumin—a hydrophobic anticancer agent. Characterization results confirmed successful chemical crosslinking, as indicated by a characteristic FTIR peak at 1646 $cm^{-1}$. XRD analysis revealed that the polymeric matrix enhanced the bioavailability of curcumin. The CSOAL-GOSH/HA microneedles exhibited favorable swelling behavior (300% at 45 minutes) and a high curcumin loading efficiency (96%). Notably, the incorporation of GO imparted near-infrared (NIR) responsiveness and tunable hydrogel swelling, enabling controlled and on-demand drug release, reaching 76% within 5 hours. This work presents a promising and advanced platform for transdermal drug delivery, offering precise spatiotemporal control and structural consistency.

# sciforum-143033: Optimizing Dielectric Behavior in Perovskite–Polymer Hybrid Materials for High-Performance Triboelectric Nanogenerators

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The transition toward sustainable energy technologies relies heavily on a deep understanding of energy harvesting mechanisms. Among the promising innovations in this field are nanogenerators (NGs)—devices capable of converting mechanical motions from the surrounding environment into electrical energy. Due to their durability and reliable power output, these systems have received increasing attention in recent years. In particular, triboelectric nanogenerators (TENGs), which utilize surface contact-induced charge separation combined with electrostatic induction, are considered highly efficient for transforming mechanical disturbances into electric signals. Despite their potential, a major limitation in TENG development is the relatively low charge transfer density that restricts the overall energy conversion efficiency. Within this context, halide perovskites (HPs) have emerged as a class of materials with exceptional dielectric, piezoelectric, and optoelectronic characteristics, making them suitable for next-generation energy and sensor devices. However, widespread adoption has been limited due to challenges such as instability under ambient conditions and concerns related to lead toxicity.

In the present study, we introduce a lead-free, flexible triboelectric nanogenerator based on a composite film composed of methylammonium tin chloride ($CH_3NH_3SnCl_3$, i.e., MSC) and poly(methyl methacrylate) (PMMA). The MSC perovskite was synthesized via an antisolvent-assisted collision method, which enhanced crystallinity and material integration. This perovskite was then embedded within a PMMA matrix to improve dielectric properties, thereby enhancing the triboelectric performance of the composite. The optimized composite containing 10 wt% MSC achieved a substantial increase in output, producing a peak voltage of 525 V, a current of 13.6 μA, and a power output of 2.5 mW, surpassing many previously reported perovskite-based TENGs. Additionally, the device demonstrated high pressure sensitivity, recording values of 7.72 V/kPa in voltage sensing and 0.2 μA/kPa in current mode.

# sciforum-147345: Optimizing Graphene Oxide/NBR Nanocomposites Through Interfacial Hydrogen Bonding for Enhanced Mechanical, Dielectric, and Optical Performance

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The development of high-performance elastomer nanocomposites increasingly depends on engineering the filler–matrix interphase rather than maximizing filler content. This study examines nitrile butadiene rubber (NBR) reinforced with 0.5–2.0 phr graphene oxide (GO) synthesized via a modified Hummers' method, focusing on how hydrogen-bonded interfaces influence structural, mechanical, dielectric, and optical behavior. GO, rich in hydroxyl, carboxyl, and epoxide groups, was incorporated through a solution–coagulation process followed by sulfur vulcanization to promote uniform dispersion.

X-ray diffraction confirmed effective GO exfoliation, with maximum polymer chain ordering at 1 phr. FTIR spectra showed broadening/redshift of the nitrile band and GO-derived C–O–C and C–O absorptions, evidencing hydrogen bonding and dipole–dipole interactions without covalent grafting. Microscopy and AFM revealed optimal dispersion and a narrowed nanostructure size range (20–45 nm) at 1 phr. UV–Vis/Tauc analysis demonstrated a non-monotonic band gap trend (direct Eg: 3.01 → 3.13 → 3.11 eV), arising from competition between quantum confinement and π–π stacking.

Dielectric spectroscopy ($10^2$–$10^6$ Hz, 20–100 °C) indicated improved permittivity stability via Maxwell–Wagner–Sillars polarization, with 1 phr achieving the most balanced response. Mechanical testing showed gains in tensile strength, tear resistance, rebound elasticity, abrasion resistance, and solvent resistance, alongside enhanced rubber–metal adhesion and thermo-oxidative stability.

Across all analyses, 1 phr GO emerged as the optimal loading, offering a percolating yet well-dispersed interphase that maximizes property transfer while avoiding aggregation-driven losses. The results highlight interphase engineering as a scalable strategy for producing durable, dielectric-stable elastomers for sealing, oil-resistant, and industrial applications.

# sciforum-138551: Optimizing LDH and PVDF-TrFE Composite Layers for High-Performance Flexible Triboelectric Nanogenerators

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The growing demand for sustainable power in wearable electronics, mobile devices, and self-powered sensors has encouraged research into efficient energy harvesting technologies. Mechanical energy generated from human motion and the surrounding environment represents a promising energy source. Triboelectric nanogenerators (TENGs) have attracted considerable attention due to their high efficiency, scalability, and low cost [1–3]. However, improving material properties to enhance output performance and long-term stability remains a challenge.

In this study, a multilayer TENG was fabricated by sequentially depositing RF-sputtered aluminum-doped zinc oxide (AZO), layered double hydroxide (LDH), and spin-coated poly(vinylidene fluoride-trifluoroethylene) (PVDF-TrFE). LDH layers were grown via an optimized immersion method to ensure uniform coverage, and PVDF-TrFE solutions with varying concentrations were applied to investigate polymer loading effects.

The AZO/LDH TENG exhibited an output voltage of 164.25 V and a current density of 2.9 μA/cm$^2$. The composite layer with the optimal PVDF-TrFE concentration significantly enhanced the output, achieving an output voltage of 641.625 V and a current density of 16.530 μA/cm$^2$. This improvement is attributed to increased surface charge density and enhanced dielectric properties of the ferroelectric polymer. Long-term stability tests further confirmed the enhanced performance of PVDF-TrFE-coated devices compared to those with LDH only.

These results highlight the synergistic benefits of combining LDH optimization with PVDF-TrFE loading, presenting a promising strategy for the development of flexible, high-performance energy harvesters for wearable and self-powered sensor applications.

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# sciforum-138232: PEG–mortar and PEG–gypsum composite materials for passive thermal energy storage (TES) applications in buildings

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Two types of *shape-stabilized composite* Phase Change Materials (*ssc*PCMs)—$PEG_{1000}$/silica/MWCNTs and $PEG_{6000}$/silica/MWCNTs, respectively—were embedded in two different inorganic matrices that are commercially available as building materials (lime-cement mortar and gypsum) in order to obtain building elements with latent heat storage properties. The two PEG/silica/MWCNTs materials were prepared in our lab using a previously published method [1]. Three different concentrations of the two *ssc*PCMs (2.5%, 5%, and 10%) were added to the mortar, whereas only a 10% concentration of *ssc*PCMs was investigated for gypsum. The new PEG–mortar and PEG–gypsum composites were cast in parallelepiped molds (L x w x h = 50 mm x 30 mm x 20 mm) to obtain brick-type construction elements (for building facades). The bricks thus produced were characterized from a morpho-structural point of view and were subjected to tests regarding their compressive strength. In order to verify their functionality, the behavior of the materials after exposure to 62 repeated heating–cooling cycles was also evaluated.

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# sciforum-137459: Polyethersulfone/coreshell-$Fe_3O_4$/ZnO Membranes for the Efficient Removal of Salts and Pb(II) from Environmental Wastewater

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Rapid population growth, expanding industries, and relentless economic development contribute significantly to water contamination which is a major obstacle to achieving sustainable quality water. The increasing presence of water contamination like heavy metals, salts and industrial effluents exacerbates the global water crisis, demanding advanced water filtration solutions. Therefore, the architectural evaluation for effective performance of nanofiltration (NF) membranes is of paramount importance. NF technology offers a promising avenue due to its ability to remove multivalent ions, organic and micro -pollutants efficiently while operating at relatively low pressure compared reverse osmosis (RO). This study focuses on the morphological structure, analysis of chemical composition, permeation and rejection of Polyethersulfone/coreshell-$Fe_3O_4$/ZnO membranes. The SEM images showed porous, interconnected tunnels and finger-like morphological structures of NF membranes. The water uptake, porosity and thickness contributed to the performance of the membranes. The contact angle of the membranes was improved significantly with the incremental addition of trimesoyl chloride. 0.50 wt % of PES/$Fe_3O_4$/ZnO was highly hydrophilic with a contact angle of 55.22˚. This membrane also offered maximum rejection of $Na_2SO_4$ (50.91 %), NaCl (52.64 %), and 80.39 % Pb(II) rejection . In addition, this study highlights that the synergistic effects of the pore-former, solvent evaporation time, metal oxides and monomers are crucial for effective performance of nanofiltration membranes.

# sciforum-138646: Polymer blends based on poly(lactic acid) (PLA) and poly(caprolactone) (PCL) for engineering applications

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Self-healing materials have garnered significant interest in the industry due to their potential for various applications, particularly in the automotive sector, including exterior parts and interior components. In this context, multiple strategies have been implemented to develop sustainable materials, especially for interior vehicle elements. Additionally, consumers demand constant improvements in material quality, as well as innovations in design, shapes, and colors.

In the automotive field, polylactic acid (PLA) has been proposed as a suitable material for this industry, with modifications or incorporations of other materials aimed at improving its properties. Self-healing polymers offer a good solution for maintaining the appearance of interior car components. By combining PLA with polycaprolactone (PCL), a more flexible material is obtained, and the incorporation of murexide (Mu) particles contributes to enhancing its self-healing capabilities.

To evaluate the properties of the resulting material, reactive extrusion was carried out using maleic anhydride as a grafting agent for PLA, likewise improving its compatibility with PCL and murexide (Mu) particles. Characterizations were performed using nuclear magnetic resonance (NMR), Fourier Transform infrared (FT-IR) spectroscopy, X-ray diffraction (XRD), thermogravimetric / differential scanning calorimetry (TGA)/(DSC), and confocal laser scanning microscopy (CLSM) techniques to analyze the morphology, structure, and thermal behavior of the material. The observed results show that the extrusion process alters the system's crystallinity, favoring an amorphous structure and achieving adequate dispersion of the constituent materials. However, no significant changes were observed between the samples and the raw materials when analyzed by NMR and FT-IR. Based on the collection of all analyses, it can be inferred that a self-healing material is obtained, though further studies are required to confirm that the material meets the necessary properties.

# sciforum-138822: Polyvinylpyrrolidone-Mediated Engineering of $NiMn_2O_4$ Nanocubes for Enhanced Energy Storage and Non-Enzymatic $H_2O_2$ Detection

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**Abstract**

Developing polymer-assisted advanced materials for multifunctional energy storage and sensing platforms offers a viable path to address future energy demands and associated economic constraints. In this context, inverse spinel-structured $NiMn_2O_4$ has gained attention as a next-generation electrode material due to its high energy density, superior power delivery, and robust cycling stability. The incorporation of polyvinylpyrrolidone (PVP) as a polymeric surfactant during hydrothermal synthesis plays a pivotal role in tailoring the material's nanoscale architecture. PVP not only modulates nucleation and growth to achieve a mixed morphology of nanocubes and nanoflakes, thereby optimizing the surface-to-volume ratio, but also facilitates a shift from diffusion-controlled to surface-driven capacitive behavior. This transition significantly improves charge transport dynamics, energy density, and structural durability. The resulting electrodes deliver a high specific capacitance of 816 F $g^{-1}$ at 1 A $g^{-1}$ and retain excellent cyclic stability over 5000 cycles in 1 M KOH. The assembled asymmetric supercapacitor (ASC) device demonstrates 96% capacitance retention after 10,000 cycles, delivering an energy density of 8.8 Wh $kg^{-1}$ at 6400 W $kg^{-1}$ and reaching a peak energy density of 36.55 Wh $kg^{-1}$ at 400 W $kg^{-1}$. Complementary density functional theory (DFT) analysis provides insights into the polymer-modulated electronic structure and redox behavior. In addition, the non-enzymatic NiMn4/GCE-based $H_2O_2$ sensor showcases excellent sensitivity, a low detection limit, and high selectivity against various biological interferences, demonstrating the polymer-engineered $NiMn_2O_4$'s dual functionality in sustainable energy and biosensing applications.

# sciforum-147371: Processing technology for polymer composites in biomedicine

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Polymer structures are essential in biomedical applications, such as tissue engineering and regenerative medicine, due to their properties of biocompatibility and biodegradability. The use of polymer composites is particularly significant for various applications, as a combination of mechanical, chemical and biological properties can be achieved. The intended application determines the selection of the biopolymer materials. In addition, the method used to process the materials should produce scaffolds that deliver the required therapeutic effect. Electrospinning is a well-established technique for producing fibres from a spectrum of polymer feedstock with diameters ranging from micrometres to nanometres. Moreover, electrospun fibres may exhibit a variety of biomimetic surface features (such as porosity) and orientations. The present review is aimed at describing the synthetic and natural polymers commonly used in biomedical applications, with particular focus on composite polymers. The processing of polymer composites using various electrospinning techniques is also discussed, as well as the biomedical application of the electrospun polymer composites. Although polymer composites and electrospinning have seen significant growth in biomedicine, making them suitable candidates for Industry 4.0, recent advances have shown great potential in propelling them into Industry 5.0 applications. These advances include the fabrication of smart 3D multi-functional scaffolds with tailored mechanical and biological properties, and the inclusion of machine learning technologies.

# sciforum-123690: Regime Kinetics of Poly Ethylene Terephthalate/Thermotropic Liquid Crystalline Polymer PET/TLCP Polycomposites

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**Abstract:**

The crystallization behavior of polyethylene terephthalate (PET) and PET/Thermotropic liquid crystalline polymer (TLCP) composites was analyzed under isothermal conditions using calorimetric kinetic data, with thermodynamic parameters derived from the Lauritzen–Hoffman (L-H) model. The crystal growth process, dominated by secondary nucleation, deviates from simple spherulitic radial growth, instead reflecting a complex interplay of nucleation and lamellar growth phenomena. The temperature dependence of the linear crystal growth rate (G) follows a biexponential form as per the L-H relation, integrating both segmental transport and thermodynamic driving forces. Through kinetic modelling, values of nucleation constants (Kg), pre-exponential growth factors ($G_0$), and surface free energies ($\sigma$ and $\sigma_e$) were obtained. The analysis confirmed crystallization in Regime II across all compositions and temperatures studied (195–210°C), characterized by a chain-folding mechanism where growth occurs on pre-existing crystalline substrates. The substrate length (L), estimated via the Lauritzen Z test, increases with TLCP content and crystallization temperature, indicating enhanced nucleation and hindered chain folding in composites. PET/TLCP blends exhibited higher fold surface energy and work of chain folding compared to neat PET, revealing the inhibitory effect of TLCP on PET crystallization kinetics. These findings offer a comprehensive understanding of the crystallization regime transitions and underlying thermodynamics in PET/TLCP systems.

# sciforum-146244: Rheological Properties of Ultra-high-Molecular-Weight Polyethylene and Its Blends with Linear Low-Density Polyethylene

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Ultra-high-molecular-weight polyethylene (UHMWPE) has attracted substantial scientific attention since its inception in industrial production owing to its exceptional properties, such as high tensile strength, superior wear resistance, chemical inertness, and a low coefficient of friction. Of particular importance are the rheological characteristics of this material, as well as the processing conditions.

This study examines two industrial grades of UHMWPE that had been previously investigated in [1], where the potential for plastic deformation development within the processing temperature range was demonstrated. The rheological and thermal properties of the materials were analyzed. Additionally, blends of two UHMWPE grades with linear low-density polyethylene (LLDPE) were prepared across a wide concentration range (0 to 50 wt.%). The rheological and physico-mechanical properties of the resulting samples were investigated.

Plasticity, a key parameter for processing high-molecular-weight materials, is largely determined by the breadth of the molecular weight distribution rather than the absolute molecular weight values. Experimental results demonstrate that blending UHMWPE with LLDPE significantly improves plasticity and processability without substantially degrading the material's physico-mechanical properties.

The findings indicate the feasibility of using UHMWPE/LLDPE blends in conventional processing methods, such as injection molding. It was established that the UHMWPE content in such blends can reach up to 50 wt.%, though an optimal concentration of 30 wt.% ensures a balance between processability and retention of physico-mechanical properties. These results open new prospects for developing advanced UHMWPE-based composite materials with enhanced processing characteristics.

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# sciforum-131713: Simulating Polymer Behavior in Silica Nanocomposites

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Polymer chain behavior in polymer/silica nanocomposites was explored using long-term atomistic molecular dynamics simulations. The study focused on two polymers: poly-(butadiene) (PB) and poly(ethylene oxide) (PEO). Both cis-1,4-PB and trans-1,4-PB nanocomposite systems contain 30 wt% silica nanoparticles with a diameter of about 4 nm. The overall size of the PB polymer chains remained unaffected, except for a small number of chains that wrapped around the nanoparticles. However, both the segmental and terminal dynamics of the PB chains were found to be slower in the nanocomposites compared to the corresponding bulk melts. Additionally, the PB chains within the nanocomposites exhibited highly heterogeneous dynamics, and a coupling between the dynamics and the conformation of PB chains was observed.

In the case of PEO nanocomposites, the effects of chain adsorption and the spatial confinement from the nanoparticles on the polymer's structure and dynamics were investigated. The analysis of static properties showed a heterogeneous polymer density layer near the interface of the PEO and silica. For systems with a low volume fraction of silica nanoparticles, a thin layer of slow-moving polymer chains forms on the nanoparticle surface. The polymer chains farther away from the surface move similar to a bulk material system. Conversely, in systems with a high volume fraction of nanoparticles, the dynamics of all the PEO polymer chains were predicted to be slower than in the bulk due to a strong confinement effect.

# sciforum-133961: Sol–gel complements conventional strategies for the synthesis of self-extinguishing hybrid silica–epoxy nanocomposites

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**Introduction.** Growing industry demand, together with rising pollution and the depletion of phosphorus, is moving the scientific community towards the development of flame-retardant (FR) epoxy nanocomposites (ENCs) containing low P contents and more sustainable additives.

**Methods.** High-resolution transmission electron microscopy (HRTEM) analysis was carried out to study the morphology of ENCs. Cone calorimetry (CC) and UL-94 vertical flame spread tests were performed to investigate the fire response of all ENCs.

**Results.** The reaction of DGEBA (Bisphenol A diglycidyl ether)- or Novolac-based resins with APTES (3-aminopropyltriethoxysilane) allows the production of organic–inorganic silanized epoxy moieties. The hybrid moieties can condense with tetraethyl orthosilicate (TEOS), a silica precursor, to form an in situ silica phase through sol–gel reactions. HRTEM analysis revealed that in the case of DGEBA, the silica phase was composed of well-ordered multi-lamellar nanoparticles (NPs). In contrast, the investigation of Novolac highlighted that fully amorphous silica NPs were embedded in the hybrid co-continuous polymer network. The incorporation of DOPO-based FRs into silica–epoxy systems based on DGEBA/Novolac resin produces aliphatic nanocomposites with high transparency, no-dripping UL-94-V0 rating, and a strong decrease (up to 80%) in the peak of the heat release rate in CC tests, with up to 3 wt.% of P loading. Regarding Novolac, the transparency is remains even at loadings of silica NPs beyond 4 wt.%, thanks to their amorphous nature. More waste-to-wealth approaches involve the use of humic acids or biochar from spent coffee grounds, together with ammonium polyphosphate and urea, in APTES-modified DGEBA-based epoxy systems to obtain no-dripping self-extinguishing systems, even with only 1 wt.% of P content.

**Conclusions.** The sol–gel in situ generation of inorganic phases has been explored in combination with DOPO-based FRs, bio-wastes, and other synergists to prepare no-dripping self-extinguishing (V-0 rating in UL-94 flammability tests) aliphatic ENCs, even keeping P at low loadings (1-3 wt.%).

# sciforum-129366: Solution Blow Spun Quercetin-Loaded Polylactic Acid Nanofibers for Active Food Packaging

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Currently, there has been a growing interest in the development of smart and active packaging materials that can protect food from external environmental factors. Ideally, these materials should combine antibacterial and antioxidant properties with biodegradability. However, most biodegradable and biocompatible polymers inherently lack active properties. As a result, it becomes essential to incorporate functional compounds that can enhance their protective capabilities, improve interaction with food, and ultimately extend shelf life [1].

Polylactic acid (PLA) is a well-known biocompatible and biodegradable polymer. PLA-based nanofibrous materials can be manufactured by mixing the polymer with various additives or particles to tailor their final properties [2]. Among these additives, quercetin, a naturally occurring polyphenol found in plants, is recognized for its strong antioxidant activity, which stems from its redox potential and structural configuration [3]. Incorporating quercetin into PLA nanofibers holds promise for the development of more effective smart packaging solutions.

This study aims to investigate the influence of quercetin on the properties of PLA-based nanofibers. The nanofibers were prepared by mixing a PLA solution with quercetin powder and processing the mixture using Solution Blow Spinning (SBS) [4,5]. To examine the effect of quercetin concentration, samples were prepared with varying quercetin contents (0.0, 1.0, 3.0, 5.0, and 7.0 wt%).

A comprehensive series of characterizations, including antioxidant, structural, morphological, antibacterial, and water vapor transmission tests, was conducted to evaluate the influence of quercetin on the final properties.

The outcomes of these characterizations were used to assess the effect of quercetin on the performance of the PLA nanocomposites. The findings provide insights into the potential application of these materials in active food packaging systems.

# sciforum-139215: STUDY OF NOISE ISOLATION IN POLYMERIC MATERIALS BASED ON CELLULOSE

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Noise pollution provoked by vehicles is a growing problem that negatively impacts health. For this reason, it is necessary to explore the possibility of improving sound insulation of some parts of the vehicle, such as commercial automotive paints or panels. This work deals with studying the incorporation of natural fibers into an acrylic commercial paint. Dispersions of microcrystalline cellulose (C) and nanocellulose (NC), extracted from commercial cellulose, type Iα, obtained by chemical methods (hydrogen peroxide and sodium hydroxide) and acid hydrolysis (sulfuric acid), were prepared at different concentrations (0.1, 1, 3, and 5 wt%). These formulations were applied onto 3003 aluminum substrates and characterized by Raman spectroscopy, X-ray diffraction (XRD), and optical microscopy. Moisture resistance and sound absorption capacity were also evaluated. Raman and XRD analyses confirmed the presence of cellulose and paint components such as titanium dioxide ($TiO_2$) in anatase and rutile phases. On the other hand, optical microscopy showed that NC presents better dispersion and less agglomerates than C. In acoustic performance, the results showed that the addition of C at 5 wt% lead to the best noise attenuation compared to NC. C displays values c.a. 2.4 dB (3.15%) in the minimum value and 1.7 dB (2.05%) in the maximum value compared to the paint. However, the incorporation of both materials increases moisture absorption. In conclusion, the addition of microcrystalline cellulose to automotive paints may be promising for automotive sound insulation.

# sciforum-139261: Sustainable composites based on bioplastics and hydrothermally carbonized wood waste

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Implementing sustainability and circularity concepts involves the conscious use and treatment of various types of waste to promote the transition from a linear to a circular economy and reduce the carbon footprint. This study explores the use of wood waste that has undergone hydrothermal treatment as a sustainable filler in bioplastics, with the aim of formulating composite biomaterials as an alternative to fossil-based materials. Wood waste was subjected to a sustainable hydrothermal carbonization treatment at a temperature of 210 °C, the limiting temperature to avoid cellulose decomposition. The produced particles were then introduced into the poly(butylene succinate) (PBS) matrix via melt mixing, varying the processing time (2 min and 5 min) and screw rotation speed (20 rpm and 60 rpm), at different weight ratios. For comparison, biocomposites based on PBS and micro-crystalline cellulose have been produced following the same processing protocols.

The obtained composite materials were characterized using thermal (TGA/DTG), calorimetric (DSC), mechanical (tensile and DMTA tests) and rheological (oscillatory tests) analyses. Additionally, the materials were subjected to a degradation process to evaluate their resistance to hydrolytic and photo-oxidative degradation, as well as to burial in soil. All the results obtained highlight that the wood waste particles, subjected to hydrothermal carbonization (HTC), were dispersed uniformly and have a reinforcing action on the bioplastic matrix. The calorimetric analysis suggests a clear nucleating effect of both fillers, leading to a significant increase in the crystalline degree of the PBS matrix. The elastic modulus values of the biocomposites are significantly higher than the value of the neat matrix, and this increase is more pronounced for the materials containing hydrothermally treated particles.

In conclusion, hydrothermally treated wood particles can be considered as a valuable alternative to high-cost conventional micro-crystalline cellulose.

# sciforum-125408: Synergistic improvement in fire performances of polyamide 6 hybrid composites using phosphonium ionic liquid and phosphine oxide as halogen-free flame retardants

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The flame retardancy of thermoplastics used in the automotive sector has been a topical challenge for a long time. Halogenated flame-retarded systems have been the additive of choice for several decades. The main issues include the recycling of polymers containing such halogens and the burning of such plastics releasing toxic fumes. Due to recent regulations, their use is now prohibited and halogen-free solutions are well researched. This study aims to investigate the influence of the combination of phosphonium-based ionic liquid (IL-P) and phosphine oxide (PO) as non-halogenated flame retardants on the mechanical and flame retardancy properties of polyamide 6. Different compounds were prepared in the melt state to ensure a good homogeneity between different constituents. The pelletized strands were transformed into sheets using a cast extrusion film line. To compensate the loss of stiffness caused by the plasticizing effect of flame retardants, 20wt% of unmodified sodium montmorillonite (Na+MMT) was added as a reinforcing filler. Flammability tests were conducted on humid and dry conditioned samples according to UL-94 and FMVSS 302 standards. It was found that PA6/PO compounds only achieved a V-2 classification, whereas the incorporation of IL-P made PA6/PO films attain a UL-94 V-0 ranking. Moreover, the two compositions pass the FMVSS 302 burning rate test. Although the addition of nanoclay made it possible to recover the initial mechanical performances, its inflammability rating deteriorated in UL-94 burning tests. In fact, the presence of clay platelets promoted the combustion of PA6/Na+MMT composites due to the hydrolysis effect initiated by the presence of hydroxyl groups on the surface of the clay lamellae. Nevertheless, the obtained data highlighted that the phosphine oxide combination with a phosphonium ionic liquid was very efficient in improving the flame resistance performance of polyamide 6 and could be transposed to design new halogen-free flame-resistant engineering plastics.

# sciforum-138521: Synthesis and characterization of stimuli-responsive niosomes functionalized with chitosan incorporating folic acid and hyaluronic acid for anticancer drug delivery

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The development of targeted anti-cancer therapies is a critical area of research, aiming to overcome the limitations of conventional treatments that often cause severe side effects and damage to healthy cells. In this study, we report the synthesis and characterization of a novel, smart nanoparticle-based drug delivery system designed for enhanced cancer cell targeting. Specifically, niosomes were surface-functionalized with a dual-modified chitosan (CS) incorporating folic acid (FA) and hyaluronic acid (HA), targeting receptors that are commonly overexpressed on cancer cells. Importantly, the modification preserved free amino groups on the CS backbone, enabling pH responsiveness in acidic environments such as the tumor microenvironment. This design confers the system with triple targeting capabilities: receptor-mediated (FA and HA) and pH-sensitive (CS) targeting. Two bioactive compounds were co-encapsulated within the niosomes: hydrophobic curcumin, known for its anti-cancer properties, and hydrophilic ascorbic acid (10 mg/mL), offering potential synergistic therapeutic effects. FTIR analysis confirmed the successful dual modification of CS with FA and HA, its effective coating onto the niosomes, and the presence of unmodified amino groups. Dynamic light scattering (DLS) analysis demonstrated optimal formulation with cholesterol and surfactants (Span 60 and Tween 60 at a 0.2:1:1 ratio), producing unloaded niosomes of 101 nm in diameter. Surface coating with modified CS increased the particle size to 174.5 nm, with further size increase upon drug encapsulation. Scanning electron microscopy (SEM) revealed a morphology suitable for cellular uptake, while in vitro cytotoxicity studies confirmed enhanced efficacy against cancer cells. The proposed multifunctional niosomal system exhibits promising features for targeted anticancer therapy, combining receptor-specificity, pH responsiveness, and synergistic drug action for improved therapeutic outcomes.

# sciforum-127027: Tensile electromechanical properties of carbon nanotube/poly (lactic acid)–polyhydroxyalkanoate filaments and additive manufactured coupons

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Additive manufacturing and the development of electro-conductive nanocomposites via fused deposition modeling (FDM) are prominent research topics. Polymers such as polylactic acid (PLA), polyhydroxyalkanoates (PHAs), and PLA-PHA blends are commonly employed to this aim. To achieve electrical conductivity, fillers such as carbon nanotubes (CNTs) and carbon black are commonly incorporated. The analysis of the filaments prior to FDM is particularly relevant, as their electromechanical properties directly influence the final performance of FDM-manufactured parts. However, there is a notable lack of research addressing this aspect. This study focuses on manufacturing CNT/PLA and CNT/PLA-PHA conductive filaments and their electromechanical characterization. The filaments are produced by melt blending followed by extrusion and are used to fabricate monolayer tensile coupons via FDM in order to evaluate and compare their electromechanical behavior. The inclusion of CNTs led to a slight increase in tensile strength in both the filament and the FDM-manufactured specimens, but elongation at break decreased in the FDM coupons. A reduction of three orders of magnitude in the electrical conductivity of the filaments was observed after FDM, along with a significant change in their piezoresistive response. These findings indicate that, while the incorporation of CNTs may improve tensile strength, the FDM process reduces electrical conductivity and alters the material's electromechanical sensitivity. Differential scanning calorimetry indicated polymer degradation, which is associated with thermal processes during extrusion and FDM. Such degradation resulted in a variation in the mechanical properties of the nanocomposites after FDM. These results underscore the importance of characterizing the polymeric filaments and the final FDM-manufactured parts to better understand and optimize the functional performance of conductive components produced by additive manufacturing.

# sciforum-135618: The Effect of Filler Type and Raditation Dose on the Mechanical Properties of HNBR Composites Prepared by Thermal and Thermo-Radiation Vulcanization

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In this work, elastomeric composites based on hydrogenated nitrile butadiene rubber (HNBR) were obtained using both thermal and thermo-radiation vulcanization in the presence of two different fillers: clay and carbon black.

The main component is HNBR 3606. An elastomer mixture was obtained on laboratory rollers in sheet form with thickness of 2 mm. The thermal vulcanization process was carried out at 150 °C for 20 minutes. Radiation-thermal vulcanizates were obtained by preheating in an electric press at 150 °C for 5 minutes and in next step samples were exposed to 100, 200, 300 and 400 kGy doses of ionizing radiation. The goal was to estimate the effectiveness of the reinforcement of each filler under various conditions of vulcanization and determine the optimal dose of radiation to achieve maximum mechanical strength.

Experimental results showed that HNBR vulcanizates with carbon black consistently demonstrated higher tensile strength than samples with clay. This is explained by the strong interaction of carbon black particles with the elastomeric matrix, which contributes to the formation of a more homogeneous and densely crosslinked network. In contrast, samples filled with clay showed weaker interfacial bonding and lower stress transfer efficiency, leading to decrease in mechanical performances.

With an increase in the dose of radiation, the tensile strength of all samples increased, reaching a maximum at 300 kGy (optimal dose) due to an increase in the crosslinking density and the formation of a network structure. However, at a dose of 400 kGy, a slight decrease in strength was observed, probably caused by excessive chain scission and molecular degradation. Elongation at break showed the opposite trend, decreasing with the increase in radiation dose, which confirms the progressive strengthening of the network.

# sciforum-147109: The Role of Multifunctional Octaspherosilicate Additives in Designing Polylactide (PLA)-based Materials: Structure–Property Optimization

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Polylactide (PLA), a biobased polymer, has gained significant attention due to its favorable mechanical properties, processability, and applicability in both Fused Deposition Modeling (FDM) 3D printing and conventional manufacturing techniques such as injection molding. However, PLA exhibits pronounced brittleness, necessitating the development of effective property-enhancing modifiers. The incorporation of hybrid inorganic–organic functionalized octaspherosilicates represents a promising strategy to overcome this limitation. Polyhedral oligospherosilicates (RSiMe2O)8Si8O12, analogs of polyhedral oligosilsesquioxanes R8Si8O12, possess a well-defined cubic Si–O–Si core with organosilyl subunits forming a functional crown, enabling modification of polymer properties. Variation in peripheral functional groups (R = H or organic moieties) allows for fine-tuning of material behavior. This study investigates the impact of multifunctional octaspherosilicates on PLA-based materials and their suitability for FDM 3D printing and injection molding.

Organosilicon additives were synthesized via catalytic hydrosilylation and incorporated into molten PLA. A 15% masterbatch was prepared, ground, and subsequently used to produce samples with lower additive concentrations (1 wt% and 2.5 wt%). The modified PLA was processed via two routes: (i) extrusion into filaments followed by 3D printing of test specimens, and (ii) direct fabrication by injection molding. Samples were characterized for their mechanical, rheological, and thermal properties (DSC).

Incorporation of multifunctional octaspherosilicates markedly enhanced the impact resistance of injection-molded samples, reflecting increased ductility. By contrast, 3D-printed specimens exhibited limited improvement in impact strength due to their anisotropic internal structure. Tensile and flexural strengths of 3D-printed samples were only slightly lower than those of injection-molded specimens, demonstrating the efficacy of the modifiers across both processing routes. Rheological measurements and SEM-EDS analysis confirmed good phase homogeneity and strong interfacial compatibility. Organosilicon additives functioned as lubricating agents, promoting polymer chain disentanglement and increasing free volume in the melt, thereby contributing to the observed enhancements in material properties.

# sciforum-125189: The thermal behavior of epoxy–siloxane amine composites

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To obtain composite materials using epoxy-functional siloxanes, direct amine addition to epoxy groups is thought to be a particularly useful approach for crosslinking epoxy, and they are used as the most popular curing agents.

In this study, we focused on an epoxy–siloxane amine composite obtained by the reaction between 1,3-Bis(3-glycidyloxypropyl)tetramethyldisiloxane (DS-PMO) and an aromatic amino compound, p-Phenylenediamine (PPDA). Two stages were involved in the preparation of the epoxy–siloxane amine composites. In the first stage, the hydrosilylation reaction between allyl glycidyl ether (AGE) and 1,1,3,3-tetramethyldisiloxane (TM-DS) was performed in the presence of a Karsted catalyst, resulting in the glycidoxypropyldisiloxane (GP-DS) intermediary compound. In the second stage, the GP-DS derivative was modified with PPDA to obtain the epoxy–siloxane amine composites (PPD-DS).

The polymers' structures were confirmed by FTIR, $^{1}$H-NMR, and MS spectroscopy. The morphology and surface chemical compositions were highlighted using scanning electron microscopy (SEM) coupled with energy dispersive X-ray analysis (EDX). The samples were subjected to thermal investigations using thermogravimetric analysis (TGA) as well as advanced thermogravimetric analysis, namely TGA/FT-IR/MS. In addition, the optical properties and static contact angle of precursors and the synthesized sample were investigated. The results showed that modifying epoxy–siloxane with p-Phenylenediamine allows for the production of hybrid materials with very good thermal stability, and it can also be recommended to use the PPD-DS composite material for UV-based applications.

# sciforum-139387: Thermo-Optical Characterization of PVA Films with SiO2-Au Nanocomplexes Using Photoacoustic Spectroscopy.

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Recent progress in nanoscience has enabled the development of nanostructured materials with applications in the diagnosis and treatment of diseases. Among these, silicon dioxide ($SiO_2$) nanoparticles combined with gold nanoparticles (AuNPs) have demonstrated significant promise in biomedical imaging and photothermal therapy due to their optical tunability and biocompatibility. In this study, $SiO_2$-Au nanocomplexes were synthesized and dispersed in aqueous polyvinyl alcohol (PVA) solutions to fabricate flexible films approximately 200 microns thick. The nanocomposite films were prepared with varying nanoparticle concentrations ranging from 1.50 to 4.5 mg/mL to investigate their optical and thermal behavior. Photopyroelectric (PPE) techniques were employed to determine key parameters such as optical absorption coefficient and thermal diffusivity, which are crucial for assessing their photothermal conversion capabilities. The results indicated that at specific SiO2-Au nanocomplex concentrations, the films exhibited high absorption coefficients in the visible spectrum, particularly at wavelengths of 520 nm and 660 nm. Their thermal diffusivities were recorded to determine their capacity for light-to-heat conversion. These findings highlight the potential of PVA films with $SiO_2$-Au nanocomplexes for use in minimally invasive photothermal therapies. Additionally, polyvinyl alcoholprovides biocompatibility, ease of processing, and mechanical flexibility, making this nanocomposite system a promising candidate for integration into biomedical devices and therapeutic platforms.

# sciforum-138593: Valorization of Medical Gauze Waste into Sustainable PLA/Cellulose Fiber Composites

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The main objective of using natural fibers as reinforcement phase in composites is to improve the mechanical properties and production of lightweight materials. Moreover, their biodegradability, renewability, nontoxicity, and abundance in nature make natural fibers ideal for use in composites. The valorization of biomass is one of the important ways we can control the consumption of non-renewable resources. Also, biocomposites have gained considerable academic and industrial attention due to their improved properties (thermal, mechanical and barrier, as well as fire resistance) compared to virgin polymer. Properties improved in the presence of fillers include an increase in Young's modulus, yield strength, a decrease in gas permeability, an increase in thermal resistance and an increase in biodegradability rates. Integrating cellulose fibers into PLA enables the development of advanced composites that exhibit notable improvements in mechanical strength, thermal stability, barrier performance, and overall sustainability.

The present work consists of extracting cellulose fibers from gauze strips (F-BG) for the production of PLA/F-BG biocomposites. The improvement of PLA and cellulose fibers' compatibility was achieved by adding a synthesized compatibilizer (PLA-g-MA). The fiber loading in PLA/F-BG composites varied between 1% and 3%. Rheological analysis indicated that the incorporation of F-BG fibers led to a reduction in the melt flow index, with a more pronounced decrease observed as the PLA-g-AM content increased. Moreover, mechanical characterization through impact and flexural tests showed that impact resistance decreased with higher F-BG content. However, F-BG addition significantly enhanced the flexural strength and elastic modulus of the composites.

# sciforum-134787: Valorization of Pecan Nutshell for the Design of Sustainable Polymeric Materials

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Global pecan nut production is projected to generate USD 3.54 billion by 2033, with a 7.3% CAGR between 2023 and 2033 [1]. In 2024, Mexico accounted for 50–55% of global production, mainly in the states of Chihuahua, Sonora, and Coahuila. Roughly 50% of pecan weight corresponds to the woody shell, representing 1–1.5 million tons of nutshell residue annually, of which more than 60,000 tons per year are produced in Mexico. This positions the country as a key source of raw material for the development of biodegradable materials [2].

Pecan nutshell (PNS) is an abundant agri-food byproduct, rich in lignocellulose and phenolic compounds, which has gained increasing attention for its potential in sustainable material development, particularly in food technology [3]. Research efforts have focused on its valorization through hydroalcoholic extraction, chemical modification, and physical treatments, resulting in materials with enhanced functional properties.

This presentation highlights research progress since 2013 on the use of PNS in polymeric materials for active and biodegradable packaging. Its structural and functional attributes enable the incorporation as a reinforcing agent or bioactive source in polymer systems, improving mechanical strength, barrier performance, and bioactivity.

Overall, PNS emerges as a versatile functional ingredient, aligned with the principles of the circular economy, sustainability, and food safety. Its valorization not only reduces agricultural waste but also supports the transition toward responsible, eco-friendly solutions in the agri-food sector.

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# sciforum-128074: Valorizing henequen bagasse by obtaining cellulose and using it to obtain acrylic composite films

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Sustainable management of agricultural waste is crucial for environmental protection and economic viability. This work investigates henequen bagasse, a residue from henequen fiber processing, as a source of cellulose to produce reinforced acrylic composite films. Two distinct cellulose extraction methods were assessed: an alkaline hydrothermal treatment (AHTP) and an alkaline extraction procedure (AEP). Comparative analysis of the extracted cellulose was performed, which included evaluations of yield efficiency, crystallinity index, fiber dimensions, and structural morphology. The results demonstrated that AEP provided higher cellulose yields (approximately 43%) with fibers exhibiting a higher aspect ratio (L/D = 73), compared to 37% yield and an aspect ratio of 55 obtained via AHTP. Crystallinity measurements indicated that AHTP cellulose predominantly retained a cellulose I structure with 63% crystallinity, whereas AEP cellulose showed partial transformation to cellulose II, with crystallinity reducing to 44%. Cellulose–acrylic composites were prepared by incorporating the isolated fibers into a commercial acrylic latex. Thermogravimetric analysis (TGA) results showed that adding cellulose did not significantly affect thermal stability. The mechanical performance indicated superior reinforcement for AHTP-derived cellulose at 10 wt%, achieving a maximum elastic modulus of 111 MPa and tensile strength of 6 MPa, albeit with a significant decrease in elongation at break from 435% to 77%. These findings highlight the potential of henequen waste valorization for advanced material development.

# Session 5. Polymer Physics and Theory

# sciforum-136158: Exploring the Optoelectronic Potential of Polyaniline via DFT and VASP Simulations

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In this study, the electronic and optical properties of polyaniline were systematically investigated using density functional theory (DFT) within the Vienna Ab Initio Simulation Package (VASP). Structural optimization was performed to ensure the stability of the polymer configuration prior to electronic and optical analyses. The calculations revealed a characteristic density of states and an electronic band gap of approximately 3.77 eV, indicating semiconducting behavior with the potential for optoelectronic applications. From an optical standpoint, several key parameters were extracted, including the absorption coefficient and dielectric function, both showing a pronounced absorption peak in the ultraviolet (UV) region, suggesting strong photon–matter interactions in this energy range.

The strong UV absorption, combined with the wide band gap, positions polyaniline as an excellent candidate for a range of optoelectronic devices. These properties make it particularly attractive for organic solar cells, UV photodetectors, optical sensors, and light-emitting devices, where materials with high optical stability and strong absorption are critical for efficient performance. Additionally, the intrinsic structural tunability, high environmental stability, and chemical versatility of polyaniline enable easy processing, doping, and functionalization, broadening its applicability in flexible electronics, wearable technologies, and advanced photonic systems.

Overall, the results highlight polyaniline as a promising and versatile material for next-generation optoelectronic and photonic technologies, offering a desirable balance between performance, scalability, and cost-effectiveness. Future research directions could involve experimental validation, exploration of doped or composite forms of polyaniline, and the investigation of device-level integration to fully harness its potential for commercial applications.

# sciforum-155581: Biphasic Modeling of Fluid-Microstructure Interactions in Fiber-Reinforced Biological Polymer Networks

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Soft biological tissues can be viewed as natural polymeric composites - hydrated, porous, and reinforced by networks of collagen and elastic fibers embedded in a proteoglycan-rich matrix. Their mechanical response under rapid or cyclic loading arises from complex interactions between fluid transport, fiber recruitment, and matrix deformation, reminiscent of the coupled behavior observed in cross-linked polymer gels. In this work, we develop a biphasic finite element model to capture the time-dependent mechanics of fiber-reinforced biological polymer networks [1-2]. The model integrates a porous, fluid-saturated matrix with nonlinear anisotropic fiber families, accounting for regional variations in orientation and stiffness. Built upon biphasic-swelling theory, the formulation explicitly couples fluid flow and solid deformation, enabling the prediction of strain-rate sensitivity, relaxation behavior, and energy dissipation under cyclic loading. The model reproduces key experimental phenomena such as auxetic-to-non-auxetic transitions and hysteresis loops linked to fluid redistribution within the microstructure. This analogy between polymer physics and biological tissue biomechanics provides a unified framework for interpreting viscoelasticity, anisotropy, and permeability-driven effects in hierarchical soft materials. By extending theoretical concepts from polymer network mechanics to living biological systems, this study contributes to the multiscale understanding of fluid-structure interactions in complex, multiphase materials.

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# sciforum-147733: Comparison of the ultrafast phenomena between eosin Y (EY) and palladium (II) octaethylporphyrin (PdOEP) as sensitizers and bis(terpyridine-4'-yl) terthiophene as an annihilator on thin films for optoelectronic applications

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This study presents a comparative investigation of ultrafast photophysical processes in thin-film of eosin Y (EY) and palladium (II) octaethylporphyrin (PdOEP) as triplet sensitizers, combined with bis(terpyridine-4'-yl) terthiophene (T) as an annihilator. Thin films were fabricated by spin-coating on quartz substrates using chloroform ($CHCl_3$) and hexafluoroisopropanol (HFIP) solvents. Excitation wavelengths were chosen based on the absorption maxima of the individual and mixed components.

Steady-state spectroscopy revealed distinct fluorescence and absorption features, with emission maxima ranging from 600 to 750 nm. Transient absorption spectroscopy (TAS) further confirmed efficient triplet energy transfer from both sensitizers to T, as evidenced by the characteristic ground-state bleaching (GSB) and excited-state absorption (ESA) signals spanning the 400-700 nm range. Global analysis of TAS data revealed multiexponential decay dynamics, with EY+T and PdOEP+T mixtures showing significantly extended triplet lifetimes compared to isolated components. Specifically, the EY+T system (1:4 ratio in HFIP, spin-coated) exhibited a rapid initial decay followed by a long-lived state exceeding 6 ns, while PdOEP+T (1:4 ratio in HFIP, spin-coated) displayed broader ESA bands related to triplet–triplet transitions.

These results demonstrate the effectiveness of EY and PdOEP as sensitizers for triplet state generation and energy transfer to T. The insights gained provide valuable guidance for optimizing triplet–triplet annihilation mechanisms in next-generation optoelectronic and photonic devices.

# sciforum-130501: Effect of hyperbranched epoxy resin grafting on the interfacial and mechanical properties of carbon fiber/epoxy composites

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In this work, experimental and theoretical methods were used to investigate the effect of hyperbranched epoxy resin (HPE) grafting on the interfacial and mechanical properties of carbon fiber (CF)/epoxy composites. Experimentally, the HPE was grafted onto the CF surface by chemical grafting method to prepare the CF-HPE reinforcement. Results show that compared with the unmodified CF, the surface roughness and wettability of CF-HPE reinforcement increase significantly. The CF/epoxy composites were prepared by compression molding method. Compared with the unmodified CF reinforced epoxy composites, the interfacial shear strength (IFSS), the interlaminar shear strength (ILSS) and the flexural strength of CF-HPE/epoxy composites are increased by 117.2%, 34.2% and 13.5%, respectively. Furthermore, the HPE grafting can also improve the thermal stability of CF/epoxy composites. The behind enhancement mechanisms can be attributed to the improvement of surface roughness and wettability of CF-HPE, thereby further enhancing the interfacial interaction and mechanical interlocking between CF-HPE and epoxy resin. In addition, the epoxy groups in HPE can react with the epoxy resin matrix and form stronger chemical bonding between the CF and epoxy. Theoretically, molecular dynamics (MD) method was used to reveal the internal mechanism of enhancing the interfacial properties of CF-HPE/epoxy composites from the molecular level. Results show that HPE grafting can improve the interfacial interaction energy between CF and epoxy, and decrease the mean-square displacement (MSD) value and the free volume fraction of CF/epoxy composites. This work provides valuable insights to the material design of epoxy composites containing reinforcements grafted with HPE.

# sciforum-142569: First-Principles Analysis of the Optoelectronic Properties of Polyaniline Using VASP

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In this study, the electronic and optical properties of polyaniline were systematically investigated using density functional theory (DFT) within the Vienna Ab Initio Simulation Package (VASP). Structural optimization was performed to ensure the stability of the polymer configuration prior to electronic and optical analyses. The calculations revealed a characteristic density of states and an electronic band gap of approximately 3.77 eV, indicating semiconducting behavior with potential for optoelectronic applications. From an optical standpoint, several key parameters were extracted, including the absorption coefficient and dielectric function, both showing a pronounced absorption peak in the ultraviolet (UV) region, suggesting strong photon–matter interaction in this energy range.

The strong UV absorption, combined with the wide band gap, positions polyaniline as an excellent candidate for a range of optoelectronic devices. These properties make it particularly attractive for organic solar cells, UV photodetectors, optical sensors, and light-emitting devices, where materials with high optical stability and strong absorption are critical for efficient performance. Additionally, the intrinsic structural tunability, high environmental stability, and chemical versatility of polyaniline enable easy processing, doping, and functionalization, broadening its applicability in flexible electronics, wearable technologies, and advanced photonic systems.

Overall, the results highlight polyaniline as a promising and versatile material for next-generation optoelectronic and photonic technologies, offering a desirable balance between performance, scalability, and cost-effectiveness. Future research directions could involve experimental validation, exploration of doped or composite forms of polyaniline, and investigation of device-level integration to fully harness its potential for commercial applications.

# sciforum-137506: How to use Kelvin Forces to tune dynamically the interaction between colloids and dipolar polymers

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Using Langevin Dynamic simulations we show two examples of how the competition between entropic forces and interactions arising from the mismatch between the non-polar and dipolar moieties present in a media (Kelvin Forces) can be used to tune the interaction between colloids and polymers via an external field. Results are important for both electric and magnetic systems. In a first example [Polymers 17, 366, (2025)], we show that it is possible to create dipolar polymer brushes whose interaction with colloidal particles can be switch from a repulsive to an attractive nature by just adjusting the strength of the external field. This effect can be used to favour applications of polymer brushes in which the entrapping and retention of colloidal particles for a later release is required. In a second example [Polymers 16, 820 (2024) ], we show that the depletion interaction of colloidal particles immersed in a bath of dipolar polymers can be also modulated using an external field. In many cases it is possible to switch from typical depletion force profiles between two colloidal particles to force profiles that contain one or several stationary points depending on the strength of the external field. Furthermore, the inter-particle distance at which these stationary points occur can be also controlled to a certain extend by adjusting the strength of the external field. These findings can be useful in the development of magnetic colloidal tweezers, and colloidal ratchets. We thank the funding support of the Spanish Ministry of Economy and Competitiveness (MINECO/AEI/FEDER,UE) via grant number DPI2017-86610-P, and MCIN/AEI/10.13039/501100011033 through grants number PID2020-118317GB-I00, and , PID2021-123723OB-C22.

# sciforum-147205: Natural and Petroleum-Based Resins: Impact on SBR Dynamics by Solid-State NMR Spectroscopy and Relaxometry

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In the tire industry, tackifying resins are essential ingredients because they modulate green tack and green strength of the uncured rubbers, facilitating their manipulation and preventing creep and tear of the final products. From a molecular perspective, the presence of the resin alters the dynamics of the polymer chain, resulting in the modification of the rheological and viscoelastic behaviour of the rubber compounds. Since the mechanical response of the final compounds varies depending on the type of resin added, it is important to dissect the molecular origins of such differences. In this research, we compared the effect of a natural- and a petroleum-origin resins on the dynamics of Styrene-Butadiene Rubber (SBR) in compounds of interest for the tyre industry. To this end, we employed a variety of Solid-State Nuclear Magnetic Resonance experiments (SS-NMR) at variable temperature. These include 1H Field Cycling NMR, DIPolar chemical SHIFT correlation and Centerband Only Detection of Exchange experiments. These techniques enabled the study of polymer dynamics on a wide range of motion time scales, form the fast segmental motions related to glass transition to the slower and collective motions of the polymer chains. In addition, measurements of $^{1}H$ $T_1$ and $T_{1\rho}$ relaxation times provided information on the polymer-resin miscibility on the nanometer scale, which is essential for achieving compounds with the desired mechanical properties. Dipolar-Filtered Magic Sandwich Echo experiments were also carried out to obtain information on the presence of domains with different degree of mobility, as well as on the onset of their motions with temperature. The SS-NMR results were compared with those from dynamic-mechanical, rheometric, calorimetric and chemical characterization. This approach provided valuable information to elucidate the complex relationship between molecular and macroscopic properties in rubber compounds, aiding the design of formulations with improved performances.

# sciforum-124054: Nonequilibrium effects on the association of an anionic polysaccharide and a cationic surfactant

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Mixtures of oppositely charged polyelectrolytes and surfactants play a crucial role in various industrial applications,. The interactions between these components influence key physicochemical properties, making it essential to develop a thorough understanding of the mechanisms governing their association. In particular, their bulk interactions and adsorption at fluid/fluid interfaces are of great interest due to their impact on emulsification, foaming, and other stabilization processes. However, the study of these systems remains challenging, as their complexation is often influenced by nonequilibrium phenomena, leading to kinetically trapped aggregates that exhibit distinct physicochemical properties compared to their equilibrium counterparts.

Among the many polyelectrolyte–surfactant systems, the interaction between sodium alginate (SA) and hexadecyltrimethylammonium bromide (CTAB) serves as a model for investigating these phenomena. Sodium alginate, a natural anionic polysaccharide, interacts strongly with the cationic surfactant CTAB, forming aggregates with diverse morphologies depending on factors such as concentration, ionic strength, and mixing protocol. The resulting structures exhibit a wide range of sizes and interfacial behaviors, significantly affecting their adsorption at fluid/fluid interfaces. Understanding these processes is critical for optimizing their use in industrial applications, where controlling interfacial properties is key to achieving desired functionalities.

This study aims to provide, by combining bulk characterization techniques (electrophoretic mobility, fluorescence spectroscopy, conductimetry and UV/visible spectrosctopy) with surface tension measurements, new insights into the complexation mechanisms of SA-CTAB mixtures, with a special focus on the formation of nonequilibrium states and their impact on interfacial properties. Our results highlight the importance of kinetic effects in determining the final properties of polyelectrolyte–surfactant complexes. In fact, the presence of Marangoni stresses during the preparation of the solution results in a very different association process compared to that appearing when Marangoni stresses are absent. This presents strong implications in the nature of the systems, which can influence the final application.

# sciforum-155582: Physically Based Modeling of Anisotropic and History-Dependent Behavior in Multi-Network Polymers

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This work advances the modeling of complex polymer systems by developing physically based constitutive frameworks capable of predicting the nonlinear, anisotropic, and history-dependent mechanical behavior of multi-network materials such as double-network hydrogels and filled elastomers [1-2]. These soft materials exhibit remarkable toughness and resilience due to intricate energy dissipation mechanisms involving chain scission, interfacial sliding, filler debonding, and viscoelastic relaxation. A multiscale modeling approach is proposed, combining molecular-level statistical mechanics with homogenization techniques to link microscale deformation mechanisms to macroscopic responses. The resulting models account for anisotropic softening, directional damage, and the influence of deformation history, achieving excellent agreement with multiaxial experimental observations. For filled elastomers, the framework incorporates visco-hyperelastic effects by representing the material as coupled elastic-viscous networks subjected to strain amplification from the filler phase. This description captures key phenomena such as the Mullins effect, hysteresis, and the evolution of anisotropy under cyclic loading. A comprehensive formulation is also proposed to explicitly represent the interaction between polymer and filler subnetworks, integrating mechanisms like chain-cluster debonding and interfacial viscous sliding. The finite element implementation of the hydrogel model demonstrates its robustness for simulating heterogeneous deformation fields. Altogether, this research establishes a unified and predictive basis for the design of architectured polymer materials, opening pathways toward multiphysics extensions coupling mechanical, electrical, or thermal effects for advanced functional applications.

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# sciforum-138463: Prediction of the Fatigue Life of Medical Polymers with the Help of Statistical Models: A Systematic Review

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The mechanical strength, as well as the responsiveness to stimuli, of photosensitive polymers makes these materials exceptionally useful in the reconstruction of hard tissues, although their clinical effectiveness over extended periods of cyclic loading remains unclear. This work systematically reviews 86 research articles that estimate the fatigue life of medical-grade photosensitive polymers using three different techniques: adaptation of the Weibull distribution, Paris–Erdogan crack propagation models, and hybrid statistical–machine learning methods. Data collection comprised standardized bending and tensile fatigue tests performed under physiologically relevant loading conditions. Throughout 2010 to 2024, I found and screened 1247 records while adhering to PRISMA guidelines, eventually yielding 86 studies from sources like PubMed, Google Scholar, and Web of Science. Erdogan models reached accuracy rates of 83–86% ($R^2$ range: 0.80–0.84), while the highest performing hybrid statistical–machine learning methods achieved 91–94% accuracy ($R^2$ range: 0.88–0.91). These hybrid approaches outshone other models in capturing nonlinear degradation trends in high-cycle fatigue (>10^5 cycles) where traditional models overestimated fatigue life by 12–18%. Regardless of the model used, fatigue resistance was observed to strongly correlate crosslinking density (Pearson's r = 0.79) and filler composition (r = 0.74). While statistical models have merit, especially during the preliminary stages of design, their predictive accuracy is often limited. In contrast, the machine learning component in hybrid models improved performance under varying load conditions and material complexity, resulting in more clinically reliable estimates of the device lifetime. Key limitations of the study included absent standardized protocols for fatigue testing and difficulties simulating in vivo degradation conditions. Supporting the conclusions of this study are the interdisciplinary efforts required to improve photosensitive polymer fatigue life testing that are guided by real-time clinical predictions and test standardization.

# sciforum-141377: The effect of alkylbutoxyethyladipates on the rheology of PVC melts

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Esters of dicarboxylic acids and oxyethylated alcohols are an important class of plasticizers. Plasticizers based on them are considered environmentally friendly. Plasticization remains the key method of PVC modification. Studying the process of processing PVC into materials by melting requires knowledge of the relationship between the process parameters and the properties of the flow. For this purpose, measurement of rheological properties using the melt fluidity index is widely used. Two esters butylbutoxyethyladipate and decylbutoxyethyladipate were synthesized and their properties were investigated. Evaluation of the effect of the ether structure on intermolecular interactions and the magnitude of the energy barrier of the transition state revealed a clear dependence of the properties on the length of the alkyl radical. Thus, the introduction of BBEA reduces the viscosity of the PVC melt by 30-50% compared to DOF, for example, at 190 °C and 50 wt. The MFI of a PVC composition with a BBEA content is 7.0 g/10 min versus 1.4 g/10 min for a composition with DOP. There is a pronounced temperature dependence of viscosity for compositions with BBEA, as a result of the high mobility of PVC chains in its presence and the thermodynamic stability of the mixture, and a less pronounced dependence using DBEA due to limited conformational mobility. Compositions with BBEA retain their white color up to 195°C (at 50-70 wt.h.), which is associated with better homogenization and screening of labile chlorine-containing PVC groups. When using plasticizers, an enthalpy-entropy compensation effect was revealed: high ΔH values of the viscous flow of PVC melts are accompanied by less negative ΔS. The Gibbs energy (ΔG) remains stable (1.85–2.15 kJ/g), confirming the universality of the flow mechanism. The concentration dependence of the thermodynamic parameters is to reduce Ea by 20-40% with an increase in the plasticizer content to 70 wt.h.

# sciforum-147749: Ultrafast Excited-State Dynamics and Aggregation Behavior of 2,5-Bis(2,2':6',2"-Terpyridine-4'-yl)-Thieno[3,2-b]Thiophene: Experimental and DFT Study

**Pınar Güloğlu [1,*], Petr Toman [1], Miroslav Menšík [1], Andrei Chernyshev [2], Jiří Zedník [2], Jiří Vohlídal [2], Jiří Pfleger [1]**

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The aggregation behavior of π-conjugated molecules critically influences their excited-state dynamics and thus their performance in optoelectronic applications. In this work, we deal with the title substance (hereafter referred to as **Tt**), used as a unimer for metallo-supramolecular polymers, and study the dynamics of its photophysical properties in various solvents using femtosecond transient absorption spectroscopy (fs-TA), steady-state absorption and emission spectroscopy, and dynamic light scattering (DLS). Experimental studies are completed with DFT and time-dependent DFT calculations, providing more detailed insight into the electronic structure of **Tt** and excited-state processes in it.

In aprotic solvents such as toluene and DMSO, **Tt** predominantly exists as free solvated molecules, exhibiting long-lived excited states with lifetimes extending up to hundreds of picoseconds. In contrast, different types of aggregation behavior have been observed in proton-donating solvents. In pure and aqueous hexafluoropropan-2-ol, HFIP and HFIP (*aq*), the formation of nanoaggregates ranging from 12 to over 1000 nm in size has been observed by DLS. These aggregates exhibit blue-shifted absorption bands characteristic of H-type aggregation and show significantly accelerated excited-state decay due to enhanced nonradiative relaxation pathways. Interestingly, in the more acidic solvent mixture of pH 1 (HFIP/0.01 M $HClO_4$ in $H_2O$ (4:1)), a red-shifted absorption band characteristic of J-type aggregation has been observed.

Solvent polarity and hydrogen bonding strongly modulate excited-state lifetimes, with the fastest internal conversion observed in acidic HFIP/water mixtures. Solvation dynamics in HFIP/0.01 M $HClO_4$-$H_2O$ mixtures completed within 1.2 ps, further influencing relaxation processes. In the most acidic environment tested (HFIP/0.01 M $HClO_4$ in $H_2O$ (4:1); pH=1), relaxation is considerably faster than in other solvent systems due to hydrogen bonding.

The combination of experimental and theoretical analyses reveals how hydrogen bonding and aggregation govern the photodynamics of **Tt,** providing valuable insights for designing polymeric materials with tailored optoelectronic properties.

# sciforum-133031: Unlocking the first few seconds of the Injection Moulding Cycle using operando X-ray scattering Measurements

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Injection moulding is the most common technology employed for shaping polymers. Despite its long history dating back to 1872, it remains a remarkably under instrumented technology. The vast majority of quality control and scientific study takes place on products postproduction. There is a substantial body of studies using simulation, but again there is little data to validate the predicts of simulations. In this work, a recent project performed at CDRSP in partnership with the ALBA Synchrotron Light Source focused on developing an industrially relevant operando X-ray scattering during injection moulding capability is presented. The challenges in such a project are identified and the design of the equipment to meet those challenges are described. In fact, the powerful integration of this equipment with the NCD-SWEET beamline, the SAXS/WAXS beamline at ALBA, enabled the capture of time-resolved structural information during dynamic processes. The advantages of these operando measurements are identified, in which the different processes are separated in time, rather than consolidated into a single average data set available from post-product analysis. The operando system is equipped with pressure and temperature sensors, and we correlate these measurements with the data available from X-ray scattering, which also includes a transmission monitor that enables the thickness of material in the mould cavity to be evaluates as a function of time. We contrast the transformation from the melt to the solid state for both synthetic and biobased polymers. The scope for dynamic measurements during the moulding cycle is explored and future planned work for detecting moulding defects such as weld lines will be critically discussed. The role of this equipment in enhancing sustainability will be underlined.

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# sciforum-155580: Bioinspired Lattice-based prostheses: A New Approach for Accurately Mimicking Multiaxial Mechanics of Intervertebral Discs

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Despite the significant advancements in intervertebral disc prostheses in recent years [1], they remain, to this day, the least favored medical solution among surgeons and the least appreciated by patients for treating damaged discs [2]. The current prostheses are still unable to accurately replicate several fundamental mechanical properties of the natural disc, such as auxeticity, energy absorption, and nonlinear stiffness [3]. This inability prevents them from mimicking correctly the natural mechanical behavior of the disc, adversely affecting the post-operative health and well-being of patients. To address these challenges, the current study explores novel bioinspired lattice-based polymeric architected structures, designed to mimic the complex mechanical behavior of the human annulus fibrosus. New cellular structures are developed to introduce complex mechanical functionalities into the lattices, whose performance is investigated using different polymers (hydrogels such as poly(ethylene glycol) diacrylate, alginate and gelatin methacrylate, and soft thermoplastics such as thermoplastic polyurethane and polylactide) to assess the coupled influence of cellular architecture and material microstructure. By tailoring cellular geometry, thickness, and material, these structures can reproduce nonlinear stiffness and axial-circumferential behaviors, including regional variations observed in natural discs. This precise control leads to sophisticated behaviors that conventional prostheses cannot achieve. The first derived replacement systems succeeded in replicating key mechanical characteristics of the natural annulus fibrosus, including auxeticity, nonlinear stiffness and region-dependent responses. These biomimetic lattices provide a promising pathway for the development of personalized, high-performance disc prostheses.

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