# المؤتمر العاشر لكيمياء الحالة الصلبة
# والمؤتمر الخامس للكيمياء التناسقية

# 10th Solid Chemisry Conference
# 5th Coordination Chemistry Conference

# SCC-ICC 2025

**21-24 December 2025**

***Iberostar Selection Kantaoui Bay Hotel,***
***El Kantaoui, Sousse, Tunisia***

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## Abstracts of Lectures and Communications
## List of Participants

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# Foreword

We are delighted to welcome you to the Joint Conference SSC & JCC 2025, proudly organized by the Tunisian Chemical Society. This prestigious event seamlessly combines two major scientific gatherings: the 10th Solid State Chemistry Conference (SSC) and the 5th Conference on Coordination Chemistry (JCC). By bringing together these two vibrant fields, we aim to foster dialogue, exchange, and robust collaboration across disciplines, strengthening the bonds between researchers who have graciously accepted our invitation.

The Organizing Committee, in close collaboration with the Scientific Committee, has prepared a rich and diverse program. This program addresses the latest advances and emerging topics in both Solid-State Chemistry and Coordination Chemistry, thereby reflecting the dynamism and creativity of our scientific community. We are profoundly grateful to the distinguished plenary speakers and researchers who have chosen to travel from their home countries, especially during this festive season, to join our conference. Their willingness to share their valuable expertise and insights is deeply appreciated, as it significantly enriches our scientific discussions.

This meeting is specifically designed to encourage active participation through plenary lectures, oral communications, and dedicated poster sessions. It represents a unique opportunity to explore new frontiers, exchange innovative ideas, and build bridges between complementary areas of research. We are particularly committed to offering young scientists an inspiring environment where scientific rigor and collegiality meet, ensuring an experience that is both highly educational and enjoyable.

Our program features distinguished contributions from leading experts and rising talents from various countries, thus emphasizing the truly international dimension of this event. With a comprehensive program composed of 11 plenary lectures, 73 oral communications, and 112 poster presentations, and welcoming almost 227 attendees, the conference is set to be a highly stimulating platform for scientific exchange and collaboration.

We extend our best wishes to all attendees for a highly productive scientific meeting and a truly memorable conference. We sincerely hope your stay in our beautiful country will be both scientifically rewarding and personally enjoyable, enhanced by the famous hospitality of Tunisia and the charm of El Kantaoui-Sousse, a wonderful destination all year round.

**Adel MEGRICHE**
University of Tunis El Manar
*Chair of the SCC 2025*

**Mohamed Taieb BEN DHIA**
University of Tunis El Manar
*Chair of the JCC 2025*

**Mohamed DAMMAK**
University of Sfax
*Co-chair of the SCC 2025*

**Med Abderrahmane SANHOURY**
University of Tunis El Manar
*Co-chair of the JCC 2025*

# SCIENTIFIC COMMITTEE

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**Mohamed DAMMAK** (Co-chair SCC 2025)
FSS - Sfax, University of Sfax, Tunisia

**Mohamed Abderrahmane SANHOURY** (Co-chair JCC 2025)
Member of the TCS Coordination Chemistry Group

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EPFL - Swiss Federal Institute of Technology, Lausanne, Switzerland

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Florida State University, Florida, USA

**Mohamed BOUOUDINA**
Prince Sultan University, Riyadh, KSA

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**Jesús CANALES-VAZQUEZ**
Universidad de Castilla-La Mancha, Spain

**Gilles LERONDEL**
University of Technology of Troyes, Troyes, France

**Habib BOUGHZALA**
IPEIN - Nabeul, University of Carthage, Tunisia

**Anne-Marie CAMINADE**
Research Director in CNRS, Toulouse, France

**Latifa LATROUS**
IPEIEM - El Manar, University of Tunis El Manar, Tunisia

**Essebti DHAHRI**
FSS - Sfax, University of Sfax

**Béchir CHAOUACHI**
ENIG - Gabès, University of Gabès, Tunisia

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# ORGANIZING COMMITTEE

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**Halim HAMMI**
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**Mohamed Mouldi ABDELKAFI**
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**Imed LAAJIMI**
Tunisian Chemical Society

# SCC - JCC 2025 Program

| | ***Sunday 21 December 2025*** |
|---|---|
| **14.00 - 17.00** | **Registration and Check in** |
| **17.00 - 17.30** | **Opening Ceremony** |
| **17.30 - 18.15** | **Plenary Lecture 1** **Jesús CANALES-VÁZQUEZ** **Chair**: Adel MEGRICHE.<br>*University of Castilla-La Mancha, Albacete, Spain*<br>**Low cost 3D-printing of Materials for Energy Applications: Li-ion batteries and SOFCs** |
| **18.15 - 19.00** | **Plenary Lecture 2** **Jason LOVE** **Chair**: Mohamed Taieb BEN DHIA<br>*University of Edinburgh, Edinburgh, UK*<br>**Chemical Solutions for Recycling Metals from Electronic Waste** |
| **19.00** | ***Dinner*** |
| **20.00 - 23.00** | **WORKSOP ON RIETVELD REFINEMENT**<br>**Workshop animated by Professor Habib BOUGHZALA**<br>Technical training course on Rietveld refinement in solid-state materials using X-ray diffraction<br>**Detailed program at the end of this document.** |

| | ***Monday 22 December 2025 (Morning)*** | | | | | |
|---|---|---|---|---|---|---|
| **09.00 - 09.45** | **Plenary Lecture 3** **Gillian REID** **Chair**: Mohamed Abderrahmane SANHOURY<br>*School of Chemistry and Chemical Engineering, University of Southampton, UK*<br>**Electrodeposition of 2D Transition Metal Dichalcogenide Semiconductors Using Single Source Precursors** | | | | | |
| **09.45 - 10.30** | **Plenary Lecture 4** **Alessandro CASELLI** **Chair**: Nizar BELLAKHAL<br>*University of Milan, Italy*<br>**Sustainable Catalysis via Iron and Zinc Complexes: from Photochemical Reactivity to Tunable Metallate Systems** | | | | | |
| **10.30- 11.30** | **Poster Session 1 (P 1 - P 28) Alphabetical Order** \| Evaluators: Imen ABDELHEDI & Jesús CANALES-VAZQUEZ | | | | | |
| | **Oral Communications - Session 1** | | | | | |
| | **Room A - Chair**: Béchir CHAOUACHI | | **Room B - Chair**: Fathi TOUATI | | **Room C - Chair**: Rym ABIDI | |
| | *Com.* | *Communicating \| Topic A - D* | *Com.* | *Communicating \| Topic B - J* | *Com.* | *Communicating \| Topic Coord.* |
| **11.30 - 11.45** | **OC-01A** | AROUA Nourhene | **OC-01B** | BEN AMOR Sarra | **OC-01C** | AKREMI Narmine |
| **11.45- 12.00** | **OC-02A** | BEN AMOR Wala | **OC-02B** | BOUHAJEB Oumayma | **OC-02C** | DHIFET Mondher |
| **12.00 - 12.15** | **OC-03A** | BEN SOLTAN Wissem | **OC-03B** | KTIFA Skander | **OC-03C** | MAJDOUB Sarra |
| **12.15 - 12.30** | **OC-04A** | JEBALI Sami | **OC-04B** | HAMRAOUI Khouloud | **OC-04C** | MOHAMED Hayder |
| **13.00** | ***Lunch*** | | | | | |

## *Monday 22 December 2025 (Afternoon)*

| | | | | | | |
|---|---|---|---|---|---|---|
| **14.30 - 15.15** | **Plenary Lecture 5** **Mohammad Khaja NAZEERUDDIN** Chair: Ridha Ben SALEM<br>*Swiss Federal Institute of Technology, Lausanne, Switzerland*<br>**The Influence of Additive-Engineering and Charge Transporting Layers in Perovskite Solar Cells** | | | | | |
| | **Oral Communications - Session 2** | | | | | |
| | **Room A - Chair**: Mahmoud CHEMINGUI | | **Room B - Chair**: Abderrahmen GUESMI | | **Room C - Chair**: Thouraya BARHOUMI | |
| | *Com.* | *Communicating \| Topic D* | *Com.* | *Communicating \| Topic C - J* | *Com.* | *Communicating \| Topic Coord* |
| **15.15 - 15.30** | **OC-05A** | HAMROUNI Abdessalem | **OC-05B** | LABIADH Houcine | **Keynote:** 15.15 - 15.40 | **Valentina PIROVANO**<br>*University of Milan, Italy*<br>**Unlocking Multifaceted Chirality through Gold-Catalyzed Enantioselective Transformations** |
| **15.30 - 15.45** | **OC-06A** | LABIADH Lazhar | **OC-06B** | SOUEMTI Ahmed | | |
| **15.45 - 16.00** | **OC-07A** | MANSOURI Badreddine | **OC-07B** | TOUBANE Amel | **OC-05C** | ACHECH Amel |
| **16.00 - 16.15** | **OC-08A** | LANSARI Imane | **OC-08B** | MEKAHLIA Leila | **OC-06C** | GHARIANI SYRINE |
| **16.15 - 17.15** | **Coffee break + Poster Session 2 (P 29 - P 56) Alphabetical Order** \| Evaluators: Mohamed Mehdi RAMMEH & Gilles LÉRONDEL | | | | | |
| | **Oral Communications - Session 3** | | | | | |
| | ***Room A* - Chair**: Haykel GALAI | | ***Room B* - Chair**: Mohamed BELHOUCHET | | **Room C - 17.00 - 23.00** | |
| | *Com.* | *Communicating \| Topic C - D* | *Com.* | *Communicating \| Topic B, G, Coord* | **WORKSOP ON RIETVELD REFINEMENT**<br>**Workshop animated by Professor Habib BOUGHZALA**<br>Technical training course on Rietveld refinement in solid-state materials using X-ray diffraction<br>**Detailed program at the end of this document.** | |
| **17.15 - 17.30** | **OC-09A** | MEJRI MARS Alma | **OC-09B** | MADDOURI Alaeddin | | |
| **17.30 - 17.45** | **OC-10A** | SALHI Sourour | **OC-10B** | WALHA Sandra | | |
| **17.45 - 18.00** | **OC-11A** | NAIFAR Amine | **OC-11B** | MESSAOUDI Olfa | | |
| **18.00 - 18.15** | **OC-12A** | HAJJI Melek | **OC-12B** | DJOUDI Ferhat | | |
| **19.00** | ***Dinner*** | | | | | |

## *Tuesday 23 December 2025 (Morning)*

| | | | | | | |
|---|---|---|---|---|---|---|
| **09.00 - 09.45** | **Plenary Lecture 6** **Anne-Marie CAMINADE** **Chair**: Houcine AMMAR<br>*Research Director in CNRS, Coordination Chemistry Laboratory, Toulouse, France*<br>**Phosphorus dendrimers for the functionalization of materials and as soluble supports of coordination complexes** | | | | | |
| **09.45 - 10.30** | **Plenary Lecture 7** **Gilles LÉRONDEL** **Chair**: Rached BEN HASSEN<br>*University of Technology of Troyes, France*<br>**Chemistry based sustainable nanophotonics** | | | | | |
| **10.30 - 11.30** | **Poster Session 3 (P 57 - P 84) Alphabetical Order** \| Evaluators: Halim Hammi & Aicha Beya MAMMERIA | | | | | |
| | **Oral Communications - Session 4** | | | | | |
| | **Room A - Chair**: Kais ANTAR | | **Room B - Chair**: Mohamed ABDELHEDI | | **Room C - Chair**: Nejib MEKNI | |
| | *Com.* | *Communicating \| Topic D - E* | *Com.* | *Communicating \| Topic F, H, J* | *Com.* | *Communicating \| Topic Coord* |
| **11.30 - 11.45** | **OC-13A** | DHIEB Sihem | **OC-13B** | FATTOUM Arbi | **OC-07C** | TOUMIA Hiba |
| **11.45 - 12.00** | **OC-14A** | HADDAD Larbi | **OC-14B** | BEN SLIMEN Aya | **OC-08C** | BELLALI Saher |
| **12.00 - 12.15** | **OC-15A** | MASMOUDI Amani | **OC-15B** | BEN AMMAR Nour Elhouda | **OC-09C** | EL GHARBI Safa |
| **12.15 - 12.30** | **OC-16A** | HADDED Rahma | **OC-16B** | VALERA-JIMÉNEZ José Fernando | **OC-10C** | ELAOUITI Sahbia |
| **13.00** | ***Lunch*** | | | | | |

## *Tuesday 23 December 2025 (Afternoon)*

| | | | | | | |
|---|---|---|---|---|---|---|
| **14.30 - 15.15** | **Plenary Lecture 8** **Hédi MATTOUSSI** **Chair**: Latifa LATROUS<br>*Florida State University, USA*<br>**Interfacial manipulation and control of colloidal nanomaterials via coordination chemistry** | | | | | |
| | **Oral Communications - Session 5** | | | | | |
| | **Room A - Chair**: Mostafa KOLLI | | **Room B - Chair**: Walid REKIK | | **Room C - Chair**: Fatma ZOUARI | |
| | *Com.* | *Communicating \| Topic E* | *Com.* | *Communicating \| Topic A, B, G, K* | *Com.* | *Communicating \| Topic Coord* |
| **15.15 - 15.30** | **OC-17A** | SNOUSSI Aziza | **OC-17B** | HAJJI Asma | **OC-11C** | GUEBEBIA Salma |
| **15.30 - 15.45** | **OC-18A** | ESSALEM Soulef | **OC-18B** | FATNASSI Ameni | **OC-12C** | HALLAB Wissem |
| **15.45 - 16.00** | **OC-19A** | MARS Abdelmoneim | **OC-19B** | CHELLI Chaima | **OC-13C** | AGOUILLAL Farid |
| **16.00 - 16.15** | **OC-20A** | KETIR Wahiba | **OC-20B** | BESKRI Ali | **OC-14C** | MOUSSA Marwa |
| **16.15 - 17.15** | **Coffee break + Poster Session 4 (P 85 - P 110) Alphabetical Order** \| Evaluators: Semy BEN CHAABENE & Makki ABDMOULEH | | | | | |
| | **Oral Communications - Session 6** | | | | | |
| | **Room A - Chair**: Abdelmoneim MARS | | **Room C - 17.00 - 23.00** | | | |
| | *Com.* | *Communicating \| Topic J* | | | | |
| **17.15 - 17.30** | **OC-21A** | AJARI Hanene | | | | |
| **17.30 - 17.45** | **OC-22A** | AMAIRIA Wahiba | | | | |
| **17.45 - 18.00** | **OC-23A** | AOULED ABDALLAH Marwa | | | | |
| **18.00 - 18.15** | **OC-24A** | BAABOURA Ghaya | | | | |
| **19.00** | ***Dinner*** | | | | | |

**WORKSOP ON RIETVELD REFINEMENT**
**Workshop animated by Professor Habib BOUGHZALA**
Technical training course on Rietveld refinement in solid-state materials using X-ray diffraction
**Detailed program at the end of this document.**

## *Wednesday 24 December 2025 (Morning)*

| | | | | | | |
|---|---|---|---|---|---|---|
| **09.00 - 09.45** | **Plenary Lecture 9** **Mohamed BOUOUDINA** **Chair**: Mustapha HIDOURI<br>*Prince Sultan University, Riyadh, KSA*<br>**Hydrogen Powering the Future. Global Energy Solutions** | | | | | |
| | **Oral Communications - Session 7** | | | | | |
| | **Room A - Chair**: Souhaira HBAIEB | | **Room B - Chair**: Fouad FERKOUS. | | **Room C - Chair**: Saoussen CHERNI | |
| | *Com.* | *Communicating \| Topic C, E, G, I* | *Com.* | *Communicating \| Topic F, G, J, Coord* | *Com.* | *Communicating \| Topic Coord* |
| **09.45 - 10.00** | **OC-25A** | MANGA Moise | **OC-21B** | MOUMEN Youssra | **OC-15C** | FLISS Outaf |
| **10.00 - 10.15** | **OC-26A** | AMMARI Hanen | **OC-22B** | BOUHARB Narjess | **OC-16C** | GASSOUMI Bouzid |
| **10.15 - 10.30** | **OC-27A** | CHEMEK Mourad | **OC-23B** | BOUAZIZI Ikram | **OC-17C** | ZOUAGHI Mohamed Oussama |
| **10.30 - 10.45** | **OC-28A** | ABDELAZIZ Balkis | **OC-24B** | MANCER Daya | **OC-18C** | DIAKHATE Aichetou |
| **10.45 - 11.00** | **OC-29A** | ACHOUR KHEDHIRI Arwa | **OC-25B** | CHAKER Hanen | **OC-19C** | BEN ABID Halima |
| **11.00 - 11.45** | **Plenary Lecture 10** **Essebti DHAHRI** **Chair**: Mohamed DAMMAK<br>*Faculty of Science of Sfax, University of Sfax, Tunisia*<br>**Impact of Preparation Method on the Functional Properties of Metal Oxides for Technological Applications** | | | | | |
| **11.45** | **Closing Ceremony**<br>**Remarks and Best Posters Awards** | | | | | |
| **12.00** | ***Lunch*** | | | | | |

| | | | | |
|---|---|---|---|---|
| **TOPICS** | **A** | **Innovation in Synthesis and Preparation**<br>Advances in solid-state materials synthesis, new solids, and compounds<br>Preparation and synthesis of new inorganic solids | **G** | **Functional, Sustainable, and Emerging Materials**<br>Functional materials<br>Sustainable, emerging and biomaterials |
| | **B** | **Characterization and Optical Properties**<br>Advances in characterization of solid-state materials properties<br>Photonic and optical properties of solids | **H** | **Advances in Glasses, Ceramics, and Polymers** |
| | **C** | **Computation, Modeling, and Next-Generation Devices**<br>Computation and theoretical aspects<br>Design, modelling and device fabrication | **I** | **Metals and Alloys: Properties and Applications** |
| | **D** | **Catalysis and Environmental Applications**<br>Catalysis, environment | **J** | **Nanomaterials, Nanocomposites, and Hybrid Structures**<br>Nanomaterials, nanocomposites and microporous/mesoporous materials<br>Surfaces, interfaces, hybrid, and nanostructured solids |
| | **E** | **Materials for environmental protection** | **K** | **Thin Films and Deposition Techniques** |
| | **F** | **Energy Materials for a Sustainable Future**<br>Energy and sustainable materials<br>Materials for renewable energy production and storage | **L** | **Electrochemistry and Corrosion Science in Solids** |

## Joint Conference SCC-JCC 2025 | Workshop Rietveld

Programme du 22 au 23 décembre 2025 | Animateur : **Pr. Habib Boughzala**

| Horaire | Dimanche 21 décembre | Lundi 22 décembre | Mardi 23 décembre |
|---|---|---|---|
| **17.00 – 19.00** | | Identification des phases.<br>Analyse<br>de la pureté d'une phase.<br>Outil : **QUALX** | Détermination des taux de substitution (TS)<br>Outil : **EXPO**<br>Exemple 1, 2, 3 |
| **19.00 - 20.00** | **Diner** | **Diner** | **Diner** |
| **20.00 - 21.30** | Installation des logiciels :<br>**EXPO**, **POWDLL** & **QUALX**<br>Installation des données de traitement<br>Installation de la base des données<br>**COD_database** | Indexation - Pattern matching.<br>Outil: **EXPO**<br>Exemple 1, 2 | TS & QPA. Outil: **EXPO** |
| **21.30 - 21.45** | **Break** | **Break** | **Break** |
| **21.45 - 23.00** | Découverte d'un diffractogramme.<br>Outil : **EXPO** | Analyse Quantitative<br>des Phases (QPA).<br>Outil: **EXPO** Exemple 1, 2, 3 | Questions particulières des participants<br>Evaluation et clôture |

# Speakers' Abstracts

# Jesús CANALES-VÁZQUEZ

Jesús Canales-Vázquez is currently Full Professor of Materials Science & Engineering at the University of Castilla-La Mancha, Albacete (Spain). Canales is a multidisciplinary researcher with a consolidated background in Materials Science & Engineering, especially in Materials for Energy Applications, mostly Solid Oxide Fuel Cells and Li-batteries. He holds a BSc (Universidad Complutense Madrid, Spain) and a PhD in Chemistry (University of St Andrews, UK) (2003), From 2003 to 2004, he was a research fellow at the University of St Andrews working and then moved to the Materials Science Institute in Barcelona. In 2006, he was appointed as Head of the Fuel Cell Department at the Albacete Science & Technology Park to design and set up new brand research labs. In 2007, he was awarded with Ramón y Cajal fellowship (tenure-track) at the Renewable Energy Research Institute in Albacete (UCLM) and in 2011 appointed as Associate Professor.

Canales has been principal investigator (PI) of multiple research projects devoted to Materials for Energy Applications (Solid Oxide Cells, Batteries) and Additive Manufacturing, including some relevant contracts with companies and international research centres. Canales runs an Instrumentation Unit dedicated to the characterisation of materials, including electron microscopy, thermal analyses, electrochemical testing, XRD, etc, for both UCLM research groups and companies. As a result of his work, Canales has published 120+ JCR articles and licensed 2 patents, which have resulted in the creation of 2 successful spin-off companies: one devoted to the development of 3D printing technologies and a second dedicated to the production at industrial scale of sodium carbonate using biogenic CO2 from fermentation processes.

# Low cost 3D-printing of Materials for Energy Applications: Li-ion batteries and SOFCs

J. Canales-Vázquez[a], J.F. Valera-Jiménez[b], I.M. Peláez-Tirado, J.I. García-Jiménez, H. Gueddari-Aourir, J.R. Marín-Rueda, M.Castro-García & J.C. Pérez-Flores

[a)] *Materials for Energy & 3D Printing Lab (3D-ENERMAT,) Renewable Energy Research Institute, University of Castilla-La Mancha, C/ Investigación 1, 02071 Albacete (Spain)*

In the European context of transition towards decarbonization of the energy model, the development of highly efficient and environmentally friendly/sustainable technologies for energy production and storage is crucial [1]. Both fuel cells and batteries are at the forefront of such technologies, and they have undergone phenomenal progress in the last decades. However, there is room for improvement as the conventional processing routes to produce these devices exhibit certain limitations regarding geometries, as most of the active materials are ceramics, excessive use of critical raw materials, etc.

In the present work, we demonstrate the use of a low-cost 3D printing technology based on the extrusion of ceramic-loaded filaments [2-4] that allows the production of free-form electrodes and electrolytes for Li-ion batteries and solid oxide fuel cells. The formulation of the filaments allows the introduction of additives such as carbon black to increase the electronic conductivity of the resulting 3D object or pore formers to modulate the microstructure. After debinding and sintering, the crystal structure is maintained and the electrochemical properties of the resulting ceramics compete with the state-of-the-art. In the case of Li-ion batteries, we have been able to produce LTO anodes displaying reversible capacities of 168 mAh $g^{-1}$ at C/2 (96% of the theoretical), or LFP cathodes with capacities as high as 152 $mAhg^{-1}$ at C/2 or 139 $mAhg^{-1}$ at 1C showing stable responses after 100 cycles in all cases [4]. As per SOFCs, we have been able to produce 3D printed cells with power densities exceeding 200 $mWcm^{-2}$ at 900°C.

**Key words:** 3D-Printing, Ceramic Filaments, Li-ion batteries, Solid Oxide Fuel Cells, Electrochemical performance.

## References

[1] European Commission: Directorate-General for Research and Innovation, Horizon Europe strategic plan 2025-2027, Publications Office of the European Union, 2024, https://data.europa.eu/doi/10.2777/092911

[2] J.R. Marín Rueda, V. Yagüe-Alcaraz, J. J. López-López, G. Sánchez-Bravo, J. Canales-Vázquez, Procedure for 3D printing of ceramics via FDM (ES 2 640 930 B1, PCT/ES2017/070202

[3] J.F. Valera-Jiménez, J.C. Pérez-Flores, M. Castro-García and J. Canales-Vázquez, "Development of full ceramic electrodes for lithium-ion batteries via desktop-fused filament fabrication and further sintering", Applied Materials Today, 25, 101243 (2021)

[4] I.M. Peláez-Tirado, J.R. Marín Rueda, J.M. Ramos-Fajardo, M. Castro-García, J.C. Pérez-Flores and J. Canales-Vázquez, "Fused Filament Fabrication and Characterisation of 3- and 8-YSZ-based SOFC electrolytes", Journal of the European Ceramic Society, 44(8),5031-5040 (2024)

# Jason LOVE

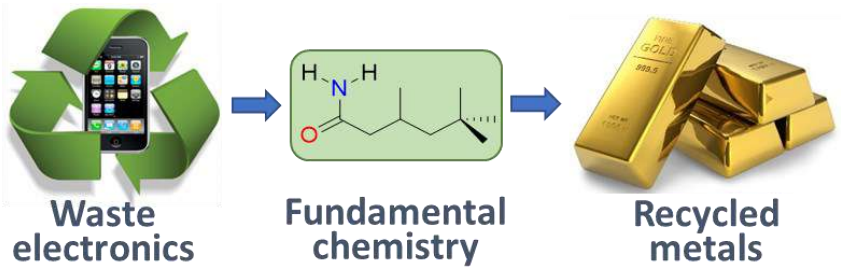
**Jason B. Love BSc(Hons) PhD CChem FRSC** is Professor of Molecular Inorganic Chemistry at the University of Edinburgh and Head of the School of Chemistry. He has published 165 peer-reviewed articles and patents and has delivered over 90 international, national, and public invited lectures. His primary research interests focus on the recovery and recycling of valuable and critical metals, making use of an in-depth chemical understanding to deliver new technologies and processes, a research effort that is supported by research council and industry funding. He is also a pillar lead on the UKRI Accelerating the Green Economy Centre REACT (U of Glasgow, HWU, U of Edinburgh) for responsible electronics and is a Member of the Board of the Incorporation of Goldsmiths of the City of Edinburgh. Love is an expert contributor to governmental and society initiatives in materials recycling and circularity for clean technologies and has contributed to magazine and radio commentary articles on gold recycling and urban mining.

# Chemical Solutions for Recycling Metals from Electronic Waste

Jason B. Love

*EaStCHEM School of Chemistry, University of Edinburgh, Edinburgh EH9 3FJ, U.K.*

Metals are critical to modern technologies and their recycling from sources such as electronic waste, magnets, and high-performance materials is crucial to achieve circular economy ambitions and to ensure that wastes are minimised and environmentally benign.[1] In this presentation, the application and significance of coordination and supramolecular chemistry in metal recycling processes will be highlighted. New selective precipitation routes to the separation of gold,[2] copper,[3] and rare-earth metals,[4] from electronic waste will be described. These case studies rationalise the need to understand separations processes at a fundamental chemical level and the ability to exploit ligand design to achieve new and useful metal separation technologies.[5]




**Keywords:** .gold, rare-earth elements, sustainable, metal separations

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# Gillian REID

Gill received her BSc and PhD in chemistry from the University of Edinburgh in Scotland (UK). She moved to the University of Southampton as a lecturer in 1991, becoming professor in 2006 and has held various leadership roles in Southampton, including being Head of School from 2016-2020.

Her research focuses on experimental coordination and organometallic chemistry, mainly with ligands from groups 15 and 16, motivated by understanding the properties and reactivities of their metal complexes, and with a focus on their applications.

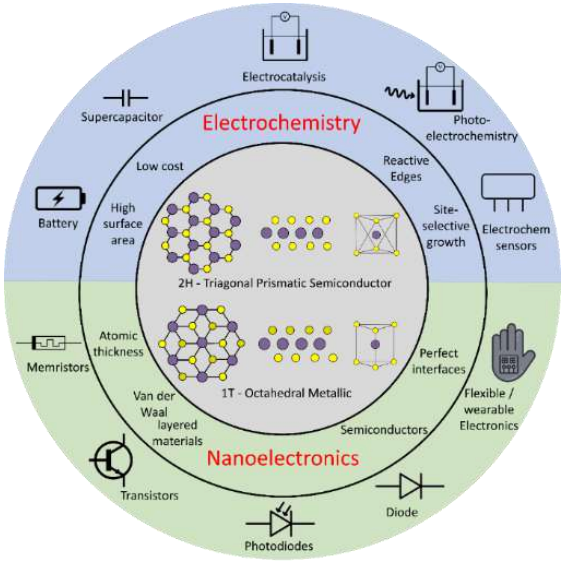
Gill served as the President of the Royal Society of Chemistry between 2022–2024. She was elected to Fellow of the Royal Society of Edinburgh in 2022, Fellow of the European Academy of Sciences in 2023 and received the IUPAC Distinguished Women in Chemistry award in 2023. In 2025 she was appointed to CBE for services to the chemical sciences and to inclusion and diversity.

# Electrodeposition of 2D Transition Metal Dichalcogenide Semiconductors Using Single Source Precursors

Gill Reid

*School of Chemistry and Chemical Engineering, University of Southampton, UK*

Transition metal dichalcogenides (TMDCs) are an important family of 2D-layered semiconductors of formula $ME_2$ (M = metal; E = chalcogen = S, Se, Te). With strong covalent in-plane bonding, weak van der Waals inter-layer bonding and readily tuneable bandgaps, they are attracting great interest for use in next-generation electronic and optical devices. However, to realise this it is necessary to grow monolayer or few-layer TMDCs with well-defined compositions, defect-free and with a high degree of crystallinity. The area-selective growth of high-quality mono/few-layer TMDCs is therefore a key target.[1,2] This lecture will discuss our recent collaborative work on the development and application of single source precursors (i.e. molecular complexes containing the pre-formed $ME_2$ sub-unit that defines the TMDC) for the area-selective electrodeposition of 2D TMDCs. [3-6]

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# Alessandro CASELLI

Full Professor of Inorganic Chemistry at the University of Milan since 2022, he currently serves as the Rector's Delegate for the UNITECH platforms (UNIMI Research Infrastructures). He graduated in Chemistry from the University of Milan (1995) and obtained his PhD from the University of Lausanne (2000) under the supervision of Professor Carlo Floriani, with a dissertation titled "The Chemistry of d²-Metal Carbenoids Over an Oxo Surface Modeled by Calix[4]arene."

His research focuses on inorganic and organometallic chemistry, with particular emphasis on sustainable catalytic processes aimed at the synthesis of high value-added fine chemicals and structural motifs of biologically relevant compounds. His work places strong emphasis on innovative technologies and on elucidating the mechanistic aspects of catalytic transformations to improve catalyst design and performance. Priority is given to the use of reagents that meet atom-efficiency criteria (e.g., CO2, O2, H2O2, carbenes, azides) and to the employment of eco-sustainable catalysts based on first-row transition metals. In recent projects, his interests have expanded toward the development of new catalytic methodologies that combine the ease of catalyst recovery typical of heterogeneous systems with the high activity and selectivity of homogeneous catalysts, also integrating continuous-flow techniques. More recently, his research has included the design of nanostructured solids featuring controlled release of bioactive species for crop protection.

He is the author of nearly 100 ISI-indexed publications, with over 3,500 citations and an H-index of 34, as well as one book chapter and one patent.

He has held several significant institutional roles, including Coordinator of the Scientific Committee of COSPECT (2021–2024), two terms as a member of the Academic Senate, and Coordinator of both the Mass Spectrometry Service and the Instrumentation and Technical Gases Committee within the Department of Chemistry.

He is a Fellow of the Royal Society of Chemistry (FSC) and has served as principal investigator on multiple competitively funded research projects, as well as on research contracts with industrial partners.

# Sustainable Catalysis *via* Iron and Zinc Complexes: From Photochemical Reactivity to Tunable Metallate Systems

Alessandro Caselli

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The development of sustainable catalytic systems based on earth-abundant metals has guided recent work in my group on iron and zinc complexes supported by pyridine-containing macrocycles[1] and ammonium metallate frameworks. Iron(III) pyclen and related complexes catalyse the selective oxidation of alkenes[2] and alcohols[3] with hydrogen peroxide, with anionic ligands controlling spin state, electronic structure and product distribution. Their photochemical behaviour was also investigated: $[Fe(III)(X)_2(pyclen)]X$ complexes display visible-light LMCT transitions that promote Fe–X homolysis and halogen-radical generation (Fig. 1),[4] enabling selective aerobic oxidation of aromatic alkenes and alcohols under mild conditions.
A second line of research concerns $CO_2$ valorisation via atom-economic cycloaddition to epoxides[5] and aziridines. Ammonium ferrates and zincates efficiently yield cyclic carbonates[6] and carbamates[7] under mild or ambient conditions, and their immobilisation on ion-exchange resins affords heterogeneous catalysts with synergistic effects, improved selectivity, recyclability and gram-scale applicability (Fig. 2).[8] Overall, these tunable iron and zinc systems provide versatile and cost-effective platforms for sustainable oxidation chemistry and $CO_2$ utilisation.

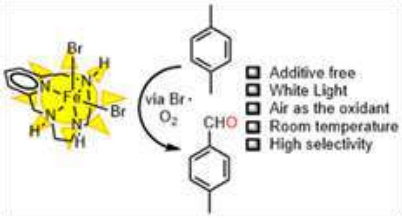


**Figure 1**: $[Fe(III)(X)_2(pyclen)]^+$ complexes as photocatalysts

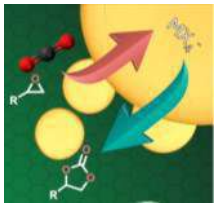

**Figure 2**: Supported metallates

**Key words:** Sustainable catalysis; Iron and zinc complexes; Photochemical oxidations, $CO_2$ valorization; Metallates

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# Mohammad Khaja NAZEERUDDIN

Nazeeruddin is a Professor of Chemistry at the EPFL Sion campus, and his current research at EPFL focuses on Perovskite Solar Cells and Light-emitting diodes. He has published more than **927 peer-reviewed papers**, ten book chapters, and he is the inventor/co-inventor of over 103 patents. His work's high impact has been recognized by invitations to speak at over 450 international conferences. He appeared in the ISI listing of most cited chemists and has more than 193394 citations with an h-index of 197 (https://scholar.google.com/citations?user=3c4Y1ycAAAAJ&hl=en&oi=ao). Several industrial partners, Panasonic, NEC, TOYOTA-AISIN, TOYOTA-Europe Motors, Solaronix, and ABENGOA, have funded his research. His total funding during the last 10 years is CHF 18.5 million.

He teaches the "Functional Materials" course at EPFL and Korea University. According to the Web of Science in 2016, he is the fifth most cited chemist in the world and is one of the 19 scientists identified by Thomson Reuters as the World's Most Influential Scientific Minds in 2015. One of the 24 Highly Cited researchers was named in **three ESI fields** in 2018. https://hcr.clarivate.com/. He was named Thomson Reuters' "Highly Cited Researcher" from 2014 to 2025 and was listed among the top 10 researchers in the perovskite solar cell research field by the Times Higher Education. Based on the Career Long Impact, Nazeeruddin has been ranked among the top 2% of most cited scientists worldwide, according to the list published by Stanford University in October 2022. He directs and manages several industrial, national, and European Union projects. He has been appointed a world-class university professor by Korea University, an adjunct professor by King Abdulaziz University in Jeddah, Imam Abdulrahman Bin Faisal University (IAU), Southeast University in China, and the Chinese Academy of Sciences (in Haixi Institutes). He is an **elected member of the European Academy of Engineering, the European Academy of Sciences (EURASC), a member of the Swiss Chemical Society, a fellow of the Royal Society of Chemistry, and a fellow of the** Telangana Academy of Sciences. **He won the 34th Khwarizmi International Award (KIA) for Laureates in Fundamental Sciences in 2021 and The 2025 Mustafa (pbuh) Prize in Basic and Engineering Sciences. He serves on the editorial boards of several journals.**

# The Influence of Additive-Engineering and Charge Transporting Layers in Perovskite Solar Cells

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# Valentina PIROVANO

Valentina Pirovano was born in Bergamo, Italy, in 1986. In 2010, after a six-month research stay in the group of Prof. Lutz Ackermann at the University of Göttingen, she obtained her Master's degree in Chemistry and Pharmaceutical Technology at the University of Milan, Italy.

From 2011 to 2014, she pursued a co-tutored Ph.D. under the supervision of Prof. Elisabetta Rossi (University of Milan) and Dr. Rubén Vicente (University of Oviedo, Spain). Since 2014, she has worked as a postdoctoral researcher in the group of Prof. Elisabetta Rossi, focusing on transition-metal catalysis for the synthesis and functionalization of heterocyclic scaffolds.

In 2020, she started her independent career as an Assistant Professor at the University of Milan, and in 2023 she was promoted to Associate Professor. Her current research interests include the photocatalytic functionalization of complex indole derivatives and the enantioselective synthesis of hetero- and macrocycles beyond classical central chirality.

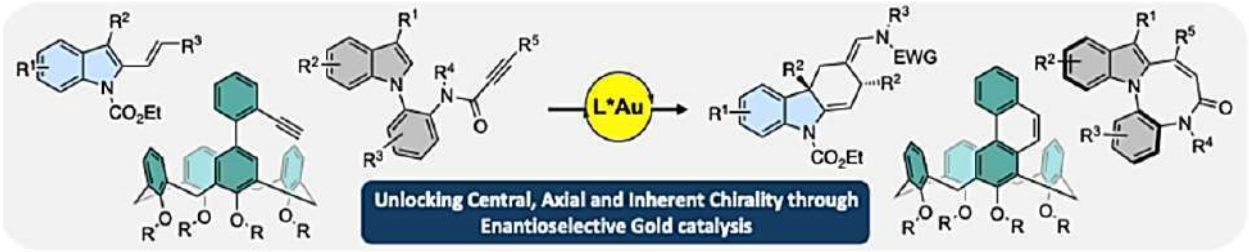
**Scopus Author ID: 36136255200**

# Unlocking Multifaceted Chirality through Gold-Catalyzed Enantioselective Transformations

Valentina Pirovano, Silvia Meraviglia, Giorgio Abbiati

*Dipartimento di Scienze Farmaceutiche, Sez. di Chimica Generale e Organica "A. Marchesini", Università degli Studi di Milano, Italia*

Chirality manifests in several forms in organic molecules, most commonly as central chirality arising from tetrahedral stereogenic centers, but also as axial, planar, and helical chirality, where stereochemical information is encoded in conformational or topological features. While asymmetric catalysis has long focused on central stereocenters, the controlled construction of more complex chiral elements is an emerging frontier.[1] Gold catalysis provides a privileged platform, combining π-activation with tunable chiral ligands, and has been exploited for central chirality,[2] while its application to axial, planar, and inherently chiral architectures remains less explored.[3] This work highlights the use of chiral gold(I) catalysts to access indole-based scaffolds with central or axial chirality and inherently chiral calix[4]arenes,[4] demonstrating the versatility of gold catalysis in shaping multiple chiral elements with high stereocontrol.




**Key words:** homogeneous catalysis, gold, enantioselectivity, hetero- and macrocycles

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# Anne-Marie CAMINADE

Anne-Marie CAMINADE is Director of Research, Exceptional Class at the CNRS (the highest grade of the Centre National de la Recherche Scientifique), at the Laboratoire de Chimie de Coordination in Toulouse (LCC), of which she is also Deputy Director (DUA) and Head of the “Dendrimers and Heterochemistry” team.

She has spent almost her entire scientific career in Toulouse, including 2 theses. She did a post doc after each of her theses, the first at the Institut Français du Pétrole (IFPEN) near Paris, the other in Germany, where she obtained an Alexander von Humboldt fellowship.

Her entire career has been devoted to the chemistry of phosphorus, in different aspects, such as coordination chemistry, supramolecular chemistry, but especially phosphorus macromolecules, such as macrocycles and above all, dendrimers.

She is co-author of 508 publications, 55 book chapters, editor of 2 books on dendrimers, she has an h index of 76 (over 18,000 WOS citations).

She has received numerous awards, including very recently the nomination as "Chevallier de la Légion d'Honneur" (the highest civilian award in France), the Grand Prix Achille Le Bel from the Société Chimique de France (SCF) and the Victor Grignard – Georg Wittig Prize of the German Chemical Society (GDCh).

# Phosphorus dendrimers for the functionalization of materials and as soluble supports of coordination complexes

Anne-Marie Caminade

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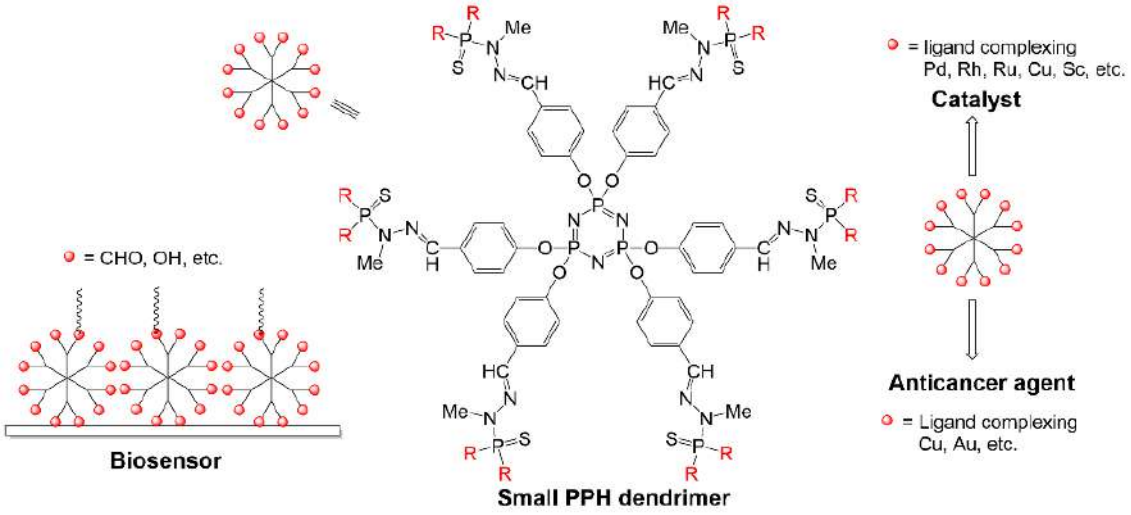
Dendrimers are a special type of hyperbranched polymers, synthesized radially and stepwise from a central core to afford structures reminiscent to that of trees. The properties of dendrimers essentially depend on the type of their periphery functions. Polyphosphorhydrazone (PPH) dendrimers are a special type of macromolecules, having a phosphorus atom at each branching point [1], and can be easily functionalized on their periphery to give them the desired properties. PPH dendrimers have been grafted to different types of materials, in particular to glass slides to create biosensors [2]. PPH dendrimers complexing different metals on their periphery are efficient and reusable catalysts [3], and have also anticancer properties, including *in vivo* [4].




**Key words:** dendrimers, polyphosphorhydrazone (PPH), sensor, catalysis, anticancer

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# Gilles LÉRONDEL

Gilles Lérondel is a condensed matter Physicist, currently Full Professor at the University of Technology of Troyes he joined in 2000 and former head of the Physics, Materials, Mechanics and Nanotechnology department. He is member of the Light, nanomaterials and nanotechnology laboratory associated with the CNRS. He is the founder and head of the center for Innovative Nanostructured industrial Foils and related applications, an industry joint laboratory. From 2004 to 2018 he was responsible of the ONT graduate program in optics and nanotechnology. Since 2020 he has been involved in EUT+ (European University of Technology) initiative. Gilles has also served as UTT Vice-president for international relations.

After receiving his PhD in condensed matter physics, from the University Joseph Fourier (Grenoble) in 1997, he moved to Italy and Japan respectively as INFM (Italian Condensed Matter Research Institute) fellow at the IENGF (now INRiM) and JSPS fellow at the Institute for Materials Research, Tohoku University. In 2001 and 2002, he was awarded an Australian Research Council fellowship and co-appointed visiting fellow at UNSW. Gilles has also been visiting professor of National Central University, Taiwan in 2011. More recently from 2014 to 2000, Gilles was temporary visiting Professor at the department of energy science, SungKyunKwan University in South Korea.

Author of more than 215 publications in refereed journals and 17 patents, his general research interest lies in light-matter interaction control at nanoscale including the development of nanostructured multifunctional materials and surfaces and near field optics. He serves as topical editor of the journal of Applied Optics (OSA) and editor of the Springer series in nano-optics and nanophotonics. As part of his interest for the societal and multidisciplinary issues associated with nanotechnology i.e. innovation and sustainable development (nanogreen), he has been from 2007 to 2010 involved in the former French-Taiwanese multidisciplinary Frontiers of Science program. Since 2011, he is member of the organizing committee of the SPIE "Optics and Photonics" conference and co-chair of the nanophotonic materials and UV and higher energy photonics conference. (contact: lerondel@utt.fr)

# Chemistry based sustainable nanophotonics

Gilles Lérondel, Hind Kadiri, Anisha Gokarna, Hyun Jeong, Komla Nomenyo, Ilhem Elgargouri

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The control of light-matter interaction at nanoscale relies on the ability to nanostructure materials. In this context, chemistry-based processes are often presented as low cost and low energy processes.

After introducing sustainability in the context of nanophotonics, we will in this presentation review different examples of nanostructuring based on chemistry alone or combined with other physical techniques. These examples will include porous silicon multilayers like omnidirectional mirrors obtained by means of electrochemistry [1], Self-assembly for nanomasking, (Photo) chemical etching of multifunctional materials [2], chemical growth of nanowires for 2D materials integration [3, 4] and finally sol-gel based coating of perovskite oxides and associated optoelectronic devices [5].

We will then conclude by emphasizing the advantages of these chemistry-based approaches compared to the physical ones.

**Key words:** nanophotonics, sustainability, chemistry, self-assembly, Chemical bath deposition, sol-gel coating, Reactive Ion etching, 2D materials, Integration, silicon, ZnO, perovskite oxides

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# Hedi MATTOUSSI

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**Hedi Mattoussi** is a Distinguished Research Professor at the Florida State University, Department of Chemistry and Biochemistry, Tallahassee, FL. Prior to joining FSU in 2009, he spent 12 years working as a senior Research Scientist at the US Naval Research Laboratory (Washington, DC). After graduating with a Bachelor in Physics from the University of Tunis El Manar (Tunis) in 1982, he moved to Paris where he earned a Ph.D. in Condensed Matter Physics in 1987 and a Habilitation to direct Research in Materials Physics in 1994, both from Sorbonne University, University of Pierre & Marie Curie Campus. He presently focuses on the development of inorganic nanocolloids and transition metal clusters and interfacing them with biological systems. Professor Mattoussi is a fellow of the American Chemical Society, ACS (class of 2011), the American Physical society, APS (class of 2013) the Royal Society of Chemistry, RSC (class of 2014), and the Materials Research Society, MRS (class of 2020). He was awarded the 2022 Kuwait Prize (sponsored by the Kuwait Foundation for the Advancement of Sciences, KFAS) and the 2024 American Chemical Society (ACS) Award in Surface Chemistry.

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# Interfacial Manipulation and Control of Colloidal Nanomaterials via Coordination Chemistry

Hedi Mattoussi

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Nanocolloids made of transition metal cores, prepared via bottom-up solution growth reactions, offer great promises for use in a wide range of applications, including optoelectronic devices and as functional platforms for integration into biomedicine. Implementation of those concepts requires access to coating strategies that can readily interface those materials with various molecules, such as dyes, metal complexes and proteins. We have developed several metal-coordinating small molecules and polymers as ligands that can surface functionalize an array of inorganic nanocrystals with varying core composition, size and shape.

In this presentation we first introduce a few coating strategies, relying on ligand substitution with multifunctional coordinating ligands, to interface inorganic nanocrystals with various target molecules. These include luminescent quantum dots, plasmonic nanocolloids and magnetic nanoparticles. In particular, we stress the ability of ligands combining mixed coordination and multidentate interactions to achieve high affinity binding and colloidal stabilization under a wide range of conditions.[1] In the second, we discuss a few representative examples where the surface-stabilized nanocrystals (such as semiconductor QDs and Au nanoparticles) have been used to investigate energy transfer interactions between the nanocolloids and proximal dyes or fluorescent proteins. We will also introduce a few examples using these concepts to develop sensing platforms that target enzymatic activity or/and allow visualization of cellular structures.[2]

**Key words:** inorganic nanocrystals, coordination, ligands, surface functionalization, sensing

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# Mohamed BOUOUDINA

Mohamed Bououdina holds a PhD in Physics from Grenoble Alpes University in France. He is the Aid to the President for Research Governance, Associate Director for the Research and Initiatives Center, and the Leader of the Energy, Water, and Environment Lab at Prince Sultan University in the Kingdom of Saudi Arabia. He has over 25 years of experience in teaching and research, occupying several positions at leading research institutions and academia in France, Spain, Japan, the UK, Bahrain, and Saudi Arabia. In addition, he was a Visiting Professor at the Chinese Academy of Sciences - China, and Petronas University - Malaysia. He has a broad background and extensive expertise in Physics, Materials Science & Engineering, Nanotechnology, and Energy, specifically in materials fabrication, analytical and spectroscopic characterizations, and functional properties for cutting-edge technologies. His research interests include energy (like hydrogen production, storage, & applications), CO2 capture & conversion, water treatment, biowaste transformation, biomedical field, and so on. He published over 600 papers in ISI journals, more than 40 book chapters, and two indexed books. He is a member of the editorial board of international journals.

# Hydrogen Powering the Future - Global Energy Solutions

Mohamed Bououdina [a], Sajjad Ali [a], Muhammed Humayun [a], Chao Zeng [b], Chundong Wang [c]

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[b)] *Institute of Advanced Materials, College of Chemistry and Chemical Engineering, Jiangxi Normal University, Nanchang 330224, People's Republic of China*

[c)] *School of Integrated Circuits, Wuhan National Laboratory for Optoelectronics, Huazhong University of Science and Technology, Wuhan 430074, China*

Hydrogen ($H_2$) technology is rapidly emerging as a cornerstone for achieving global energy sustainability, offering clean solutions for sectors ranging from transportation to industrial applications. This presentation will explore the multifaceted landscape of $H_2$ technology, beginning with an overview of current $H_2$ production methods, including electrolysis and natural gas reforming, and their role in reducing carbon emissions. The discussion will then focus on advancements in hydrogen storage solutions, including solid-state and compressed gas technologies, which are critical for safe and efficient energy transport. Key challenges in hydrogen transportation will be examined, with a particular focus on innovations in pipeline infrastructure and the emerging potential of hydrogen liquefaction for long-distance delivery. The application of $H_2$ in various sectors, including automotive, aviation, and power generation, will also be highlighted, showcasing its versatility as an alternative fuel source. Additionally, the presentation will address the risks and safety concerns associated with $H_2$ technology, emphasizing the importance of safety protocols, material compatibility, and risk mitigation strategies. Finally, the business and marketing potential of $H_2$ as a key player in the global energy market will be discussed, exploring investment trends, government policies, and the potential for hydrogen to revolutionize the clean energy economy. Selected research activities on hydrogen production will be presented, including doped ZnS, single atom catalysts, and MXenes.

**Keywords:** Hydrogen production; Storage; Transportation; Applications; Risk & Safety; Marketing.

# Essebti DHAHRI

**Professor Essebti DHAHRI** is a distinguished solid-state physicist specializing in magnetic materials, widely recognized for his significant contributions to the understanding and development of compounds with unique structural, electronic, and magnetic properties. His research spans a broad spectrum of materials — from the ternary phosphides and arsenides investigated in his doctoral work to the magnetic oxides he has synthesized through diverse preparation routes, including solid-state reaction and sol–gel methods.

In recent years, Professor Dhahri's research has focused on ferrites, manganites, cobaltites, and related oxides exhibiting promising multifunctional properties for advanced applications such as magnetic refrigeration, gas sensing, and photovoltaics. A highly productive and internationally engaged researcher, he has established numerous collaborations worldwide and co-authored more than 500 scientific papers, which have been cited over 11,000 times (h-index: 54). He is frequently invited to deliver lectures at international conferences and serves as a respected and active referee for leading scientific journals and research projects.

# Impact of Preparation Method on the Functional Properties of Metal Oxides for Technological Applications

Essebti DHAHRI

Laboratory of Applied Physics

Magnetic refrigeration is an emerging field of research that offers an environmentally friendly and cost-effective alternative to conventional cooling technologies. Cooling plays a vital role in numerous applications, such as air conditioning, industrial and domestic refrigeration, as well as food preservation and medical storage. Current systems mainly rely on gas compression–expansion cycles involving greenhouse gases, which contribute to global warming. To overcome this limitation, new approaches are being explored to design systems with high energy efficiency and low environmental impact. Among these, magnetic refrigeration near room temperature appears as a promising technology, capable of achieving efficiencies 20–30% higher than those of conventional systems while remaining economically competitive. Considering the growing energy demand associated with refrigeration technologies (air conditioning, freezing, cryogenics, gas liquefaction, etc.), the adoption of such low-energy-consumption technology could lead to significant energy savings. The main challenges today lie in the development of new functional materials and in understanding the underlying physical phenomena. Addressing these issues requires both fundamental and applied research efforts within a multidisciplinary framework involving physicists, chemists, and materials engineers. The design of new materials with properties relevant to energy and environmental applications is central to this effort. Combining elements with distinct chemical characteristics can induce new functionalities, paving the way for multifunctional materials. In this context, precise control of the synthesis and processing methods is a crucial step.

The present work falls within this research theme. It aims to deepen the study of the magnetocaloric properties of various phases already investigated in the laboratory (materials based on rare earths, transition metals, manganites, ferrites, etc.). The objective is to examine the influence of rare-earth and/or transition-metal substitutions, as well as oxygen vacancies, on the structural, magnetic, and electronic properties. The study combines experimental investigations with *ab initio* electronic structure calculations in order to better understand the parameters governing the magnetocaloric effect and to identify optimization strategies for applications operating near room temperature.

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| **A. Achech**, H. Zrida, R. Yu Kyoug, A. Haj Said, J.M. Rodrigo<br>*FSM - Monastir*<br>Synthesis of LIG-MOF composite materials for supercapacitor application | **OC 05C** |
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| **F. Agouillal**, I. Laoufi, T. Chaabane<br>*CRAPC, Tipasa, Algeria*<br>Modeling, optimizing and mechanistic study of the CR-401 catalyst behaviour in naphtha continuous catalytic reforming using artificial neural networks | **OC 13C** |
| **H. Ajari**, K. Hidouri, M. Romdhan, B. Chaouachi<br>*ENIG - Gabès*<br>Harnessing recycled polymers for high-performance microporous membranes in sustainable water treatment | **OC 21A** |
| **N. Akremi**, A. Rayes, I. Ayed<br>*FSG - Gabès*<br>Guanidinium-templated cubic Keggin crystals via reflux: Full spectroscopic profiling and photocatalytic activity | **OC 01C** |
| **W. Amairia**, M. Mezni, N. Hamdi<br>*CNRSM - Borj Cédria*<br>Removal of toluene from waster using high quality zeolite prepared from clay minerals. | **OC 22A** |
| **H. Ammari**, M. Chemingui, V. Optasanu<br>*FSS - Sfax*<br>Influence of spark plasma sintering parameters on the microstructure, mechanical and tribological properties of air-milled aluminum | **OC 26A** |
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| **N. Aroua**, M. Boukhris, S. Choura, M. Chamkha, R. Ben Salem, G. Rigane<br>*FSS - Sfax*<br>High-performance liquid chromatography analysis of phenolics in Casuarina glauca: Extraction, quantification, and antioxidant evaluation | **OC 01A** |
| **G. Baaboura**, K. Zehani, H. Maghraoui Meherzi, T. Ben Nasr, N. Bousserrhine<br>*FST - Tunis*<br>Design of PEGyllated CuNi nanoalloys with enhanced antibacterial efficiency | **OC 24A** |
| **S. Bellali**, H. Kahri, P.K. Jha, H. Barhoumi, C. Kvarnström<br>*FSM - Monastir*<br>Electrochemical performance of PEDOT–ZIF-8 composite electrodes for symmetric supercapacitors in neutral aqueous electrolytes | **OC 08C** |
| **H. Ben Abid**, A. Mechria<br>*FSG - Gabès*<br>Synthesis, structural characterisation, Hirshfeld surfaces and RDG-NCI analyses of new thiophene-based azomethine ligands | **OC 19C** |
| **N.E. Ben Ammar**, A.H. Hamzaoui<br>*CNRSM - Borj Cédria*<br>Etude de l'impact de l'intégration de polymère recyclé sur les propriétés de la matières plastique en vue de son utilisation dans l'injection des pièces automobiles | **OC 15B** |
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| **W. Ketir**, M. Trari, A. Amrane<br>*Houary Boumediane University, Algiers, Algeria*<br>Photocatalytic reduction of Cr(IV) on the $CuCrO_2$/ZnO heterojunction | **OC 20A** |

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| **L. Mekahlia**, Y. Hadef, S. Alleg, A. Merah, A.D. Lalaouna, A. Labouiz<br>*Badji Mokhtar University; Annaba, Algeria*<br>Eco-designed green synthesis of hydroxyapatite-magnetite nanocomposites assisted by carbohydrate-based agents: Influence of the saccharide type on structure and magnetism | **OC 08B** |
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| **Y. Moumen**, K. Hassine, K. Hriz, E. Deniau, H. Baroumi<br>*FSM - Monastir*<br>Triazole-functional conjugated polymers for metal-ion sensing: Synthesis and photophysical properties | **OC 21B** |

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| **A. Souemti**, A. Jraba, L. Latrous, A. Megriche<br>*FST - Tunis*<br>Nanomaterials based on molybdenum trioxide ($MoO_3$): Pioneering new strategies for environmental remediation and energy storage | **OC 06B** |
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| **S. Walha**, H. Naïli<br>*IPEIG - Gabès*<br>Structure-activity relationship of organic salts: Synthesis, photonic properties, and biomedical potential | **OC 10B** |
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# Abstracts of Oral Communications

# Program of Monday 22 December 2025

# High-Performance liquid chromatography analysis of phenolics in *Casuarina glauca*: Extraction, quantification, and antioxidant evaluation

Nourhene Aroua [a], Maher Boukhris [b], Sirine Choura [c], Mohamed Chamkha [c], Ridha Ben Salem [a], Ghayth Rigane [a,d]

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*Casuarina glauca*, a member of the Casuarinaceae family, is an underexplored species with potential pharmacological and ecological importance. In this study, the bioactive compounds of leaves, stems, fruits, and seeds of *C. glauca* collected from Djerba (Tunisia) were investigated using maceration and ultrasound-assisted extraction (UAE) techniques. The obtained aqueous extracts were analyzed by high-performance liquid chromatography coupled with a diode array detector (HPLC-DAD) to identify and quantify phenolic and flavonoid compounds. Fifteen metabolites were identified, including eight phenolic acids, six flavonoids, and one phenylethanoid glycoside. Catechin was the most abundant compound, particularly in the leaf extract (139.7 mg/mL). The UAE method yielded the highest total phenolic (17.53 mg GAE/g DW) and flavonoid contents (15.43 mg QE/g DW), as well as the strongest antioxidant activity in DPPH and FRAP assays. These findings provide the first phytochemical characterization of *C. glauca* from Tunisia and highlight its potential as a rich natural source of antioxidant compounds for green pharmaceutical and nutraceutical applications.

**Key words:** *Casuarina glauca*, phenolic compounds, HPLC-DAD, maceration extraction, Ultrasound-assisted extraction, antioxidant activity

# Optimized Ultrasound-Assisted Extraction and HPLC-DAD Profiling of Bioactive Phenolics from *Cucumis metuliferus*

Wala Ben Amor [a], Wissal Ayouni [a], Sinine Choura [b], Mohamed Chemkha [b], Ridha Ben Salem [a], Ghayth Rigane [a,c*]

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This work investigated the optimization of ultrasound-assisted extraction (UAE) of phenolic compounds from the peel and pulp of *Cucumis metuliferus* (Kiwano) grown in Tunisia. Response surface methodology (RSM) was applied to maximize total phenolic and flavonoid contents and antioxidant activities, measured by FRAP and DPPH assays. A central composite design (CCD) examined the influence of extraction time (6.59–23 min), temperature (33.18–66.81°C), and liquid-to-solid ratio (13.18–46.81 mL/g). Optimal conditions for pulp extraction were 30 min, 50°C, and a solvent-to-solid ratio of 30 mL/g. HPLC-DAD analysis identified gallic acid, chlorogenic acid (as the main compound), and caffeic acid as predominant phenolics in the peel extracts. The results highlight an environmentally friendly and efficient extraction approach, suitable for industrial applications and contributing to the valorization of *Cucumis metuliferus* as a source of antioxidant-rich compounds.

**Key words:** *Cucumis metuliferus*, phenolics, antioxidant activity, HPLC-DAD

# Co-modified H-ZSM-5 zeolites with Fe and Mn metals for excellent VOCs catalytic oxidation at low-temperatures: Synergistic effects and catalytic mechanisms.

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The development of catalysts with high adsorption and low-temperature catalytic characteristics for the decomposition of volatile organic compounds (VOCs) is of great importance for air purification. Herein, H-ZSM-5 zeolite supported Fe-Mn elements were synthesized via a two-step procedure. These zeolite-supported bimetal Fe-Mn catalysts exhibited a mesoporous structure, uniform distribution of Fe-Mn elements, excellent catalytic oxidation capacity for toluene at low-temperatures, and high stability. Due to interactive synergies between the bimetallic Fe and Mn, the $Fe_2$-$Mn_1$/H-ZSM-5 (ratio of Fe and Mn was 2:1 with a total amount of 15 % to H-ZSM-5) exhibited 100 % tolueneconversion at 200°C and $T_{90}$ = 195°C with GHSV = 20,000 mL/(g•h). Its distinguishing catalytic oxidation abilities at low temperatures were due to abundant oxygen vacancies, adequate acidic-sites and various active oxygen-species, which improved the adsorption of toluene and expedited its degradation. The $Fe_2$-$Mn_1$/H-ZSM-5 catalyst also demonstrated a good resistance to humidity and renewable catalytic properties over five cyclic tests. The in-situ DRIFTS and LC-MS results revealed that toluene was decomposed to benzyl-alcohol, benzaldehyde, benzoate-acid, formates or/and acetate step by step, and finally $CO_2$ and $H_2O$. The mechanism of toluene oxidation over $Fe_2$-$Mn_1$/H-ZSM-5 catalysts was proposed and elucidated via the Mars-van-Krevelen (MVK) model. This study comprehensively explored the adsorption and decomposition kinetics of VOCs over bimetal decorated H-ZSM-5, which was useful toward the design of highly efficient catalysts for the removal of VOCs.

**Keywords:** H-ZSM-5 zeolites, Bimetal Fe-Mn, Catalytic activity, Toluene, Stability.

# Dissolution Enhancement of Indapamide in Binary and Ternary stable Combinations with Perindopril and Amlodipine Drugs in Oral Tablets.

Sami JEBALI, Sana YAKOUBI, Galai HAYKEL

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Management of hypertension often requires a combination therapy approach, with fixed-dose formulations supporting patient adherence for better outcomes. However, some challenges need addressing concerning their solubility, the limitations posed by dissolution rates, and the possible drug-drug interaction, the key obstacles in optimizing the efficacy and the stability of these formulations. This study evaluates the physicochemical stability and solubility enhancement of indapamide in mono formulation as well as the combined form with perindopril and amlodipine. A rapid UPLC-DAD method was established and validated for profiling dissolution across three media mimicking physiological pH: 1.2, 4.5, and 6.8. Infrared Spectroscopy (FT-IR) and Differential Scanning Calorimetry (DSC) techniques were utilized to assess physical and chemical stability while molecular docking simulations offered insight into drug-drug interactions as well as toxicity risks associated. For solubility enhancement and bioavailability improvement of indapamide, two amorphization techniques, quench cooling and milling, were investigated. The relative bioavailability was notably increased with the co-formulation of indapamide (BCS II) with perindopril (BCS III) and amlodipine (BCS I); in conjunction, stability studies assessed that no significant degradation or adverse interaction has taken place. Computational modeling elaborated on the contributions of hydrogen bonding and hydrophobic interactions to a combined formulation stability and pharmacokinetic behavior. These will provide insight necessary for a rational design of fixed-dose combinations for the treatment of hypertension: enhanced bioavailability, stability, and therapeutic efficacy.

**Key words:** Indapamide, Perindopril, Amlodipine, Stability, Dissolution profile, Molecular interactions, Toxicity predictions.

# Development of a Synergistically Co-Doped Pt–S–g-$C_3N_4$ Photocatalyst for Efficient Hydrogen Generation under Visible Light

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Advancing solar-driven hydrogen production requires the engineering of photocatalytic systems that simultaneously deliver high conversion efficiency, long-term operational stability, and cost-effectiveness—criteria rarely achieved in conventional materials. This work introduces a synergistically optimized photocatalyst for visible-light-driven hydrogen evolution, based on platinum-loaded, sulfur-doped graphitic carbon nitride (Pt–S-g-$C_3N_4$). Comprehensive characterization revealed a pronounced interaction between Pt and S dopants, which effectively addressed the limitations of pristine g-$C_3N_4$ and conventional Pt–g-$C_3N_4$ systems. The material was synthesized via thermal polycondensation of melamine, urea, and thiourea, followed by platinum deposition using the incipient wetness impregnation method. Anisyl alcohol and benzyl alcohol (0.05 M) served as sacrificial agents to facilitate $H_2$ evolution. Sulfur incorporation promoted uniform Pt dispersion, increased specific surface area, improved hydrophilicity, and enhanced charge carrier separation. Compared to Pt–g-$C_3N_4$, the Pt–S–g-$C_3N_4$ composite exhibited a 150% increase in $H_2$ production rate, with activity reaching 1.5 times higher under both AA and BA conditions. Elemental mapping and band structure analyses confirmed the role of sulfur in narrowing the bandgap, suppressing electron–hole recombination, and optimizing the reduction potential for $H^+$ protons. These findings underscore the potential of Pt–S–g-$C_3N_4$ as a robust and efficient photocatalyst for solar-driven hydrogen generation and contribute to the rational design of doped carbon nitride systems for sustainable energy applications.

**Key words:** Pt-S-g-$C_3N_4$, $H_2$ production, Pt dispersion, visible light, aromatic alcohols

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# Removal of antibiotic tetracycline by heterogeneous electro-Fenton process using a magnetic $Fe_3O_4$@UiO-66 composite as sustainable catalyst

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Antibiotic contaminants in water pose a significant environmental challenge [1], requiring effective treatment solutions. Although electro-Fenton (EF) effectively degrades these pollutants [2], its implementation is constrained by the generation of iron sludge and the requirement for low pH settings. Herein, we synthesized a new $Fe_3O_4$@UiO-66 composite and evaluated its performance in the heterogeneous EF (HEF) method for the removal of tetracycline (TC) from aqueous solutions. TC could be nearly eliminated entirely after 0.5h, and the total organic carbon (TOC) removal efficiency exceeded 99% within 4 h. The $Fe_3O_4$@UiO-66 catalyst exhibited remarkable stability and reproducibility, sustaining approximately 87% of TC removal efficiency after 10 cycles. It demonstrated efficacy in many water matrices, such as tap and lake water, showing its flexibility to natural environmental conditions. Furthermore, the examination of energy consumption revealed that the optimal conditions for TOC reduction concurrently minimized consumption of energy, offering the $Fe_3O_4$@UiO-66/EF process a promising and economical method for wastewater treatment.

**Key words:** $Fe_3O_4$@UiO-66 catalyst; Heterogeneous electro-Fenton; Tetracycline; Water remediation; Stability.

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# Photocatalytic Degradation of Ciprofloxacin Using a $BiFeO_3/TiO_2$ Heterostructure with Peroxymonosulfate Activation

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The widespread presence of the antibiotic ciprofloxacin (CIP) in aquatic environments poses a significant ecological threat due to its persistence and low biodegradability. This work investigates the enhanced photocatalytic degradation of CIP using a $BiFeO_3/TiO_2$ heterostructure, activated by peroxymonosulfate (PMS). The $BiFeO_3/TiO_2$ composite was synthesized via the sol-gel method and its performance was evaluated under both UV and visible light irradiation. The synergistic combination of the heterostructure and PMS resulted in the highly efficient generation of reactive oxygen species, primarily sulfate ($SO_4^{\bullet -}$) and hydroxyl ($OH^{\bullet}$) radicals, leading to superior CIP degradation. Remarkably, the system demonstrated near-identical degradation efficiency under visible light compared to UV irradiation, highlighting the catalyst's effective utilization of solar energy. Control experiments confirmed the essential role of both light irradiation and the catalyst in the oxidation process. The high performance under visible light underscores the potential of the $BiFeO_3/TiO_2$/PMS system as a sustainable and energy-efficient advanced oxidation process for the remediation of organic pollutants in water.

**Keywords:** Photocatalysis, Heterostructure, $BiFeO_3/TiO_2$, Ciprofloxacin, Peroxymonosulfate, Advanced Oxidation Processes, Water Treatment.

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# Removal of Reactive Violet and Bemacid Yellow dyes from aqueous solutions by adsorption onto activated carbon.

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Water is the main constituent of biological matter, making up roughly 70% or more of living organisms. The importance of water as a fundamental requirement for life is continually emphasized worldwide. As a heavily polluting industry according to the Central Pollution Control Board, the textile industry is the principal source of dye pollution and has become a key area of focus for industrial wastewater solution [1]. Indeed, the rapid expansion of industrialization has led to a sharp increase in the global demand for textile products. Consequently, the textile industry has substantially increased its wastewater discharge, posing a significant threat to environmental safety worldwide [2].

Activated carbon prepared from human hair using potassium carbonate ($K_2CO_3$) as an activating agent was evaluated for its efficiency in adsorbing the textile dyes *Reactive Violet* and *Bemacid Yellow* from aqueous solutions. The study examined the effects of contact time, initial dye concentration, and solution pH on adsorption performance.

The activated carbon was characterized by Fourier-transform infrared spectroscopy (FTIR) to identify its surface functional groups, and its adsorption behavior was systematically assessed [3]. The results indicated that the material exhibits strong potential for removing both dyes from solution. Adsorption equilibrium was reached within 1 hour, with maximum removal efficiencies of 45.31% for *Reactive Violet* and 65.87% for *Bemacid Yellow*. The adsorption capacity increased with rising initial dye concentration, and the optimal removal occurred at pH 6 for both dyes.

**Key words:** adsorption, textile dye, activated carbon, bemacid yellow, reactive violet.

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# Electrochemical platform based on functionalized MXENE for simultaneous sensing of pesticides

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The growing concerns over environmental and health impacts from pesticide contamination highlight a critical need for advanced sensors that are both rapid and precise. In response, this work presents a novel electrochemical sensor built on MXENE nanocomposite and transition metal dichalcogenide nanomaterials, integrated onto a screen-printed electrode [1-2]. The successful construction of this nanomaterial was confirmed through a detailed characterization process using Raman spectroscopy, SEM, XRD, and electrochemical methods, which also verified its enhanced electrochemical properties.

The resulting sensor demonstrated exceptional performance, detecting the target pesticide at nanomolar concentrations with high specificity. It also proved to be robust, showing remarkable storage stability and consistent results with a repeatability of 3.7% RSD. When applied to real-world samples, the sensor delivered accurate results, achieving a recovery rate as high as 98.3%. These compelling findings indicate that the proposed composite material is a highly promising foundation for a new class of electrochemical sensors, with potential for broad use in safeguarding environmental health and ensuring food safety.

**Keywords:** MXENE nanocomposite, Pesticide detection, Electrocatalysis, food and environmental monitoring, Portable sensor.

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# Optimization and Modeling of Photocatalytic Degradation of anionic Dye Using Co/ACBH Catalyst

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The methodology of experimental design was employed to model and enhance the operational parameters for the photocatalytic degradation of the azo dye Congo Red (CR) using the synthesised heterogeneous catalyst Co/ACBH. The heterogeneous catalyst was prepared by a simple impregnation method of activated carbon. The activated carbon and the synthesised Co/ACBH catalyst were characterized by using several techniques such as BET, XRD, FT-IR and SEM-EDX. Three experimental parameters were chosen as independent variables : the catalyst mass, the Congo Red concentration, and the pH solution. A Response Surface Methodology (RSM), specifically Box–Behnken design, was employed to create a quadratic model that describes the functional relationship between the efficiency of CR degradation (response) and three independent variables. The original dye concentration and pH had a major impact on the degradation efficiency. Based on the statistical data, the best conditions for the removal of CR dye from aqueous solution by the prepared Co/ACBH catalyst were: the mass of the catalyst 0.3 g, the CR dye concentration 50 mg/L, and the pH of the solution 3. Under optimal conditions, the degradation performance was at 97 %. A regression analysis revealed a significant connection between the experimental data and the expected values, with an R 2 value of 0.998. The regeneration experiments proved that the resulting Co/ACBH catalyst still had a high removal capacity for Congo Red dye after three regeneration cycles.

**Keywords:** Dye removal; photo-Fenton process; Activated carbon; photochemical oxidation; anionic dye

# Quantitative Analysis of Absorption and Refractive-Index Modulation in Oxidatively Coated Quantum Dots under Thermal and Pressure Stimuli

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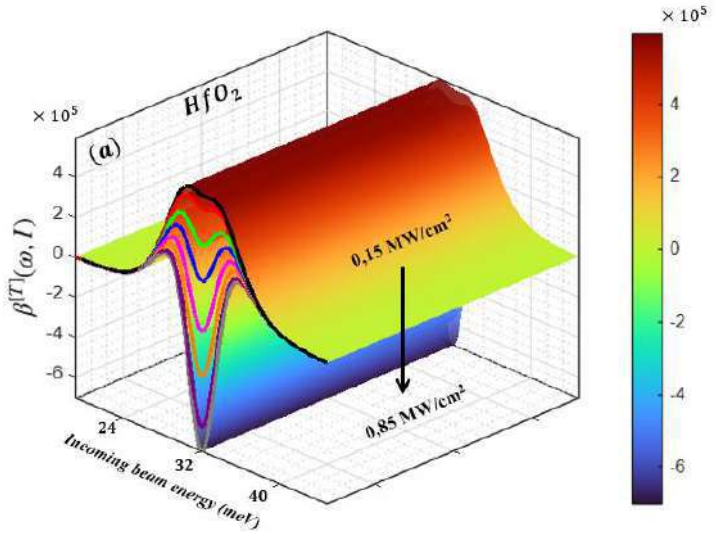
Contemporary studies seek to elucidate and model, through mathematical frameworks, the optical response of quantum dots (QDs) in oxidative environments, with emphasis on the total absorption coefficient and refractive index. These optical parameters are highly sensitive to variations in particle size, composition, surface states, electric field strength, impurity content, and surrounding conditions. Oxidative reactions can significantly reshape the electronic landscape of QDs by redistributing carrier wavefunctions, while controlled modifications of shell or core dimensions enable precise adjustment of electronic energy levels and, consequently, light–matter coupling efficiencies. Furthermore, temperature and pressure represent additional key parameters that must be incorporated into modeling approaches, as they can strongly modulate both structural and electronic properties of QDs.




**Keywords:** Core/shell QDs, Dielectric medium, Local field effects, Effective Mass Approximation and Compact density approch.

# Probing Noncovalent Interactions in Organic–Inorganic Hybrid Materials: Computational DFT-Based Approaches

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The rational design of organic–inorganic hybrid materials depends critically on understanding the noncovalent interactions that govern their structure, stability, and functionality. These interactions-often subtle yet decisive-can be effectively characterized using quantum chemical methods. In this work, we apply dispersion-corrected density functional theory (DFT-D), alongside topological and orbital-based analyses such as the Quantum Theory of Atoms in Molecules (QTAIM), Independent Gradient Model (IGM), and Natural Bond Orbital (NBO) analysis, to investigate the noncovalent landscape in a series of class I hybrid materials. Our case studies include discrete chlorometallates of cobalt(II), cadmium(II), and iron(III), paired with organic ammonium cations. These systems are ideal candidates for showcasing how noncovalent interactions-hydrogen bonding, electrostatics, dispersion, and weak orbital delocalization-shape supramolecular architecture and influence material properties. This integrated computational strategy provides a rigorous and multifaceted view of interaction mechanisms, reinforcing the central principle that *structure determines properties* in hybrid systems. The findings advance our understanding of structure–property relationships and demonstrate the utility of modern DFT-based techniques in materials research.

**Keywords:** Organic–Inorganic Hybrids, Noncovalent Interactions, Computational Chemistry, dispersion-corrected DFT-D

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# Peroxidase-Like Activity of Nanostructured Spinel Ferrites Synthesized by Auto-Combustion: Structural and Kinetic Investigations

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The development of efficient and stable nanozymes represents a promising alternative to natural enzymes for catalytic and environmental applications. In this work, nanostructured spinel ferrites ($MgFe_2O_4$) was synthesized via a low-cost auto-combustion method using glycine as a fuel [1]. The structural, morphological, and textural properties of the as-prepared materials were investigated using X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), UV–Vis spectroscopy, scanning electron microscopy (SEM), and nitrogen adsorption–desorption (BET) analyses. The results confirmed the formation of highly crystalline spinel ferrites with mesoporous sponge-like morphology and specific surface areas up to ~12 $m^2/g$ [1].

The catalytic performance of the ferrite nanoparticles was evaluated through their peroxidase-like activity using o-phenylenediamine (OPD) as a chromogenic substrate in the presence of $H_2O_2$. Kinetic studies were performed at different pH values (1-12), and the results were analyzed using Michaelis–Menten and Lineweaver–Burk models. $MgFe_2O_4$ exhibited significant catalytic activity, with high correlation coefficients ($R^2 \approx 0.97$), confirming its potential as robust peroxidase mimics. The activity was found to be strongly pH-dependent, with enhanced reaction rates under acidic conditions.

These findings highlight the efficiency and versatility of nanostructured ferrites as nanozymes for potential use in biosensing and wastewater treatment applications. Future work will focus on integrating these ferrites with functional organic matrices to develop hybrid catalytic systems.

**Key words:** Spinel ferrites, nanozymes, peroxidase-like activity, auto-combustion synthesis, Michaelis–Menten kinetics, environmental catalysis

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# Synthesis, characterization, and antibacterial evaluation of $BiFeO_3/BaTiO_3/SrTiO_3$ ternary nanocomposites

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This study reports the synthesis, structural and physico-chemical characterization, and antibacterial evaluation of compositionally tuned $BiFeO_3/BaTiO_3/SrTiO_3$ (BFO/BTO/STO) ternary nanocomposites. The BFO/BTO/STO ternary nanocomposite was synthesized via a sonochemical route and characterized using XRD, FTIR and SEM. The antibacterial activity of the ternary nanocomposite was evaluated against two different bacteria: Staphylococcus aureus (S. aureus) and Escherichia coli (E. coli) [1,2]. A greater inhibition rate was observed for S. aureus, and thus, the BFO/BTO/STO ternary nanocomposite demonstrated higher antibacterial activity against S. aureus than E. coli. These findings highlight the potential of BFO/BTO/STO ternary nanocomposite as a promising material for antibacterial applications.

**Key words:** Antibacterial activity, perovskites, ternary nanocomposite, $BiFeO_3/BaTiO_3/SrTiO_3$

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# Study of the DC sputtering power effect on its electrical properties of Ag/AlN/Si Schottky diode

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The DC sputtering power (DCSP) effect on the chemical composition, structural and electrical properties of Ag/ AlN/Si Schottky diode was studied. The AlN films grown on Si substrate were examined by X-ray diffraction (XRD), Fourier Transformed Infra-Red (FTIR), and Raman spectroscopy. The analyzes by XRD, FTIR and Raman show stability at the level of the structure and the qualitative chemical composition of the AlN layer for DCSP of 200 W and 400 W. However, the quantity of chemical compounds on the surface of AlN is affected by this variation. From Current-Voltage (I-V) measurements, the ideality factor (n), barrier height (φb), and series resistance (Rs) were extracted by adopting Cheung functions.

**Key words:** DC sputtering power, Ag/ AlN/Si, Schottky diode, Current-Voltage (I-V) measurements.

# ZnO nanoplates as efficient antibacterial agents under dark and UV conditions for aqueous applications

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Zinc oxide (ZnO) nanomaterials are promising disinfectants for controlling harmful pathogens that affect health and the environment. In this study, ZnO nanoparticles (NPs) with plate-like shapes were synthesized by a simple, eco-friendly, and low-cost co-precipitation method. Their antibacterial activity was tested in water against two Gram-negative and two Gram-positive bacteria, both in the dark and under UV-A light. The ZnO NPs showed complete (100%) antibacterial efficiency at a very low concentration of 0.5 mg/mL. This strong effect is related to their shape, small size, and optical properties. The nanoplates damage bacterial membranes through surface abrasion and by producing reactive oxygen species (ROS), which destroy key cell components such as DNA, proteins, and lipids. The results show that these green-synthesized ZnO nanoplates are effective antibacterial agents with great potential for biomedical and food packaging applications.

**Key words**: Zinc oxide nanoparticles, antibacterial activity, reactive oxygen species (ROS), green synthesis

# Physical Properties of Multifunctional $Zn_{(1-3x)}Eu_{2x}O$ Nanoparticles: Microstructural, Optical Band-gap and Dielectric Characterizations

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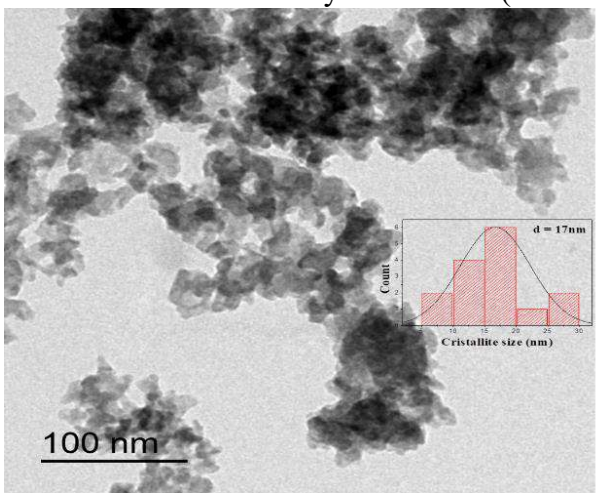
Using the concept of nucleation doping, zinc oxide (ZnO) nanoparticles were successfully prepared in aqueous phase at 80 °C for a weight percent (10%) doping and characterized by X-ray diffraction, transmission electron microscopy to determine the morphology of the obtained nanoparticles, analyzed by X-ray photoelectron spectroscopy (XPS) and FT-IR spectroscopy [1]. The energy difference (Eg) of the samples was estimated by means of the UV-visible technique by application of the Tauc equation. In addition, the electrical properties and relaxation phenomena are identical. Elliott was the first to introduce the "conductivity spectrum", which he successfully explained with the "jump correlated barrier" model. These spectra of the material obtained at different temperatures are determined by Bruce's law (double power of Jonscher) [2]. The study of the electrical conductivity in continuous mode reveals the semiconducting (SC) character of the nanoparticles. The conductivity of the SC is activated by a hopping phenomenon of small polarons at high temperature. The contribution of conductive grains and resistive boundary regions to the ZnO/Eu transport phenomena is explained by the Nyquist configuration.




**Key words** Nanoparticle, Eu doping ZnO, optical properties, electrical conductivity.

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# Nanomaterials Based on Molybdenum Trioxide ($MoO_3$): Pioneering New Strategies for Environmental Remediation and Energy Storage

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Due to their tunable physicochemical properties, $MoO_3$-based nanocomposites show promise for environmental and energy applications. This study describes the synthesis of $MoO_3$@MgO and $MoO_3$@$SnO_2$ n-n heterojunctions using a solvothermal method. Both semiconductors exhibit band gaps of approximately 2.7 eV and moderate low-temperature conductivity, which is governed by thermal electron-hole junction formation.

The environmental efficacy of the nanocomposites was demonstrated by the degradation of Rhodamine B (RhB) achieving complete degradation within 135 minutes, and following pseudo-first-order kinetics. With a higher kinetic constant of 0.0348 $min^{-1}$, $MoO_3$@MgO shows superior potential for environmental remediation and intermediate-temperature electrochemical devices such as solid oxide fuel cell electrolytes. In contrast, $MoO_3$@$SnO_2$ is better suited to chemoresistive gas sensors operating at 200–400 °C.

**Key words:** Composites, Heterojunctions, Solvothermal method, Kinetic analysis, Electrical properties

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# QbD Approach During Formulation and Stability Testing of an Unstable Polymorphic API During Tablets Direct Compression, A Combined Method Using Mathematical Modeling.

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In recent years, several generic carbamazepine drugs have had to be withdrawn from the global market due to their ineffectiveness (polymorphic transformation). Through the extensive literature review we conducted during our work, we realized that pharmaceutical operations have a dramatic influence on the polymorphism of this molecule.
We therefore needed to control the pharmaceutical operations leading to the manufacture of an effective generic drug in tablet form. Knowing that the most likely form is carbamazepine dihydrate, we developed an experimental protocol to prevent the appearance of this form, direct compression have been chosen for tablet manufacturing to limit the pharmaceutical operations. Carbamazepine was grinded and then mixed with microcrystalline cellulose, an excipient known for its ability to absorb water and therefore to protect the carbamazepine from its transformation into dihydrate form. To prepare the physical mixtures of carbamazepine – microcrystalline cellulose, we opted for a QbD approach were the Critical Process Paramrameters (CPPs) were the percentage of microcrystalline cellulose and the particle size class of carbamazepine and the Critical Quality Attributes (CQAs) were the percentage of dissolution before and after 6 months of stability under accelerated conditions. To complete the experimental design, a weibul model was used to compare the he dissolution rate of the different trials as well as that of the reference product (Tegretol). the optimum parameters were then used to manufacture carbamazepine generic tablets, the dissolution percentage have been evaluated for both the generic and the reference, and each product have been characterized by FTIR and DSC, the mathematical modeling of the dissolution profiles using a modified Noyes-Whitney equation have been used to understand the behavior of carbamazepine in contact with the dissolution medium (aqueous medium). We obtained an optimum dissolution for a carbamazepine particle size class between 72 and 100 µm and 28% microcrystalline cellulose; this optimum was intended for tablet manufacturing, but the particle size class was not suitable for compression because it exhibited very poor flow. Combining the results of experimental design and weibull model, an optium have been found at the API particle size class >100 µm and 40% of microcrystalline cellulose. The formulated generic tablet using this optimum showed amaximum dissolution rate (86%) after 60 minutes, the curves of the percentage of carbamazepine dissolved from the tablets before and after stability overlap, which indicates good stability of the tablet. We observe the same peaks between the IR spectrum of the reference and the IR spectrum of the generic tablet, which proves the stability of carbamazepine before and after pharmaceutical operations. A transition temperature of 175.9°C is observed, followed by a recrystallization peak of form I, while the second peak corresponds to the melting of form I at a temperature of 195.9°C. This demonstrates that carbamazepine does not undergo irreversible changes after pharmaceutical processing. The mathematical modeling allowed to estimate the initial solubility (metastable form), which is virtually and impossible to determine experimentally due to the transition over time to the stable form (hydrate); and secondly, the recrystallization constant of the active ingredient, which can provide information about the rate of recrystallization.

**Key words:** Polymorphism, QbD, Experimental design, Mathematical modeling

# Eco-designed Green Synthesis of Hydroxyapatite–Magnetite Nanocomposites Assisted by Carbohydrate-Based Agents: Influence of the Saccharide Type on Structure and Magnetism

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The integration of green chemistry principles into the design of functional inorganic materials represents a major challenge for modern solid-state chemistry. This work proposes an eco-designed approach for the green synthesis of hydroxyapatite–magnetite (HAp–$Fe_3O_4$) nanocomposites, using natural carbohydrate-based agents (fructose, galactose, and pectin) acting as reducing, complexing, and stabilizing agents. The synthesis relies on an aqueous co-precipitation process followed by moderate thermal treatment, during which these agents control cation complexation, nucleation, and particle dispersion. Characterization by X-ray diffraction (Rietveld refinement), FTIR spectroscopy, SEM–EDS, and vibrating sample magnetometry (VSM) revealed that the type of carbohydrate strongly influences the structure and magnetic properties. Fructose promotes the formation of well-crystallized hydroxyapatite, whereas galactose and pectin lead to partially carbonated apatites. The $Fe_3O_4$ domains exhibit a quasi-superparamagnetic behavior, characterized by low coercivity and remanence, indicating homogeneous dispersion of the magnetic particles. This study demonstrates a clear correlation between carbohydrate nature, crystalline organization, and magnetic response, highlighting that saccharide-assisted synthesis constitutes a sustainable and efficient strategy for designing biocompatible nanocomposites applicable to drug delivery and biomedical fields

**Key words:** Green chemistry, Hydroxyapatite–magnetite, Carbohydrate-based agents, Structure–property correlation, Magnetic nanocomposites.

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# Raman of 2D-$MoS_2$: Disentangling The Metallic Phase Conundrum

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Two-dimensional Molybdenum disulfide (2D-$MoS_2$) is thermodynamically stable and hence easily synthesized in its semiconducting 2H phase. In contrast, the metallic-phase 1T-$MoS_2$ is a highly sensitive, metastable and complex phase that is not naturally occurring. This heightened sensitivity and instability has resulted in a widespread misrepresentation in academic literature. Based on our current understanding, the majority of Raman investigations incorrectly identify the spectrum of $MoO_3$ as 1T-$MoS_2$ due to the samples oxidation when exposed to intense laser irradiation in the presence of air, as commonly performed.

Therefore, this work focuses on conducting a comprehensive Raman analysis of 1T-$MoS_2$ by investigating the impact of oxidizing atmosphere, laser power, irradiation time, and temperature changes on the sample. Controlling the Raman conditions has allowed us to introduce a novel spectrum that signifies a new phase triggered by laser heating. This has led to further confusion in the identification of the metallic $MoS_2$ polymorphs.

This study seeks to expose the current challenges in characterizing the metallic phase of $MoS_2$, especially when using Raman spectroscopy, which till now was considered the most reliable technique for this purpose. Our results provide guidance to the next experimental Raman studies and possible practical applications for materials engineering.

# Structure–Activity Relationship of Organic Salts: Synthesis, Photonic Properties, and Biomedical Potential

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In this work, we synthesized and characterized two salts, 1H-benzotriazolium bromide dihydrate and hexamethylenediaminium bibromide, inspired by biological compositions. Their structural and functional properties highlight promising potential for applications in the medical and pharmaceutical fields. A slow evaporation method has permitted the crystallization of the two novel crystals of 1H-benzotriazolium bromide dihydrate $C_6H_5N_3$,Br·$2H_2O$ (1) and Hexamethylenediaminium bibromide $C_6H_{18}N_2$,2Br (2). These compounds were subjected to the following characterization techniques: single crystal X-ray diffraction, FT-IR spectroscopy analysis, optical properties and biological activities. The structures of compounds (1) and (2) revealing monoclinic symmetry with space group $P2_1/c$, $C2/c$, respectively. Their crystal packing is stabilized by a network of non-covalent interactions, including N–H…Br, C–H…Br, O–H…Br and N–H…O hydrogen bonds. A 3D Hirshfeld surface analysis, complemented by 2D fingerprint plots, provided detailed insights into the intermolecular interactions within the crystalline framework. The antibacterial properties of these materials were investigated in vitro against various bacterial strains, such as *Escherichia coli*, *Pseudomonas aeruginosa*, *Klebsiella pneumoniae*, *Staphylococcus aureus*, *Bacillus subtilis* and *Enterococcus faecalis*. Their antifungal activity was also assessed using the agar disc diffusion method against *Aspergillus niger*, *Candida albicans*, and *Fusarium oxysporum*. Furthermore, the complexes exhibited significant antioxidant activity, demonstrated by their capacity to scavenge ABTS radical and their overall antioxidant potential. Molecular docking studies revealed that compounds (1) and (2) interact with bacterial DNA gyrase A and fungal chitin synthase through hydrogen bonding and π-interactions, contributing to the stability of the protein-ligand complexes.

# Investigation of Dielectric Properties of $LaNiO_3/Co_3O_4$ Nanocomposites

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This work presents an extensive examination of the dielectric characteristics, AC conductivity, electric modulus, and impedance spectroscopy of a $LaNiO_3/Co_3O_4$ nanocomposite. A modified citrate gel autocombustion process was used to create the substance.

Atomic force microscopy and transmission electron microscopy characterization revealed that the nanocomposite is made up of nonuniform nanoparticles of different sizes and shapes.

Impedance investigation confirmed the sample's semiconducting nature by revealing a negative temperature coefficient of resistance. There was only one semicircular arc in the Nyquist plot, indicating that bulk grain effects predominate.

According to Jonscher's power law, the AC conductivity was found to be dependent on both temperature and frequency, suggesting that conduction mostly happens via a hopping mechanism. A large dissipation factor that diminishes with frequency was also noted which decreased with frequency. A non-Debye relaxation type was defined for the nanocomposite.

**Key words:** $LaNiO_3/Co_3O_4$ nanocomposite, Dielectric properties, AC conductivity, Impedance spectroscopy.

# Antimicrobial activity of *Eucalyptus citriodora* fruit extracts against multi drug resistant pathogens

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**Background:** Infectious disease that affects thousands of people every day, the problem of the drugs multi-resistance and ultra-resistance has created the urgent need to find alternative anti-mycobacterial agents for the treatment of resistant pathogenic microorganisms. A large number of medicinal plants used in many researches represent an inexhaustible source of bioactive substances, which possess very important biological properties.

**Material and Methods:** For the purpose of the present study, we chose Eucalyptus citriodora among the medicinal plants for its nutritional and medical value. The aim of our work was to study the anti-mycobacterial and antibacterial properties of the methanolic extract of lemon eucalyptus seeds. The extract was tested against four strains of MTBC (*M. tuberculosis, M. bovis*), and against some Gram-positive bacterial strains (*Enterococcus feacalis, Enterococcus sp, Staphylococcus haemolyticus* and *Staphylococcus aureus*) and Gram-negative (*Escherichia coli, Pseudomonas aerogenosa*, and *Acinetobacter baumannii*) using the MIC determination method on 96-well micro-dilution at different concentrations of the extract.

**Results:** The extract showed activity against all Mycobacterium strains tested with a MIC value of 12.8mg/ml. It also showed activity against four Gram-positive strains, MIC=12.8mg/ml, and against Gram-negative strains, MIC=1.6 mg/ml. This extract could be a rich source of anti-mycobacterial and anti-bacterial agents, as well as

**Conclusion:** These preliminary results show a promoting interest for these extracts, which require further investigation in order to describe the exact active molecules and their structures.

**Key-Words:** Key words: anti-mycobacterial, anti-bacterial, methanolic extract, Eucalyptus citriodora

# Guanidinium-Templated Cubic Keggin Crystals via Reflux: Full Spectroscopic Profiling and Photocatalytic Activity

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Cubic hybrid crystals of $(CH_6N_3)_3[PW_{12}O_{40}]\cdot 4\ H_2O$ were grown in quantitative yield by refluxing $H_3PW_{12}O_{40}$ with guanidinium carbonate in water/acetonitrile (1 : 1, 100 °C, 3 h). Transparent cubes (edge 0.35 mm) were fully characterised.

Single-crystal XRD (150 K, Pm-3m, a = 11.9652(2) Å) locates the Keggin cluster on a crystallographic three-fold axis, wrapped by hydrogen-bonded guanidinium and four ordered water molecules. FT-IR: ν (W–$O_t$) shifts from 968 to 975 $cm^{-1}$ upon cation exchange while ν (P–$O_a$) remains sharp at 1081 $cm^{-1}$, confirming an intact α-Keggin core.

Solid-state $^{31}P$ MAS-NMR (121.5 MHz) shows a single resonance at -14.8 ppm (FWHM 1.1 ppm), identical to the parent acid, ruling out cluster degradation. $^{1}H$ MAS-NMR reveals two guanidinium protons at 6.8 and 7.2 ppm and a broad water signal at 4.1 ppm, consistent with the four lattice $H_2O$ found crystallographically.

Diffuse-reflectance UV-Vis gives a band-gap of 2.41 eV-0.3 eV narrower than $H_3PW_{12}O_{40}$-attributed to ligand-to-metal charge-transfer from the guanidinium ion. Solution UV-Vis ($H_2O$, $10^{-5}$ M) displays the characteristic Keggin O→W charge-transfer band at 258 nm ($\varepsilon = 1.8 \times 10^4$ $M^{-1}\ cm^{-1}$) with no additional features, confirming cluster integrity in solution.

Under visible-light irradiation ($\lambda \geq 420$ nm, $O_2$) the hybrid catalyses aerobic oxidation of benzyl alcohol to benzaldehyde with 88 % conversion and 95 % selectivity within 4 h (TOF = 11 $h^{-1}$), four-fold faster than the pristine HPOM.

The work establishes guanidinium carbonate as a green structure-director that affords millimetre-scale cubic POM crystals whose supramolecular contacts stabilise the cluster and engineer a visible-light-responsive surface for selective redox catalysis.

**Keywords:** Polyoxometalate; Keggin; guanidinium; cubic hybrid crystal; FT-IR; solid-state NMR; UV-Vis; single-crystal XRD; photoredox catalysis

# Crystal Structure and Spectroscopic Investigations (FT-IR, UV/Vis) of a Novel Hydrogensulfido Five Coordinate High-spin Iron(II) Picket Fence Porphyrin Complex

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In this work we have prepared the novel hydrogensulfido iron(II) picket fence porphyrin with the formula [K(2,2,2-crypt)][$Fe^{II}$(TpivPP)(SH)] (**I**) (where TpivPP is (α,α,α,α-terakis(*o*-pivalamidophenyl)(porphinato) anion and (2,2,2-crypt) is cryptand-2,2,2). The complex **I** was characterized by UV/Vis and IR spectroscopy and single crystal X-ray diffraction molecular structure. These techniques show that the complex (**I**) crystallizes in the $P2_1/n$ space group with one ion complex [$Fe^{II}$(TpivPP)(SH)]$^-$ and one counterion [K(2,2,2-crypt)]$^+$. Compound (**I**) exhibits a non-planar conformation with major *doomed* and *saddle* distortions. The average equatorial iron-pyrrole nitrogens [Fe—$N_p$= 2.107 (2) Å] bond length and the distance between the iron and the 24-atom core of the porphyrin ring [Fe—$P_C$ = 0.5744 (6) Å] are longer than those of all other similar five-coordinate iron(II) high-spin porphyrinates. This is probably due to the electronic repulsion of the $d_{x2-y2}$ and $d_{xy}$ orbitals by the negative charge of the pyrrole nitrogens. This structure, which is the first one reported on an hydrogensulfido-iron(II) porphyrin species, confirms the high-spin state of the hydrogensulfido derivative and shows that the coordination sphere of the iron atom is strongly affected by the monodentate axial ligand from the pocket side of the TpivPP porphyrin.

**Key words:** Iron(II) porphyrin complex; X-ray molecular structure; hydrogensulfido complex;

# Design, Synthesis, and Characterization of a Novel Discotic Liquid Crystal with Improved Dielectric Behavior.

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A new discotic liquid crystal, 4-DOBOB, was synthesized and thoroughly characterized to investigate its structural and mesomorphic properties. The compound was analyzed by Differential Scanning Calorimetry (DSC), Polarized Optical Microscopy (POM), FTIR, and dielectric spectroscopy. The thermal and optical studies confirmed the formation of a stable mesophase characteristic of discotic systems. To study the interactions between discotic and calamitic mesogens, mixtures of 4-DOBOB with the well-known nematic liquid crystal 4-cyano-4′-pentylbiphenyl (5CB) were prepared with different weight concentrations of 0.5, 1.0, and 1.5 wt%. The resulting mixtures were characterized using the same experimental techniques. The DSC results revealed noticeable variations in the transition temperatures and enthalpy values, while POM observations showed significant changes in the texture and mesophase range. FTIR spectra suggested possible intermolecular interactions between functional groups of the two components. Furthermore, dielectric measurements demonstrated a clear influence of 4-DOBOB on the dielectric anisotropy and relaxation behavior of 5CB. The overall findings indicate that the incorporation of small amounts of a discotic mesogen into a calamitic matrix can lead to hybrid systems with tunable thermal and dielectric properties, which may be useful for advanced electro-optical and display applications.

**Keywords:** discotic liquid crystal, 4-DOBOB, 5CB, dielectric properties, mesophase transitions, hybrid liquid crystal systems.

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# Synthesis, X-Ray Crystallography, Spectroscopic Characterization of a New Copper(I) Bis(2,2'-bipyridine) Chloride Complex

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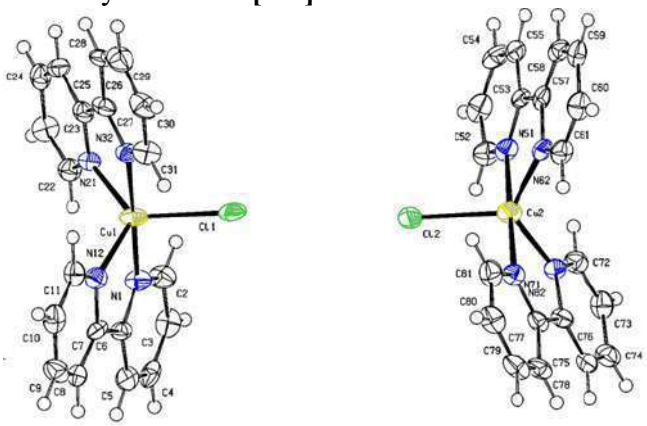
The synthesis of a copper(I) bipyridine chloride complex was successfully achieved and thoroughly investigated. Comprehensive characterization was performed using single-crystal X-ray diffraction, and various spectroscopic techniques. The crystal structure has been described in monoclinic symmetry and $P_C$ (I.T.#7) acentric space group. Cell parameters have been refined as follows: a = 12.2064(5) Å, b = 14.5937(7) Å, c=14.2523(7) Å, β = 108.650(2)°. Spectroscopic studies, including UV-Vis and IR, further validated the structural features and electronic transitions. The crystal packing is stabilized by C-H・・・N and C-H・・・Cl hydrogen bonds, forming structures. This multi-faceted approach highlights the integrative understanding of the complex's physical and chemical properties, offering potential applications in catalysis and materials science.

The photophysical and photochemical properties have led to a detailed study of the metal-2,2'-bipyridine complex and its use as a source of inspiration for the generation of inexpensive photosensitive and photocatalytic flames **[1-3]**.




Structural representation of $[Cu(Bipy)_2]Cl$

**Key words**: Copper(I) ; X-Ray ; Crystal structure ; 2,2'-bipyridine ; UV-visible.

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# Synthesis of LIG-MOF composite materials for supercapacitor application

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Supercapacitor are a promising candidate as an energy storage new generation, due to their heigh power density, fast charging, and long cycle life [1]. In this study, we present a simple and direct method for synthesizing Laser induced graphene (LIG) functionalized with metal–organic framework (MOF). These hybrid materials are highly porous crystalline compounds consisting of metal ions interconnected by organic ligands. Structural characterization confirms the successful deposition of MOF within the electrically conductive LIG surface. Therefore, this work presents an optimized set of power and scan speed laser conditions and MOF deposition time to fabricate high-quality LIG/MOF microsupercapacitors, This is achieved by correlating their structural morphology, material quality, and electrochemical performance. The fabricated devices show an increasing of the specific capacitance by up to five times compared to LIG-only electrodes (reaching values from 1.02 to 5.28 mF/cm$^2$) and high cycling stability with a capacitance retention rate of 95% after 10.000 cycles,

**Key words:** Supercapacitor, Metal Organic Framework, Laser Induced Graphene

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# Valorization of lignin extracted from *Posidonia oceanica*: From characterization to nanoparticle formation for colloidal applications

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This study focuses on the sustainable valorization of Posidonia oceanica biomass, a marine residue often regarded as coastal waste [1]. Lignin was extracted from Posidonia balls and thoroughly characterized to evaluate its physicochemical properties and potential as a natural stabilizer in Pickering emulsions. Solubility tests revealed good affinity toward polar solvents (acetone, DMSO, dioxane), while the ash content (1.8%) indicated satisfactory purity. The total lignin yield reached 20.4 %, combining soluble (7.8%) and insoluble (12.6 %) acid fractions. Boehm titration showed 5.80 mmol $g^{-1}$ of acidic functional groups, confirming high chemical reactivity. FTIR, TGA, and DSC analyses confirmed the lignin structure, thermal stability, and a glass transition at −35 °C. Lignin nanoparticles were then produced by acetone/water precipitation and characterized by DLS, zeta potential, and TEM. The average particle size ranged from 80–120 nm and decreased with increasing pH, while the zeta potential reached −36 mV at pH 9, ensuring excellent colloidal stability. These results demonstrate the potential of marine lignin as a renewable stabilizer for use in Pickering emulsion applications [2].

**Keywords:** *Posidonia oceanica*, lignin, nanoparticles, colloidal stability, sustainable valorization.

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# Program of Tuesday 22 December 2025

# Cadmium adsorption onto a composite membrane

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Cadmium contamination of water and food remains a major public-health concern due to its persistence, bio accumulative nature, and well-documented nephrotoxic and carcinogenic effects. In this study, Cellulose acetate–clay composite membranes were prepared with varying clay loadings. The adsorption process was then optimized using a Box–Behnken experimental design based on three factors: clay percentage, contact time and temperature. Batch tests on the model-predicted membranes showed an optimal formulation achieving **~94% removal** of Cd(II). Membranes were characterized by **FTIR, XRD, SEM** and **TGA**. This study demonstrates that combining inexpensive natural clays with systematic experimental design yields promising, low-cost membranes for Cd remediation.

**Keywords:** cellulose acetate membrane, clay, cadmium removal, Box–Behnken design

# Engineered Graphene Oxide for Efficient Crystal Violet Elimination: A Comprehensive Study of Adsorption Mechanisms and RSM Optimization

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The release of synthetic dyes such as crystal violet (CV) into aquatic ecosystems presents a significant environmental and public health hazard, owing to their pronounced toxicity, resistance to biodegradation, and persistent coloration that hinders light transmission and disrupts aquatic biodiversity. Among the various remediation strategies, adsorption utilizing advanced carbon-based materials has emerged as a highly effective approach to address this issue. In this study, graphene oxide (GO) was synthesized and thoroughly characterized, demonstrating the presence of abundant oxygenated functional groups that facilitate strong electrostatic and π–π interactions with cationic dye molecules. Kinetic investigations revealed that the adsorption process conformed to a pseudo-second-order model ($R^2 > 0.95$), indicating that chemisorption is the predominant mechanism, with a maximum adsorption capacity of 51.04 mg/g at an initial dye concentration of 25 mg/L. Both intraparticle and film diffusion were identified as contributing mechanisms, confirming a multi-step adsorption process. The equilibrium data were best fitted by the Toth isotherm model ($R^2 = 0.99999$), while the Langmuir model estimated a monolayer adsorption capacity of 65.98 mg/g. Optimization using response surface methodology (RSM) determined the optimal operating conditions, under which a high dye removal efficiency of 92.11% was achieved. Overall, these results highlight the remarkable efficiency, stability, and applicability of graphene oxide as a promising adsorbent for the elimination of toxic dyes from wastewater systems.

**Keywords**: Water pollution, Crystal violet, Graphene oxide, Adsorption, Response surface methodology, Biological activities.

# From Waste to Strategic Resource : Valorization of Tunisian Phosphogypsum through an Integrated Rare Earth Recovery Process

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The growing demand for rare earth elements (REEs) drives the search for sustainable secondary sources. This work presents the valorization of Tunisian phosphogypsum (PG), a major by-product of the phosphate industry, through an integrated process combining double sulfuric acid leaching and fractional precipitation.

Raw PG was first subjected to a sequential NaCl–$Na_2CO_3$ pretreatment, promoting the removal of soluble impurities and the partial conversion to calcite, a matrix more reactive under acidic conditions. Enrichment of a 15% sulfuric acid solution with REEs was achieved by double contact with pretreated phosphogypsum under controlled conditions (L/S = 3, 100 °C, 2 h). The first leaching achieved an extraction yield of about 90%, while the second leaching provided an enrichment factor greater than 2.5. This method produced a REE-rich leach liquor (4308 $mg \cdot L^{-1}$) along with two high-purity anhydrite residues suitable for industrial reuse. Progressive neutralization with 10% ammonia of the REE-rich filtrate led to three selective precipitations at pH 1.1, 2.3, and 6. The optimal recovery was obtained at pH 1.1, reaching 98.5% REE and 97% Th removal efficiencies. This integrated approach offers an eco-efficient and potentially economically viable route for the valorization of Tunisian phosphogypsum, transforming an environmentally problematic waste into a strategic resource for critical materials essential to the energy transition.

**Key words:** Phosphogypsum, Rare earth elements (REEs), Integrated process, Sulfuric acid leaching, Fractional precipitation

# Development and Characterization of Iron-Modified Bentonite for Efficient Phenol Adsorption and Regeneration

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Water contamination by toxic and persistent organic pollutants such as phenol constitutes a major environmental challenge due to its extensive use in various industrial sectors, including chemical, pharmaceutical, and petrochemical processes. In this study, natural bentonite from Djebel Stah (Gafsa region, Tunisia) was purified and modified by iron intercalation using two synthesis routes: a conventional batch method and an ultrasonic-assisted process, yielding Fe-arg1 and Fe-arg2 materials, respectively.

Comprehensive characterization using XRD, BET surface analysis, TEM, CEC, and FTIR revealed that iron incorporation significantly enhanced the surface and textural properties of bentonite. The Fe-arg2 sample exhibited superior structural homogeneity and adsorption performance, attributed to the efficiency of ultrasonic synthesis.

Adsorption experiments demonstrated high phenol removal efficiencies for all adsorbents, with Fe-arg2 showing the highest capacity. Equilibrium was reached within 20 minutes for the modified clays, compared to 30 minutes for the purified bentonite. Kinetic data followed a pseudo-second-order model, while isotherm fitting showed Langmuir behavior for Fe-arg2 and Freundlich behavior for Fe-arg1. Adsorption was most favorable under acidic pH conditions.

Regeneration studies indicated that the Photo-Fenton process effectively restored the adsorption capacity, confirming the material's reusability.

These results demonstrate that iron-intercalated bentonite, particularly Fe-arg2, is a cost-effective and sustainable adsorbent for phenol removal from industrial wastewater.

**Keywords:** phenol removal, iron-intercalated bentonite, adsorption, ultrasonic synthesis, regeneration, wastewater treatment

# Sustainable magnetic solid-phase microextraction of alkylphenols in environmental waters using a novel polymeric magnetic hawthorn nanocomposite

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A novel polymeric magnetic nanocomposite, MHSHC@PLA@C18, was synthesized via hydrothermal treatment from hawthorn seeds and applied to the extraction of alkylphenols (APs) including 4-octylphenol, 4-tert-octylphenol, and 4-nonylphenol from environmental water samples. The sorbent was characterized by SEM, TEM, FTIR, and VSM, demonstrating its suitability as an analytical adsorbent. The material was employed for magnetic solid-phase extraction (MSPE) of APs, followed by GC–MS determination after derivatization. Key extraction parameters—sample and elution volumes, ionic strength, sorbent amount, pH, and extraction time—were optimized. The method showed good accuracy (recoveries 91–116%) and precision (RSD < 20%), with limits of detection and quantification of 0.02–0.03 µg $L^{-1}$ and 0.06–0.09 µg $L^{-1}$, respectively. The procedure was successfully applied to 12 environmental samples, detecting APs in one at 0.115–0.126 µg $L^{-1}$. Evaluation using AGREE and BAGI metrics gave a sustainability score of 0.55 and an applicability score of 62.5, indicating promising potential for green and efficient AP extraction [1].

**Keywords** : Alkylphenols Polymeric magnetic silica nanocomposite Magnetic solid phase extraction Environmental samples Green analytical chemistry Applicability GC–MS

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# Mechanochemical synthesis, characterization and photocatalytic hydrogen production activity of α-$NaCuPO_4$

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The α-$NaCuPO_4$ compound was synthesized using a mechanochemical method. XRD is used to identify the crystalline phase and purity of a photocatalyst. It also provides crystallite size and structural information that directly influence its photocatalytic activity.
Subsequently, the material was characterized by Raman spectroscopy to identify molecular groups through their vibrational modes, and by UV–visible spectroscopy to investigate electronic transitions and determine the optical band gap. Scanning electron microscopy (SEM) was used to observe the surface morphology, while cyclic voltammetry (CV) measurements were performed to assess the redox behavior and electrochemical performance of the material. Furthermore, the photocatalytic activity of α-$NaCuPO_4$ was investigated through hydrogen production experiments under light irradiation, revealing its strong potential for energy conversion and environmental applications. All obtained results will be presented and discussed during the oral presentation.

# Electrocatalytic platform based on MXENE for efficient Green Hydrogen generation via Catalytic Hydrazine-Assisted Water Splitting

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The global push for sustainable energy has intensified the search for innovative materials that can efficiently produce hydrogen. Conventional water electrolysis, however, is hindered by the sluggish oxygen evolution reaction (OER), which consumes substantial energy [1]. A promising alternative is to replace the OER with more efficient anodic reactions, which can lower energy demands while co-producing high-purity hydrogen and valuable chemicals.

In this study, we developed a modified graphite electrode functionalized with a nanocomposite of MXENE and molybdenum disulfide quantum dots ($MoS_2$ QDs). This composite acts as a highly active electrocatalyst for both the hydrogen evolution reaction (HER) and hydrazine oxidation. Through a suite of characterization techniques, including SEM, Raman spectroscopy, and electrochemical impedance spectroscopy (EIS), we confirmed the material's structure and properties.

Electrochemical testing revealed strong performance for hydrogen generation and hydrazine oxidation. By successfully integrating hydrazine oxidation as a substitute for the OER, this platform significantly lowers the overpotential needed for water splitting. This approach provides a practical route to produce green hydrogen with greater energy efficiency and improved sustainability, marking a step forward in eco-friendly energy technology.

**Keywords:** Electrocatalysis, Hydrogen generation, Alternative oxidation reaction, MXENE nanocomposite.

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# Photocatalytic reduction of Cr(IV) on the $CuCrO_2$/ZnO heterojunction

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Chromium (IV) is highly toxic in water above a certain threshold (50 > µg/L). The increase in Cr (IV) concentration in water is primarily due to uncontrolled industrial discharges. This has a direct impact on human health. Current techniques (ion exchange resins, reverse osmosis, and coagulation) require sophisticated equipment and expensive materials.

In the present work, we successfully tested the reduction of dichromate by photoelectrochemistry (PEC) using the ($CuCrO_2$/ZnO) junction with the ratio (50%/50%).

Delafossite $CuCrO_2$ was prepared by sol-gel to increase its specific surface area. Physical and electrochemical characterizations of this material revealed a p-type semiconductivity with an optical band gap of 1.30 eV and an activation energy of 0.22 eV. In contrast, ZnO synthesized via the nitrate route is an n-type semiconductor with a band gap of 3.2 eV.

Cr (VI) was reduced to chromium(III) in acidic medium by photoexcited electrons from the conduction band of $CuCrO_2$ (BC) (-1.34 $V_{/SCE}$) with a reduction rate of 57%. The reduction follows first-order kinetics. Photocatalytic tests revealed that the dichromate reduction is inactive in neutral medium.

**Keywords:** chromium (VI), delafossite, photocatalysis, $CuCrO_2$, ZnO.

# Harnessing Recycled Polymers for High-Performance Microporous Membranes in Sustainable Water Treatment

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Membrane-based technologies play a critical role in addressing freshwater scarcity and sustainable wastewater management. Among these, membrane distillation (MD) offers a thermally driven approach for efficiently desalinating seawater and treating saline or contaminated effluents[1]. The efficiency of MD is strongly influenced by the membrane's nanostructure, pore morphology, surface hydrophobicity, and thermal stability[2]. In this study, flat-sheet hydrophobic membranes were fabricated from recycled low-density polyethylene (R-LDPE) using the thermally induced phase separation (TIPS) method. Butyl acetate, chosen for its lower environmental impact, served as the solvent, while hexane acted as a non-solvent. Additives including LiCl, PEG, and alumina were incorporated as pore formers to optimize porosity and mechanical strength. Characterization of the membranes included FT-IR spectroscopy for crystallinity, scanning electron microscopy (SEM) for microstructure, and measurements of porosity, pore size, bubble point pressure, thickness, contact angle, and mechanical properties. The membranes displayed high porosity (65%) and pronounced hydrophobicity (CA=115°), and the incorporation of LiCl notably enhanced mechanical performance. This approach demonstrates the potential of using recycled polymers to produce membranes with both high performance and environmental benefits[3]. By valorizing plastic waste, and employing less toxic solvents, this study supports a circular materials economy and provides a scalable, sustainable solution for water treatment and desalination applications.

**Key words:** Water scarcity, membrane distillation (MD), microporous membranes, hydrophobic properties, plastic waste, sustainable solutions.

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# Removal of toluene from water using high quality zeolite prepared from clay minerals.

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Zeolites are several microporous crystalline aluminosilicate minerals of capital importance due to their diverse range of properties. In this study, the synthesis taking into accounts the effect of the ratio (NaOH/Clay) and crystallization time. The ratio 1.6 produces pure zeolite X, after 24 hours of crystallization.-The adsorption of toluene on zeolite and the raw clay proves that the maximum adsorbed amount of toluene is accorded to pH = 6 and 5, respectively. For both adsorbents, four hours was sufficient to reach the maximum adsorption in the form of kinetics that follows the pseudo second order model. The retention modeling according to the Langmuir isotherm proves that the retention of toluene on zeolite X and raw material achieved a maximum adsorption quantity of the order of 81.96 mg/g and 34.04 mg/g, respectively. These optimum conditions of adsorption were used in order to study the retention of toluene from industrial effluent, and the results show that zeolite stands for maximum performance, reaching a retention rate of approximately 93% and would be an ideal candidate for this application.

**Key words:** Smectite, Zeolites, Toluene, Langmuir, Surface Specific $S_{BET}$.

# LC-UV Determination of Ascorbic Acid in Fruit Juices Using Magnetic Carbon Starch Nanocomposite

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A novel magnetic carbon–starch nanocomposite derived from pomegranate peels and $Fe_3O_4$ nanoparticles was synthesized and characterized for potential analytical and biomedical applications. The material was obtained through an eco-friendly process using starch as a natural stabilizer and carbon source. Its structural and magnetic properties were confirmed by SEM–EDX mapping, FT-IR, XRD [1-2].

The synthesized nanocomposite was further applied for the LC-UV determination of ascorbic acid in fruit juices using magnetic solid-phase extraction (MSPE) as a preconcentration step. The developed method showed excellent analytical performance with good linearity and recovery, demonstrating the nanocomposite's efficiency as a green and low-cost sorbent for analytical applications.

**Key words:**. Magnetic nanocomposite, Starch, $Fe_3O_4$ nanoparticles, Pomegranate peel, Green synthesis, Characterization, Magnetic Solid Extraction (MSPE).

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# Design of PEGyllated CuNi Nanoalloys with Enhanced Antibacterial Efficiency

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Magnetic bimetallic nanoalloys have attracted growing attention for their unique physicochemical properties and wide range of applications in catalysis, energy conversion, and environmental remediation. Nonetheless, their biomedical use remains limited by surface oxidation and potential cytotoxicity. In this study, we report the synthesis of copper-based magnetic bimetallic nanoalloys via a polyol-mediated chemical route, followed by surface functionalization through PEGylation to improve colloidal stability, prevent oxidation, and enhance biocompatibility. The structural properties were analyzed using X-ray diffraction (XRD), while magnetic behavior was investigated through field and temperature dependent magnetization measurements. Morphology, particle size distribution, and chemical composition were characterized by scanning and transmission electron microscopy (SEM/TEM) coupled with energy-dispersive X-ray (EDX) mapping. The colloidal stability and surface chemistry of the PEGylated systems were further assessed using optical techniques. Antibacterial assays performed against Gram-positive and Gram-negative strains demonstrated the strong antimicrobial efficacy of the PEGylated Cu-based nanoalloys. Our findings underscore the potential of PEGylated Cu-based magnetic nanoalloys as a new generation of multifunctional magnetic antibacterial agents.

**Key words:** Magnetic nanoparticle, Nanoalloy, PEGyllation, Antibacterial agent.

# Composites of crosslinked polyvinyl alcohol blended with zinc oxide nanoparticles: Conductivity and dielectric relaxation

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Cross-linked poly(vinyl alcohol)/zinc oxide (XLPVA/ZnO) nanocomposite films with improved thermal and dielectric characteristics for possible use in flexible electronics and energy storage devices are reported in this work. ZnO nanoparticles were fabricated using the sol–gel process and added in small amounts to the PVA matrix after it had been chemically cross-linked with oxalic acid at a 25% degree. X-ray diffraction, FTIR spectroscopy, thermogravimetric analysis, dynamic mechanical analysis and impedance spectroscopy were used to examine the structural, thermal, mechanical, and dielectric characteristics. The interaction between ZnO and the polymer network was validated by XRD and FTIR investigations, which also showed the decrease of the crystallinity as the ZnO content increased. PVA's increased thermal stability and decreased chain mobility as a result of crosslinking and filler incorporation were demonstrated by DMA and TGA. A charge hopping process was suggested by the behavior of AC conductivity in the 40 Hz–1 MHz range, in line with Jonscher's universal power law. Additionally, localized charge carrier dynamics were indicated by the identification of a thermally induced relaxation process utilizing modulus formalism.

**Key words:** Polymer nanocomposites, Zinc oxide, Cross-linking, Dielectric relaxation, AC conductivity, Thermal stability

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# Interfacial Engineering of ZnO Tetrapods with $Co_3O_4$ Spinel and Ag Nanostructures for Accelerated Charge Transfer in Photocatalytic and Gas Sensing Systems

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Heterojunctions have emerged as potent metal oxide semiconductor (MOS) configurations that enhance charge separation and surface reactivity, leading to improved performance in catalytic and sensing applications. This study investigates hierarchical ZnO tetrapods (ZnO-TPs) [1], which were synthesized using Flame Transport Synthesis (FTS) and subsequently decorated with Ag and $Co_3O_4$ nanoparticles through a wet-chemical deposition method [2, 3]. The coupling of n-type ZnO with p-type $Co_3O_4$ creates an effective p–n heterojunction that facilitates charge separation and accelerates surface redox reactions. The incorporation of silver (Ag) further promotes the faster migration of charge carriers, enhancing conductivity and interfacial electron transfer. Structural and morphological characterizations conducted via X-ray diffraction (XRD), scanning electron microscopy (SEM), and energy-dispersive X-ray spectroscopy (EDX) confirmed the successful formation of the ZnO/$Co_3O_4$:Ag heterostructure with uniform nanoparticle coverage. The composite demonstrated remarkable photocatalytic efficiency for the degradation of Congo Red and Methyl Orange dyes under UV irradiation, surpassing the performance of pristine ZnO and $Co_3O_4$. Additionally, gas-sensing tests revealed heightened sensitivity and expedited response/recovery behavior towards ethanol and acetone vapors, attributed to enhanced interfacial charge transport and oxygen adsorption at the ZnO/$Co_3O_4$:Ag junctions. These findings highlight the synergistic effects of $Co_3O_4$/Ag coupling in enhancing the performance of ZnO-based heterostructures for environmental and sensing applications.

**Key words:** ZnO tetrapods, $Co_3O_4$ spinel, Ag modification, heterojunction, UV photocatalysis, gas sensor.

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# Etude de l'impact de l'intégration de polymère recyclé sur les propriétés de la matières plastique en vue de son utilisation dans l'injection des pièces automobiles

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Face aux enjeux croissants de durabilité et de compétitivité dans le secteur automobile, ce projet vise à explorer l'intégration de polymères recyclés dans la fabrication de pièces plastiques techniques par injection. Réalisée au sein de la société MST s.a.r.l, spécialisée dans la production de pièces plastiques automobiles, cette étude s'attache à concilier performance mécanique, viabilité économique et réduction de l'empreinte environnementale.

L'analyse des propriétés mécaniques et thermiques des matériaux a permis de définir des seuils optimaux d'incorporation de matière rebroyée [1]. Il en ressort que le PA6-GF30 peut être recyclé jusqu'à 5 % sans altérer la résistance et la ductilité. Pour le POM, un taux de 5 % est recommandé, extensible jusqu'à 10 à 15 % selon les contraintes d'usage. Les polymères PC/ABS et PBT présentent quant à eux une bonne stabilité jusqu'à 20 %[2], démontrant leur capacité à tolérer des taux de recyclage plus élevés tout en conservant des performances satisfaisantes.

Ces résultats confirment la faisabilité technique d'une démarche de recyclage partiel dans un cadre industriel exigeant, en assurant un compromis pertinent entre qualité, coût et impact environnemental. Des perspectives d'optimisation ont également été identifiées, telles que l'ajustement des paramètres de transformation, l'usage d'additifs, et l'évaluation de la durabilité des pièces en conditions réelles.

Ce travail contribue ainsi à démontrer que l'économie circulaire peut être intégrée de manière pragmatique et efficace dans l'industrie plastique automobile.

**Mots clefs :** broyage, économie circulaire, empreinte carbone

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# Lithium-Ion Battery Electrodes with Integrated Current Collectors Enabled by Additive Manufacturing and Thermal Treatment

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Lithium-ion batteries (LiBs) are the leading energy storage technology for consumer electronics, electric vehicles, and advanced space applications. However, the growing performance demands in these fields require higher energy density, enhanced safety, and reduced production costs [1]. Conventional manufacturing of LiBs involves multiple steps and numerous components —including current collectors, binders, and conductive additives— that limit design flexibility and increase overall complexity [2]. In this context, additive manufacturing has emerged as a powerful set of technologies to directly produce functional electrochemical devices with novel architectures, fewer manufacturing steps, and improved performance [3,4].

This work investigates additive manufacturing as a route to simplify electrode fabrication and enable high-energy-density electrodes. We demonstrate LiB electrodes based on anode and cathode materials such as $Li_4Ti_5O_{12}$ (LTO) and $LiFePO_4$ (LFP), integrated with aluminum current collectors via two different strategies: i) bilayered electrode–collector architectures, and ii) composite electrodes with current collectors embedded within their microstructure. This integrated approach reduces the number of manufacturing steps while opening the door to complex electrode geometries beyond conventional planar designs. Additionally, post-processing thermal treatment yields binder-free electrodes with enhanced energy density.

**Key words:** Li-ion batteries, electrodes, current collectors, additive manufacturing, composites

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# Engineered $CaTiO_3:Ho^{3+}@SiO_2:Pr^{3+}@Au@SiO_2$ Hybrid Nanocubes for Dual-Emitter NIR Thermometry

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Near-infrared (NIR) luminescence thermometry offers substantial advantages for biological applications owing to its deeper tissue penetration and reduced light scattering compared to visible wavelengths. In this work, we report a multilayer core–shell nanoplatform composed of $Ho^{3+}$-doped $CaTiO_3$ nanocubes coated with $Pr^{3+}$-doped mesoporous $SiO_2$, further decorated with Au nanoparticles and encapsulated within an outer $SiO_2$ shell. This hierarchical architecture enables efficient photonic enhancement and improved thermal stability. The temperature-dependent luminescence intensity ratio (FIR) derived from the $Ho^{3+}$ and $Pr^{3+}$ transitions exhibits excellent sensitivity and reliable response over the physiological temperature range. The introduction of Au nanoparticles produces plasmon-mediated amplification of the emission signals, while the dual $SiO_2$ layers ensure biocompatibility and dispersibility in aqueous media. Experiments conducted using an Intralipid tissue phantom confirm the suitability of the nanostructures for biological thermal maping, demonstrating enhanced penetration depth under NIR excitation. These results highlight the promise of the proposed multishell rare-earth–plasmonic hybrid nanostructures for high-performance luminescent nanothermometry in biological environments.

**Keywords:** Lanthanides, Nano-gold@ Plasmon Optical Sensing, FIR, NIR, Relative Sensitivity, Intralipid, Tissue Phantom.

# Solid Oxide Fuel Cell Electrolytes Based on Lanthanide-Strontium Oxyapatites: Structure and Ionic Conductivity

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Fuel cells (FCs) are widely recognized as one of the most promising clean energy technologies thanks to their high efficiency in converting fuel into electricity and their reduced environmental impact. Among them, Solid Oxide Fuel Cells (SOFCs) have recently attracted renewed interest, as they employ a ceramic electrolyte capable of conducting $O^{2-}$ ions, thus enabling the generation of high power. Oxyapatites, known for their potential as oxide-ion conductors, are considered promising candidates for solid electrolytes in SOFCs.

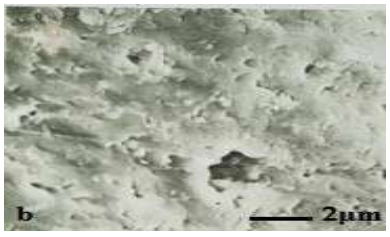
In this work, we investigate magnesium-doped rare earth–strontium silicate oxyapatites with the general composition $Sr_7–xMg_xLa_{2.5}(Nd,Gd)_{0.25}(PO_4)_2(SiO_4)_4O_{0.5}$, where the magnesium content varies (x= 0.0, 0.5, 1.0, 2.0). The compounds were synthesized using a mechanochemical method via planetary ball milling. The resulting powders were characterized by X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), and inductively coupled plasma (ICP) analysis, all of which confirmed the formation of apatite phases.

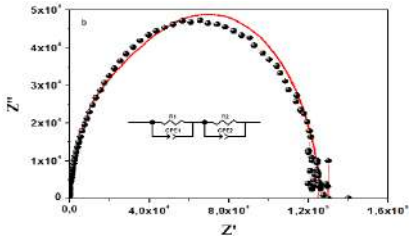
The results showed a hexagonal apatite structure (space group P63/m), with lattice parameters dependent on the ionic size of the dopant.

Rietveld refinement indicated that $Mg^{2+}$ ions preferentially occupy two sites, with a stronger tendency toward the metal (2) sites at lower doping levels. The powders were sintered without pressure, achieving dense ceramics with a maximum relative density of 90% at 1350 °C for a 6-hour dwell. Ionic conductivity was studied using impedance spectroscopy, revealing that conductivity increased with Ba substitution, reaching the highest value at x = 1. The conduction mechanism was attributed to interstitial transport, favored by an excess of oxide ions. These results suggest that the investigated oxyapatite materials are promising candidates for solid electrolyte applications in fuel cells and batteries.

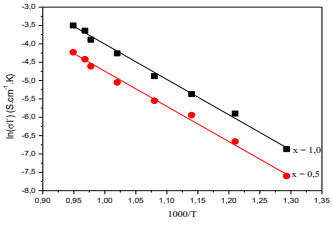
## Graphical abstract

$Sr_6Mg_1La_{2,5}(Nd,Gd)_{0,25}(PO_4)_2(SiO_4)_4O_{0.5}$




Ionic conductivity

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# An Innovative Electrochemical Platform Using Polypyrrole-Functionalized Magnetized Biochar for Anthraquinone Detection

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Screen-printed electrodes (SPEs) are widely recognized as versatile platforms for developing high-performance electrochemical sensors. In this study, biochar derived from almond shells was employed as a functional support for sensor fabrication. The biochar was magnetically modified with $Fe_3O_4$ nanoparticles and coated with polypyrrole (PPy) to enhance its electrochemical properties. The synthesized polypyrrole-functionalized magnetized biochar (MBFPPy)was thoroughly characterized by X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), and scanning electron microscopy coupled with energy-dispersive X-ray spectroscopy (SEM-EDX). Its electrochemical behavior was investigated using cyclic voltammetry (CV) and differential pulse voltammetry (DPV). The developed platform exhibited excellent electrocatalytic response towards anthraquinone detection over a linear concentration range of 3 to 100 µM, with a low detection limit of 0.04 µM. Additionally, the modified SPE demonstrated good stability and reproducibility. Recovery tests of anthraquinone in spiked water samples yielded results ranging from 99.50% to 101.58%, confirming the sensor's practical applicability.

# Development of a Biodegradation Control Protocol for EPCVD-Deposited DLC-Coated Magnesium-Based Biomedical Implants

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Magnesium (Mg) alloys are promising candidates for biodegradable orthopedic and cardiovascular implants owing to their mechanical compatibility with bone and their complete bioresorption in physiological environments. However, their high corrosion rate remains a critical challenge. To address this limitation, Diamond-Like Carbon (DLC) coatings deposited by Enhanced Plasma-Enhanced Chemical Vapor Deposition (EPCVD) have been explored as effective surface barriers to control degradation kinetics and improve biocompatibility. This study proposes a standardized biodegradation control protocol specifically designed for EPCVD-grown DLC coatings on Mg-based substrates. The protocol combines immersion testing in Simulated Body Fluid (SBF) with hydrogen evolution monitoring, pH variation tracking, and weight-loss measurements to evaluate corrosion kinetics under simulated physiological conditions. Complementary electrochemical impedance spectroscopy (EIS) and potentiodynamic polarization analyses were performed to assess coating stability and charge-transfer resistance. Morphological and chemical changes during degradation were characterized using SEM/EDS and FTIR techniques. The EPCVD-DLC coatings exhibited excellent barrier integrity, significantly reducing corrosion rate and hydrogen release while maintaining surface smoothness and chemical stability. The developed protocol provides a reliable, reproducible, and clinically relevant framework for evaluating and comparing DLC-based surface protection strategies for biodegradable metallic implants.

**Keywords :** EPCVD, Diamond-Like Carbon (DLC), Magnesium alloy, Biodegradation control, SBF testing, Corrosion resistance, Biomedical implants.

# Electrochemical Performance of Isoreticular Cu–MOFs Based on NDI and PDI Linkers for Supercapacitor Applications

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Supercapacitors outperform conventional capacitors in energy storage, offering rapid charge–discharge rates and applications in electric vehicles and large-scale energy storage. Their performance arises from electrical double-layer capacitance and/or pseudocapacitance through fast reversible redox reactions. Metal–organic frameworks (MOFs) have recently emerged as promising electrode materials, often delivering higher capacitances than conventional systems. In this work, we compare the electrochemical performance of two isoreticular copper-based MOF series constructed from naphthalene diimide ($H_2$NDI-H) and perylene diimide ($H_2$PDI-H) linkers. Electrochemical evaluation revealed outstanding performance, including high specific capacitance, excellent rate capability, and remarkable cycling stability. These findings highlight the potential of Copper-based MOFs as next-generation electrode materials for high-performance supercapacitors.

**Key words:** Supercapacitors, energy storage, Metal–organic frameworks (MOFs), NDI, PDI.

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# Electrochemical Performance of PEDOT–ZIF-8 Composite Electrodes for Symmetric Supercapacitors in Neutral Aqueous Electrolytes

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In this work, a composite material based on poly(3,4-ethylenedioxythiophene) (PEDOT) and zeolitic imidazolate framework-8 (ZIF-8) was prepared through simple self-assembly process and applied as an active electrode material for symmetric supercapacitors. The combination of the conductive polymer PEDOT and the porous ZIF-8 framework was designed to couple high electronic conductivity with a large surface area and well-developed ion diffusion pathways. The electrochemical behavior of the PEDOT–ZIF-8 composite was systematically investigated in a two-electrode configuration using cyclic voltammetry (CV), galvanostatic charge–discharge (GCD), and electrochemical impedance spectroscopy (EIS). Various neutral aqueous electrolytes were tested to explore the influence of ionic species on charge storage performance, with lithium nitrate ($LiNO_3$) used as the principal electrolyte. The device exhibited an electric double-layer capacitance (EDLC)-type behavior with enhanced specific capacitance and low internal resistance in $LiNO_3$ compared to other neutral electrolytes such as sodium nitrate ($NaNO_3$), potassium nitrate ($KNO_3$), lithium chloride (LiCl) and lithium perchlorate ($LiClO_4$). Furthermore, the symmetric cell demonstrated excellent cycling stability and good capacitance retention, confirming the structural integrity and electrochemical robustness of the PEDOT–ZIF-8 composite. These results demonstrate that the PEDOT–ZIF-8 composite is a promising electrode material for high-performance symmetric supercapacitors operating in environmentally friendly neutral electrolytes.

**Key words:** Symmetric supercapacitor, Neutral aqueous electrolyte, Energy storage, MOFs, Conducting polymer.

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# Harnessing Artificial Intelligence for the Design of a Novel Cobalt (II) Catalyst for Efficient Hydrogen Evolution

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In the pursuit of sustainable energy solutions, this work presents the design, synthesis, and characterization of a novel bidentate cobalt (II) complex with a $N_2O_2$-donor ligand, 1,2-di(furan -2-ylmethylene) hydrazine. The molecular structure and coordination environment of the synthesized complex were unequivocally established through a combination of NMR, IR, and UV-visible spectroscopic techniques.

A key innovation of this study lies in the application of artificial intelligence principles, specifically the Taguchi method, to optimize the synthetic protocol. This intelligent, systematic approach to parameter control resulted in a significant enhancement of reaction yields, demonstrating a powerful strategy for efficient catalyst development **[1]**

The synthesized cobalt (II) complex exhibits remarkable catalytic activity for hydrogen generation via the hydrolysis of sodium borohydride ($NaBH_4$), a promising chemical hydrogen storage material. A comprehensive investigation into the catalytic process was undertaken, systematically optimizing critical parameters such as temperature, catalyst loading, and substrate concentration. These meticulous adjustments allowed for the maximization of the hydrogen evolution rate, highlighting the complex's potential as an efficient and reproducible catalyst for green energy applications. This study underscores the synergy between coordination chemistry and artificial intelligence in creating advanced materials for a sustainable hydrogen economy.

**Key words:** Cobalt(II) Complex, Catalyst Design, Taguchi Method, Hydrogen Generation.

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# Allelopathic Effects of *Eucalyptus* Essential Oils on Seed Germination of *Leucaena leucocephala*, *Medicago sativa*, and *Peganum harmala*

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**Background:** Essential oils (EOs)are a complex of volatile compounds, naturally synthesized in different parts of the plant. Recently, their use as allelochemicals with bioherbicidal potential has attracted increasing interest. Some of them possess not only weed-killing properties, but also pre-harvest germination-inhibiting properties. In this study, we evaluated the allelopathic effects of EOs from two *Eucalyptus* species and four different subspecies on seed germination and root development of three plants from the Gabès region (Tunis): an invasive plant (*Leucaena leucocephala*); a cultivated plant (*Medicago sativa*) and a third spontaneous plant (*Peganum harmala*).
**Materials/Methods** EOs were extracted from *Eucalyptus* leaves - *Eucalyptus socialis subsp. socialis*, *E. socialis subsp. viridans*, *E. oleosa subsp. oleosa*, and *E. oleosa subsp. cylindreoidea* - collected from the Gabes region (southern Tunisia), using hydrodistillation in a Clevenger-type apparatus. Seeds of *Leucaena leucocephala*, *Medicago sativa*, and *Peganum harmala* were exposed to EO vapors at concentrations of 0, 30, 60, and 90 µL. Seed germination was assessed on days 3 and 5, with both germination percentage and radicle length recorded at each time point.
**Results**. EOs of *E. oleosa subsp. cylindreoidea*, applied at doses of 30, 60 and 90 µL, completely inhibited radicle length (mm) and germination rate (%) in all experiments. However, the application of 30 µL of *E. oleosa subsp. oleosa* did not significantly reduce *Leucaena leucocephala*, germination after 5 days (6,67%); but it reduced root length by 54,19 % compared to the untreated control. A marked difference in the effects of the *Eucalyptus* species and subspecies was observed, particularly at the highest dose of 90 µL. At this concentration, the Eos of *Eucalyptus oleosa subsp. oleosa* and *E. socialis subsp. viridans* significantly reduced the germination rate of *Leucaena leucocephala* seeds to 46,66% and 51,66%, respectively. In contrast, the oils of *E. socialis subsp. socialis* and *E. oleosa subsp. cylindreoidea* completely inhibited germination after 5 days of exposure. The various concentrations of the tested EOs led to a significant inhibition of *Peganum harmala* seed germination and resulted in very limited radicle growth. The control group showed a high germination rate (88.33%), which decreased notably with exposure to 30 µL of *Eucalyptus socialis subsp. viridans* oil (58.51%). This inhibition became more pronounced with *E. socialis subsp. socialis* and *E. oleosa subsp. oleosa* (22.65%), and germination was completely inhibited by *E. oleosa subsp. cylindreoidea* (0%). The highest effect was observed on *Medicago sativa* seeds, for which no germination occurred, regardless of the essential oil tested or the concentration applied.
**Conclusion:** The results obtained show an herbicidal effect that varies between species and subspecies, in addition, EO, particularly those derived from *E. oleosa subsp. cylindreoidea*, hold promise as potential natural sources for the development of bio-herbicidal products.

**Keywords:** *Eucalyptus* subspecies, essential oil, allelopathic activities.

# Spray-drying encapsulation of Bioactive Compounds of Tunisian Okra leaf extracts

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The major objective of modern pharmaceutical and food industries is the use of functional plant-based food ingredients to respond to current consumer attitudes. There has been great scientific interest in the characterization of active ingredients from natural sources, particularly from agricultural production waste. However, phenolic compounds in *Abelmoschus esculentus* L.'s leaf have an excellent bioactivities. This research records lyophilized Okra leaves samples extracted by microwave technique and microencapsulated by spray-drying using maltodextrin–pectin (10:1) as encapsulating material. The total phenolic content, antioxidant and antibacterial proprieties of *Abelmoschus esculentus* L. extracts and spray-dried samples were evaluated to verify the encapsulation efficiency. Okra microcapsules have smal Sauter mean diameter values (7.98 ± 0.12 µm). Then, scanning electron microscopy of Okra leaves microcapsules was also carried out.

These data are applicable for expanding the application of okra leaves as food additives and/or preservatives in the food industry.

**Keywords:** *Abelmoschus esculentus* L.; leaf; spray-drying; microencapsules; phenolic compounds; bioactivities.

# A Copper-Chloride Perovskite with Jahn-Teller-Distorted $CuCl_6$ Octahedra: Synthesis, Structure, and Optical Properties

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In this work, we report the chemical synthesis and comprehensive investigation of the structure–property relationship of a novel layered hybrid perovskite, ethylenediammonium tetrachlorocuprate(II), synthesized using a short-chain organic diammonium cation as a structural template. The compound crystallizes in the monoclinic $P2_1/c$ space group and exhibits a distinctive yellow color at room temperature an optical signature attributed to square-planar $[CuCl_4]^{2-}$ units arranged in two-dimensional layers. Hirshfeld surface analysis, complemented by two-dimensional fingerprint plots, reveals key intermolecular interactions governing the crystal packing. Infrared (IR) spectroscopy confirms the presence of characteristic vibrational modes at room temperature. The optical properties are further examined, with the indirect optical band gap estimated at 1.93 eV a value consistent with theoretical calculations performed using DFT within the VASP framework (1.87 eV). Thermal behavior was assessed via TGA-DTA analysis, confirming the material's stability under elevated temperatures. These results highlight the potential of short-chain diammonium cations in directing the formation of structurally stable and optoelectronically active hybrid perovskites, offering promising prospects for next-generation low-dimensional semiconductor applications.

**Key words:** Copper, Band Gap, Semiconductor.

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# Modeling, Optimizing and Mechanistic Study of the CR-401 Catalyst Behaviour in Naphtha Continuous Catalytic Reforming Using Artificial Neural Networks

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The Continuous Catalytic Reforming (CCR) of naphtha is a central refinery process for upgrading low-octane hydrocarbons into aromatic-rich reformates. The CR-401 catalyst, based on a bifunctional Pt–Re/Cl–γ-$Al_2O_3$ system, provides both metallic and acidic functionalities enabling dehydrogenation, isomerization, and cyclization reactions. However, catalyst deactivation through coke deposition remains a major limitation, resulting from condensation and polymerization of polyaromatic precursors on both metal and acid sites [1].
In this study, a data-driven modeling approach using artificial neural networks (ANNs) was developed to predict and optimize the performance of the CR-401 catalyst in the Algiers refinery (RA1G). Industrial data collected over one operational year were processed to establish correlations between reactor temperatures, hydrogen-to-hydrocarbon ratio ($H_2$/HC), catalyst circulation rate, and total chlorine content (TCl) with two key responses: Research Octane Number (RON) and coke yield ($Y_{coke}$). Forty-five ANN architectures were trained and validated (K-fold = 5 to15), hidden layers (3 to 7), and neurons per layer (10 to 30), taking the coefficient of determination ($R^2$), the mean square error (MSE), and the mean absolute error (MAE) as performance indicators [2].
A high accuracy for RON prediction ($R^2_{validation}$ = 0.9999999, $MSE_{validation}$ = 0.001672) was achieved with the configuration of 15 K-folds, 3HL and 10 neurons per layer. An accuracy of $R^2_{validation}$ = 0.9999986 and $MSE_{validation}$= 0.0006863 was obtained for coke yield applying a configuration of 15 K-folds, 7 HL and 20 neurons per layer.
Sensitivity analysis revealed that the 4th reactor temperature and TCl exert the strongest influence on both RON and coke formation. Mechanistic interpretation indicated that moderate increases in metal site activity (470–485 °C, $H_2$/HC = 1.8–2.2) enhance dehydrogenation and aromatization, whereas excessive acid site strength or reduced hydrogen partial pressure promote coke nucleation. The ANN-assisted optimization effectively captures the nonlinear behavior of bifunctional catalysis, supporting operational decisions that balance activity, selectivity, and catalyst longevity.

**Keywords:** CR-401 Pt–Re/$Al_2O_3$ catalyst, Naphtha Continuous Catalytic Reforming, Bifunctional mechanism, Research Octane Number, Coke precursors, Artificial neural networks.

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# Pt-doped g-$C_3N_4$ photocatalyst for Piperonal production under visible light

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Metal-free catalysis, particularly employing semiconducting graphitic carbon nitride (g-$C_3N_4$) is currently garnering significant attention owing to its sustainability and notable catalytic activity in various chemical transformations. Despite its application as a photocatalyst, the overall efficiency of g-$C_3N_4$ under visible light remains limited. This constraint is primarily attributed to slow charge carrier mobility, fast recombination of photogenerated electron/holes pairs ($e^-/h^+$), and limited specific surface area (SSA) [1]. A comprehensive set of strategies has been investigated to enhance the photocatalytic performance of g-$C_3N_4$, notably the deposition of noble metals to introduce highly efficient catalytic active sites. In this study, bulk g-$C_3N_4$ (CN) was synthesized via thermal polycondensation of a urea-melamine mixture. To enhance its crystallinity, optoelectronic properties, and photocatalytic activity, platinum (Pt) nanoparticles were introduced onto the CN surface using the incipient wetness impregnation method, yielding the hybrid composite denoted as Pt-CN. The synthesized samples were characterized by XRD, FTIR, SEM-EDX, and $N_2$ adsorption–desorption measurements. Photocatalytic assays demonstrated efficient piperonal synthesis under visible light irradiation. The Pt-CN composite exhibited notable activity, achieving piperonal selectivity of 48% under $N_2$ bubbling and 71% in ambient air. This enhanced performance was closely correlated to a suite of improved physicochemical properties resulting especially from Pt loading.

**Key words:** Photocatalysis, g-$C_3N_4$, Pt loading, organic synthesis, Piperonal

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# Program of Wednesday 24 December 2025

# VALORISATION OF INVASIVE PLANT SPECIES IN SENEGAL FOR THE DEVELOPMENT OF BIO-BASED MATERIALS

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The reflection on lignocellulosic invasive plant species can be a major asset for the development of socio-economic and innovative activities of populations and industry. The objective of this work is to valorize biopolymers from these species in bio-recyclable materials, low carbon and environmentally friendly for applications in the paper, construction and electronics. The study of the chemical and morphological composition of these species made it possible to select three plant materials (Mariscus, Aeschynomene and Phragmites) in order to extract by delignification the lignin used in the synthesis of conductive composites (Pani-$LG_i$) by in situ polymerization of aniline and cellulosic pulp by bleaching after filtration of black liquor for paper making. Characterization results (TGA and electrical conductivity) showed thermally stable composites (Pani-$LG_i$) up to 350°C [1], and conductivities ranging from 2.60 to 4.20 $S.Cm^{-1}$, higher than those of the conductive polymer (Pani = 0.72 $S.Cm^{-1}$) [2, 3]. The cellulose content was confirmed by the results of the chemical composition and the pulp obtained allowed the manufacture of different types of paper. Our results allow us to affirm that these plants have a promising potential in ecological materials and in the paper industry and as composites in electronic devices.

**Keywords** : invasive species, cellulose, lignin, biomaterials, papermaking

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# Influence of Spark Plasma Sintering parameters on the microstructure, mechanical and tribological properties of air-milled aluminum

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This work explores the effect of spark plasma sintering (SPS) parameters on the microstructure and mechanical behavior of high-energy ball-milled aluminum powders. Sintering was performed between 550-625 °C under 50-100 MPa. The powders and consolidated samples were characterized by XRD, SEM, laser granulometry, and Archimedes density. Mechanical and tribological properties were evaluated through Vickers microhardness, nanoindentation, and wear tests. Optimal conditions (600 °C, 100 MPa, 46 h milling) produced the highest microhardness (187.5 HV) and density. At 625 °C, excessive grain growth reduced hardness. Nanoindentation revealed distinct hard and soft regions, while tribological tests showed up to 50 % lower wear rate and 20 % lower friction coefficient compared with unmilled samples.

**Key words:** Aluminum, High-energy ball milling, Spark Plasma Sintering, microstructure, tribology, mechanical properties.

# Experimental and theoretical investigations on the photophysical and electronic properties of new synthesized organic small molecule for optoelectronic applications

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In the present work, we report the chemical synthesis of a newly π-conjugated system using a Wittig reaction. The chemical structure of the synthesized molecule named 1,4-Bis((*E*)-2-(1-methyl-pyrrol-2-yl)vinyl)benzene (**BisPyrBz**) was supported by Fourier transform infrared spectroscopy. The optical properties were investigated first using optical absorption (O.A) and steady-state photoluminescence (PLs) tools. Else, transient photoluminescence (TRPL) and emission quantum yield measurements (PLQY) were experimentally undertaken in diluted solution and condensed state. Theoretical investigations on the synthesized molecule were performed using density functional density (DFT). Experimental and theoretical data show the formation of a planar π-conjugated system. The obtained molecule presents a blue emission with high PLQY, at around 35% in the solution state. The emission is red-shifted to the green color, with a drastic decrease of the PLQY to around 1% indicating a possible aggregation-caused quenching behavior in the condensed state. The use of the synthesized **BisPyrBz** as a π linker in a newly designed A-π-D small molecule permits to obtain a newly near-infrared absorbing material with a weak energy gap $Eg = E_{LUMO} - E_{HOMO}$, which is at around 1.93 eV, and a weak optical band gap which is estimated to be 1.67 Ev. The obtained observations believes the exploitation of the designed A-π-D in the photovoltaic application.

**Keywords:** π-conjugated system, optical absorption (O.A), steady-state photoluminescence (PL), dye, density functional density (DFT).

# Innovative Computational Design of Nitrobenzofurazan Non-Fullerene Acceptors for High-Performance Organic Solar Cells

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This study presents the computational design and analysis of nitrobenzofurazan (NBD)-based non-fullerene acceptors, denoted as Ai (i = 1–5), using density functional theory (DFT) in acetonitrile solvent. These newly developed donor–acceptor (D-A) type small molecules, incorporating nitro ($NO_2$) and fluorine (F) substituents within the NBD core, aim to enhance the performance of non-fullerene organic solar cells (OSCs). The DFT and time-dependent DFT (TD-DFT) calculations at the B3LYP/6-311G(d,p) level were employed to examine their geometric, electronic, optical, and charge transport characteristics. All designed molecules exhibited narrower energy gaps (1.67–2.25 eV) and intense absorption peaks (λ_max = 463–472 nm). Their low exciton binding energies (0.48–0.55 eV) indicate efficient charge separation and donor–acceptor interactions, as confirmed by FMO, PDOS, MEP, and TDM analyses. The compounds also displayed high open-circuit voltages (V_OC) and favorable fill factors (FF), underscoring their excellent photovoltaic performance. Among them, A4 emerged as the most promising acceptor, showing optimal electronic alignment and strong charge transfer when blended with an NBD-based donor, confirming its potential for efficient real-world OSC applications.

**Key words:** Nitrobenzofurazan (NBD); DFT; DOS; TDM; OSCs; NFAs

# Design of novel bio-sourced materials derived from chitosan for piezoelectric sensor applications

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Chitosan, a cationic linear polysaccharide derived from chitin, has attracted considerable attention in recent years due to its excellent biocompatibility, biodegradability, low cytotoxicity, and ease of chemical modification **[1]**. In addition, its outstanding physical, chemical, and biological properties make it valuable for a wide range of applications. The introduction of fluorinated groups into chitosan modifies its functional and structural characteristics, enabling its use in piezoelectric applications. To enhance its functional properties, chitosan was chemically modified through O-alkylation. Two distinct modification routes were designed to introduce fluorinated and aromatic alkyl groups onto the chitosan backbone, using 2,2,3,4,4,4-hexafluorobutan-1-ol and 2-aminobenzotrifluoride.

The synthesized derivatives, CS-$M_1$ and CS-$M_2$, suffer from poor solubility, which represents a major limitation. To overcome this issue, a quaternization reaction was proposed to produce CS-$M_1$-$Q_1$ and CS-$M_2$-$Q_1$, which confers water-soluble characteristics to these materials. The obtained derivatives were thoroughly characterized using SEM, UV–Vis, FTIR, XPS, NMR, and XRD analyses. The IR spectra clearly show the appearance of new bands, confirming the successful incorporation of these groups into the chitosan side chain. XPS characterization further confirms the incorporation of functional groups and enables the determination of the degree of chitosan modification. The obtained results confirmed the successful incorporation of the targeted functional groups into the chitosan side chains.

**Keywords:** Chemical modification, Chitosan, functional biopolymer, biomass valorization

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# Triazole-Functional Conjugated Polymers for Metal-Ion Sensing: Synthesis and Photophysical Properties

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The selective detection of metal cations is an important challenge in environmental analysis and chemical sensing. In this work, we present the elaboration of three new conjugated semiconducting polymers **P$_{1\text{-}3}$**, designed to combine strong fluorescence with triazole groups capable of binding metal ions. The synthetic route begins with the preparation of the dipole and the dipolarophile. The dipole is produced by azidation of 4,4′-diamino-2,2′-stilbene disulfonic acid (DASS), a PPV-based fluorophore that shows strong emission and good-water solubility, giving the azido compound DASS-$N_3$. The dipolarophile is obtained through the propargylation of vanillin, which provides the alkyne-functionalized unit VAN-TRIP. DASS-$N_3$ and VAN-TRIP are then joined through a click reaction to generate the triazole building block DASS-Tri-VAN, known for its good coordination ability. This triazole unit is finally engaged in three separate Wittig polycondensation reactions using different phosphonium salts. These salts are prepared through sequential alkylation, chloromethylation, and phosphination, and each one leads to a distinct conjugated polymer in the **P$_{1\text{-}3}$** series. All three polymers show good solubility in polar organic solvents and strong fluorescence in solution. The molecular structures of the obtained polymers were confirmed by $^{1}H$ and $^{13}C$ NMR spectroscopies together with FT-IR analysis. Their optical behavior was examined using UV–vis absorption measurements, and the HOMO and LUMO energy levels were determined by cyclic voltammetry. These results describe a stable π-conjugated system with properties suitable for electronic and optoelectronic applications.

**Keywords**: Functional polymers, side chain effect, photophysical properties, chemical sensing.

# Heterogeneous Catalytic Reduction of Oxygenated Functions in Olive Pomace Oils for Sustainable Biofuel Production

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The valorization of olive pomace oils, abundant by-products of the Mediterranean agro-industry, offers a promising route for renewable energy production. In this study, we investigated the heterogeneous catalytic reduction of oxygenated functions in crude olive pomace oils to produce biofuel fractions with improved physicochemical properties. Two catalytic systems were explored: magnetic iron oxide nanoparticles ($Fe_3O_4$), which allow easy recovery and recycling, and supported palladium catalysts (Pd/C), known for their efficiency in hydrogenation reactions.

Experimental results demonstrated that $Fe_3O_4$ promotes partial reduction of double bonds with moderate selectivity, whereas Pd/C showed higher efficiency in converting oleic acid (C18:1) into saturated stearic acid (C18:0), leading to enhanced stability and calorific value of the obtained biofuel. Comparative analyses confirmed that prolonged sonication time (3 h, 6 h, 9 h) significantly influences both conversion rates and selectivity.

The results were critically discussed with reference to literature reports (Rylander, Harada, Qu et al.), highlighting mechanistic pathways involving C=C bond hydrogenation and progressive deoxygenation. This work confirms the feasibility of catalytic reduction as a green route for biofuel elaboration and opens perspectives for further optimization, including catalyst recycling, temperature control, and solvent effects.

**Keywords:** Biofuel, Olive pomace oil, Heterogeneous catalysis, $Fe_3O_4$, Pd/C, Renewable energy.

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# Mechanical and Biological properties of structured composite Scaffold based on Hydroxyapatite and Degraded Chitosan

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The elaboration of bone Scaffolds with integrated porous Structure, appropriate mechanical properties and excellent biocompatibility is still persisted a great challenge [1]. For that reason, in this work, structured composite has been elaborated using the freeze-drying technique based on hydroxyapatite and degraded chitosan in order to study its mechanical and biological properties comparing to the one that is composed by hydroxyapatite and chitosan which is widely illustrated [2]. Therefore, Analysis by Infrared Spectroscopy, XR Diffraction, SEM, TEM and Thermal Analysis by TGA/DSC were realized to notice the main differences in the physicochemical properties and to determine the pore size of both hybrid scaffolds. Furthermore, a study of the mechanical properties using the compression test is established of each scaffold. In addition, a cytotoxicity test had been realized in order to study the percentage of cells viability after the incubation with bioscaffolds.

**Key words:** degraded chitosan, composite, Scaffold, Hydroxyapatite

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# Design and Optimization of Ciclopirox Olamine-Loaded Solid Lipid Nanoparticles: Effect of Formulation Variables on Physicochemical Characteristics and Drug Release Behavior

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**Purpose:** Onychomycosis remains a challenging condition to treat effectively due to the limited permeability of the nail plate and the poor bioavailability of conventional topical antifungal formulations. Ciclopirox olamine (CPX), a broad-spectrum antifungal agent, has limited therapeutic efficacy primarily due to its low penetration and short retention time at the target site. The present study aimed to develop and optimize solid lipid nanoparticles (SLNs) as a novel delivery system to enhance the stability, encapsulation, and controlled release of CPX.
**Methods:** CPX-loaded SLNs were prepared using cocoa butter as the lipid matrix and Tween 80 as the surfactant, employing a high-speed homogenization followed by an ultrasonication technique. A Central Composite Design (CCD) was applied to investigate the effects of three critical formulation variables-Tween 80 concentration, homogenization speed, and sonication time—on the particle size, polydispersity index (SPAN), and encapsulation efficiency (EE%). The optimized formulation was further characterized by Fourier Transform Infrared Spectroscopy (FTIR), Differential Scanning Calorimetry (DSC), and in vitro drug release studies. The release kinetics were analyzed using Higuchi, Korsmeyer–Peppas, and Weibull models.
**Results:** The optimized SLNs exhibited a mean particle diameter of 242.87 ± 46.92 nm, a Span of 1.61 ± 0.43, and an encapsulation efficiency of 92.98 ± 2.71%, indicating successful entrapment and a narrow size distribution. FTIR and DSC analyses confirmed the absence of chemical interaction between CPX and the lipid excipients, suggesting successful encapsulation and preservation of drug integrity. Microscopic images revealed uniform, spherical nanoparticles. In vitro drug release followed Higuchi kinetics ($R^2$ = 0.9559), indicating a diffusion-controlled mechanism and demonstrating sustained release compared with free CPX.
**Conclusion:** The optimized CPX-loaded SLN formulation offers a promising nanoscale carrier for enhancing drug stability and providing controlled antifungal delivery. This lipid-based nanocarrier system could represent a potential platform for improving the therapeutic performance of ciclopirox olamine and other poorly permeable antifungal agents.

**Keywords:** Ciclopirox olamine, solid lipid nanoparticles, design of experiment, central composite design, controlled release, drug delivery.

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# Synthesis, Structural, thermal and Antimicrobial activity characterizations of PLA/BCT nanocomposite films

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This study investigates the influence of incorporating $Ba_{1-x}Ca_xTiO_3$ with x= 0.04 (BCT) nanoparticles on the structural, thermal, optical, and spectroscopic properties of nanocomposite films with PolyLactic Acid (PLA) matrix. The BCT nanoparticles were synthesized using the sol-gel method and the PLA/BCT nano-composites were prepared with solvent-casting routine. The properties of BCT nanoparticles, PLA and PLA/BCT (8 and 20 wt.%) were determined through various analyses including X-Ray Diffraction (XRD), Scanning Electron Microscopy (SEM), UV–Visible absorption and Infrared spectroscopy measurements. The tetragonal system with space group P4mm was formed by the $Ba_{1-x}Ca_xTiO_3$ with x= 0.04 composition according to the X-ray diffraction studies. The average crystallite sizes, determined by the Scherrer and W-H methods, are approximately 24 up to 27 nm.

The morphology and average grain size, analyzed using scanning electron microscopy (SEM), reveal a nanometric scale structure. The elemental analysis with energy dispersive X-ray (EDX) permitted the identification of the elemental composition of BCT compound and PLA/(20% BCT) composite. SEM revealed an homogeneous dispersion of nanoparticles within the PLA matrix with no noticeable agglomeration.

FTIR spectroscopy results confirmed the formation of the perovskite phase and the existence of vibrations bands of the polymer. Similarly, scanning differential calorimetric analysis showed that the incorporation of BCT nanoparticles had little influence on the glass transition temperatures (Tg) of different samples.

UV–Visible spectroscopy measurements revealed a pronounced absorption in the ultraviolet region, confirming the semiconducting behavior of the nanoparticles with a wide band gap. This strong UV absorption is consistent with the white appearance of the sample. The direct optical band gap of the BCT compound was determined to be approximately 3.14 eV, further supporting its classification as a wide-bandgap semiconductor material.

Moreover, the incorporation of BCT nanoparticles into the PLA matrix markedly enhanced the antimicrobial activity, achieving nearly complete inhibition against S. aureus, C. albicans, and Aspergillus sp. in the PLA/(20%BCT) composite. This result confirms the high effectiveness of this broad-spectrum material at room temperature.

In summary, incorporating BCT nanoparticles into the PLA matrix markedly improves the overall properties of the resulting nanocomposites. The methodology and findings of this work provide valuable insights into the interactions between nanoparticles and polymer matrices, which are essential for the design and development of high-performance nanocomposite materials.

This research paves the way for potential applications in advanced fields, driven by the improved structural, thermal, and optical characteristics of the PLA/BCT nanocomposites. Moreover, the findings highlight the versatility and potential of PLA/BCT nanocomposites in various innovative applications, pushing the boundaries of material science and engineering.

**Key words:** Barium calcium titanate oxide, PolyLactic Acid, Sol-gel preparation, X-Ray Diffraction, Perovskite structure, Antimicrobial activity , bioactive nanocomposite.

# DFT Calculation and Mechanism Study of the Reaction of Diethylphosphoryl Azide with Hydrocarbon isothisocyanates

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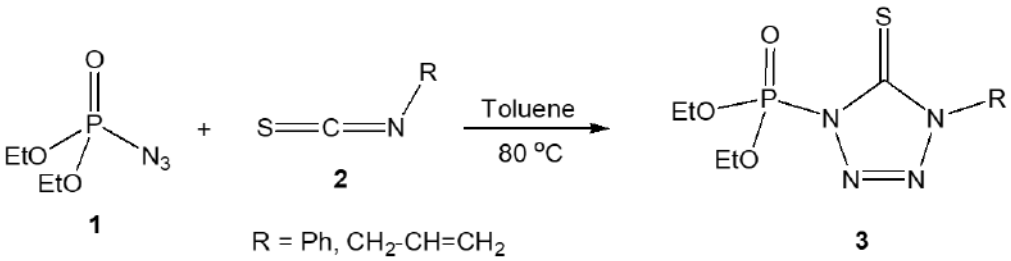
The 1,3-dipolar cycloaddition reaction of diethylphosphoryl azide with phenyl- and allylisothiocyanates carried out in anhydrous toluene at 80 °C, lead sto the corresponding 1,4-disubstituted tetrazoline-5-thiones in good yields (Scheme 1). The DFT calculations, which started by the optimisation of the substrate's energies, allowed the determination of their most stable conformations. The study of the reaction mechanism was realized by starting from the optimised stable conformations and following the evolution of the IRC values (energies, bonds length, and angles and dihedral angles), across the different states (SM, TS and Product), to show that the reaction may follow a concerted or a two steps mechanism [1]. The study of the complexing properties of the products is under investigation.




Scheme 1

**Key words:** DFT, tetrazoline-5-thione, isothiocyanate, diethoxyphosphoryl azide, 1,3-dipolar cycloaddition, asynchronous, concerted, mechanism.

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# DFT-Based Computational Modeling of Amino-Substituted n-MOF-5-$NH_2$ and n-MOF-5 for Enhanced Adsorption and Energy Storage Applications

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The characterization and synthesis of novel metal organic framework (MOF) for targeted applications have advanced significantly in recent years, owing to their status as a groundbreaking, eco-friendly material with promising applicability across diverse domain, such as adsorption or energy storage. Furthermore, beyond experimentation, DFT-computational modeling represents a sophisticated theoretical approach that elucidates and interprets phenomena through 3D-visualization, thereby enhancing comprehension of the underlying experimental mechanisms. In this investigation, we synthesized two compounds, n-MOF-5 and its amino-functionalized derivative, n-MOF-5-$NH_2$, employing a polyethylene glycol-templated, eco-friendly sol-gel synthesis technique. Comprehensive morphological characterizations were performed; encompassing, FT-IR, XRD, SEM, and TGA have been conducted. The experimental results elucidate the adsorption capacities of MOF-5, n-MOF-5-$NH_2$, for volatile organic compounds (VOCs) and hydrogen ($H_2$), which are detailed in the following references [1, 2]. To further elucidate the adsorption mechanisms of VOCs and $H_2$, density functional theory (DFT) calculations were conducted, incorporating QTAIM analysis to assess the adsorption efficacy of various entities. Non-covalent interaction (NCI) analysis and reduced density gradient (RDG) iso-surfaces were employed to delineate the functional groups implicated in the adsorptions of VOCs and $H_2$. Ultimately, electron localization function (ELF) analysis was computed to enhance our comprehension of the localized, non-localized, and lone pair's electrons on the surfaces of complexes.

**Keywords:** Metal organic frameworks (MOF), Chlorinated volatile organic compound (VOC), DFT, QTAIM, NCI, ELF-LOL

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# DFT Study and Anticancer Evaluation of Novel Benzimidazole Derivatives

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This study reports the synthesis and detailed characterization of novel benzimidazole derivatives with strong potential as anticancer agents. Density functional theory (DFT) calculations were employed to optimize the geometric structures, showing excellent alignment with experimental results. The electronic properties of these compounds were examined, and their anticancer efficacy was tested across multiple cancer cell lines, including MDA-MB-231, MCF-7, and HT-29. Among them, compound 2a demonstrated particularly high cytotoxicity against the MDA-MB-231 breast cancer cell line, highlighting its promise as a therapeutic candidate. These results underscore the relevance of benzimidazole derivatives in the pursuit of next-generation anticancer drugs and offer valuable insights for advancing molecular design and drug development.

**Key words:** Benzimidazole derivatives, Density Functional Theory (DFT), Cytotoxicity, Anticancer agents, Molecular docking

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# Synthesis and spectroscopic characterization of phosphorylated salophen and salen Schiff base ligands

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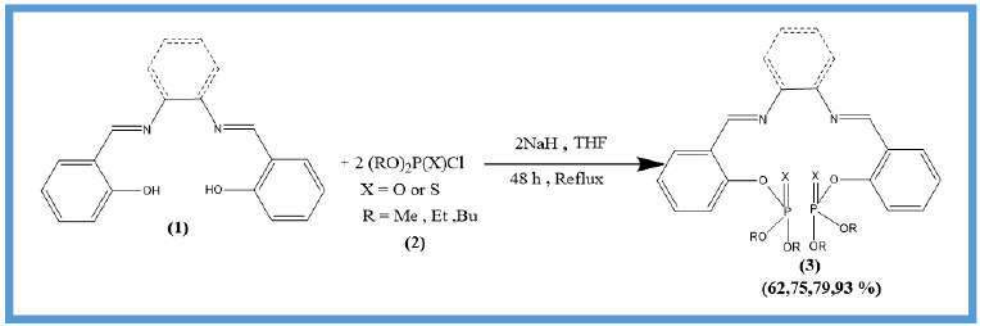
Schiff base ligands are currently attracting attention from many research groups due to their wide-ranging applications in various fields such as biology [1], coordination chemistry, and catalysis [2]. They are studied for their antioxidant, antibacterial, and antiviral properties [3]. As a continuation of our work on organophosphorus chemistry [4, 5], we turn our attention to the phosphorylation of common salophen and salen Schiff base ligands. The reaction was carried out using Schiff bases (**1**) and dialkyl phosphoro- or thiophosphorochloridates (**2**) in THF in the presence of NaH as base to give corresponding diphosphorylated Schiff base derivatives (**3**). These compounds were characterized using multinuclear ($^{1}$H, $^{13}$C and $^{31}$P) NMR and IR spectroscopic techniques. The use of these diphosphorylated Schiff bases (**3**) as potential tetradentate chelate ligands towards different metal ions is ongoing and will be also discussed in detail.




**Key words**: Salophen, Salen, O, O-diethyl chlorophosphate, phosphorylated Schiff bases, NMR

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# Synthesis, structural characterisation, Hirshfeld surfaces and RDG-NCI analyses of new thiophene-based azomethine ligands

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*Research Laboratory for Catalysis and Materials for the Environment and Processes (**LR19ES08**)*

New thiophene-based azomethine ligands were successfully synthesized via a condensation reaction between thiophene-derived carbonyl compound and aromatic amines. The ligands were characterized by FT-IR, $^{1}H$ and $^{13}C$ NMR spectroscopy. Their molecular structures were determined by single-crystal X-ray diffraction, revealing nearly planar geometries stabilized by intramolecular hydrogen bonding and π–π stacking interactions.

To further investigate the intermolecular contacts, Hirshfeld surface analysis was performed, providing quantitative insights into the nature and contributions of hydrogen bonding and van der Waals interactions governing the crystal packing. Comparative analysis showed that substituent variations around the thiophene and aromatic ring significantly influence molecular packing and crystal stability. These results highlight the structural versatility of thiophene-based Schiff bases and their potential as building blocks for coordination and materials chemistry.

Furthermore, the reduced density gradient and non-covalent interaction (RDG-NCI) analysis, in conjunction with the sign($\lambda_2$)ρ function, offers significant insights into the characteristics of intermolecular and intramolecular interactions within the examined system.

**Keywords:** Thiophene; Azomethine; Schiff base; Crystal structure; Hirshfeld surface analysis; X-ray diffraction; Spectroscopic characterization.

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| **A. Yacoub**, Z. Ksibi<br>*FST - Tunis*<br>Catalytic degradation of triclosan using $Fe/ZrO_2$ and $Fe–Co/ZrO_2$ systems | **PC 105** |
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| **D. Douadi**, M. Debiane, S. Benmbarek, A.B. Mammeria<br>*University ofAlgiers1, Algeria*<br>Bioactive profiling of Urtica dioica L. and development of a stable anti-inflammatory topical formulation | **PC 111** |
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# Abstracts of Poster Communications

# Unveiling Structure-Property Relationships in Nitrothiophenes: Strategic Amino Substitution for Tunable Optoelectronic and Nonlinear Optical Properties

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This computational study elucidates the significant effect of amino functionalization on the electronic structure and physicochemical properties of nitrothiophene derivatives. A comparative investigation of 2,4-dinitrothiophene (DNTh) and its amino-substituted analog, 2-amino-3,5-dinitrothiophene (ADNTh), was conducted using density functional theory (DFT) and time-dependent DFT (TD-DFT) at the B3LYP/6-311++G(d,p) level. The introduction of a strong electron-donating amino ($-NH_2$) group at the 2-position induces significant electronic restructuring, manifesting as a drastic reduction of the HOMO-LUMO energy gap, a pronounced enhancement of intramolecular charge transfer (ICT) character, and improved electron delocalization across the π-conjugated framework. This is evidenced by frontier molecular orbital and Natural Bond Orbital (NBO) analyses. Interrogation of the electrostatic potential (ESP) surfaces and density of states (DOS) further corroborates the increased polarity and charge mobility in ADNTh. The computational models exhibit excellent agreement with experimental spectroscopic data (IR, Raman, $^1$H-NMR), validating the predicted molecular structures. Notably, TD-DFT simulations of UV-Vis absorption and emission spectra reveal a marked bathochromic shift and elevated light-harvesting efficiency (LHE) for ADNTh, originating from strong, low-energy $\pi \rightarrow \pi^*$ excitations. These findings highlight the critical role of targeted donor-acceptor molecular engineering in tailoring optoelectronic properties, positioning ADNTh as a highly promising candidate for advanced applications in nonlinear optical (NLO) materials, organic electronics, and photonic devices.

**Keywords:** Thiophene derivatives; Density Functional Theory (DFT); Intramolecular Charge Transfer (ICT); Nonlinear Optics (NLO); Structure-Property Relationships; Donor-Acceptor Systems.

# Enhancing LIG-MOF supercapacitors performance through double pass laser processing

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Laser-induced graphene (LIG) produced by direct laser writing has become one of the most explored techniques for the fabrication of Microsupercapacitor (MSC) electrodes [1]. This study proposes a simple and cost-effective approach to enhance the performance of supercapacitors based on (LIG) functionalized with Metal organic framework (MOF). They are a class of porous, crystalline materials made of metal ions or clusters linked by organic molecules. [2] The use of two consecutive laser passes using the same $CO^2$ engraver on polyimide film led to the expansion in the size of the pores, the increase in the graphitization degree, and the densification of the produced material. The best achieved material displayed an enhancement of the areal energy density from 0.86 to 4.20 mWh/cm2 at 0.02 mA/cm2 and high cycling stability with a capacitance retention rate of 92% after 10.000 cycles.

**Key words:** Laser Induced Graphene, Supercapacitor, Metal Organic Framework,

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# In Silico Selection and Docking Evaluation of Natural Ligands from *Ricinus communis* Methanolic Extract for Antimicrobial Applications

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The identification and optimization of natural ligands from plant extracts offer a sustainable pathway for developing novel antimicrobial agents. In this study, a computational selection and docking approach was applied to explore the bioactive potential of phytochemicals extracted from Ricinus communis leaves. The methanolic extract was characterized using FTIR–NMR spectroscopy, revealing six major constituents: Ricinine (R)**,** Lupeol (L)**,** α-Amyrin (A)**,** Quercetin (Q)**,** Quercetin-3-O-β-D-glucopyranoside (QGP)**, and** Quercetin-3-O-β-rutinoside (QR) **[1].**

Ligand optimization was performed using Chimera, followed by SwissDock molecular docking simulations against twelve microbial protein receptors representing six species: *Staphylococcus aureus*, *Escherichia coli*, *Pseudomonas aeruginosa*, *Bacillus subtilis*, *Saccharomyces cerevisiae*, and *Aspergillus niger*.

The structural elucidation allows the identification of Ricinine (R), Lupeol (L), alpha-Amyrin(A), Quercetin (Q), Quercetin-3-O- β- D-glucopyranoside (QGP) and Quercetin-3-O-β- rutinoside (QR) in the obtained extract.

Our results show that binding affinities (ΔG, kcal/mol) ranged from –5.31 to –11.22, demonstrating significant variation in ligand–receptor interaction strength. Notably, quercetin derivatives (Q, QGP, QR) exhibited the most favorable energies, suggesting a high potential for hydrogen bonding and π–π stacking interactions within active sites.

For *S. aureus*, Ricinine showed strong affinity to 4URM (ΔG = –6.94), whereas QGP and QR bound more tightly to 3FRA (ΔG = –9.60). Against *S. cerevisiae*, QR and α-Amyrin displayed high stability on 4LXJ (ΔG = –11.22). Structure–activity relationship (SAR) analysis confirmed the significance of hydroxylation and glycosylation patterns in improving bioaffinity.

This study highlights *R. communis* as a promising source of natural ligands for antimicrobial drug design. The six evaluated compounds are synergically more active against *Staphylococcus aureus* and *Saccharomyces cerevisiae.*

**Keywords:** Natural ligands selection, *Ricinus communis, Molecular Docking, Antimicrobial activities.*

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# Investigation of Silyl Cation–Lewis Base Complexes: Structural Features and Stability via DFT and NBO Analysis

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This work delves into how steric and electronic influences govern the structural and energetic properties of Si–P bonds within silicon-based cationic systems coordinated to phosphine ligands. Through comprehensive computational analysis, it is shown that $(CH_3)_3Si^+$ forms the most compact Si–P linkages (2.01–2.03 Å), a result of low spatial hindrance and effective orbital overlap. Slightly elongated bond lengths (2.03–2.05 Å) occur with $(C_2H_5)_3Si^+$, while the most extended distances (2.08–2.10 Å) are associated with $Ar_3Si^+$, where both steric congestion and electron-withdrawing aromatic rings impede close approach. The angular parameters reflect similar trends; bulky phosphines such as $(C_2H_5)_3P$ induce broader Si–P–R bond angles (e.g., up to 121° with $Ar_3Si^+$) relative to less hindered analogs like $(CH_3)_3P$.
Energetically, the $(CH_3)_3Si^+\cdots(CH_3)_3P$ pair exhibits the strongest interaction (~–28 kcal/mol), a result of well-balanced spatial arrangement and electrostatic compatibility. In contrast, electron donation trends derived from charge transfer calculations reveal that $(C_2H_5)_3P$ is more effective in transferring electron density than $(CH_3)_3P$, aligning with predictions based on steric and electronic parameters. Natural Bond Orbital (NBO) evaluations further demonstrate that increased σ-donation correlates with greater interaction strength, as evidenced by more negative interaction energies. Conversely, $Ar_3Si^+$ consistently engages in weaker associations, hindered by the electron-withdrawing character of its aromatic substituents.
Altogether, this study emphasizes the nuanced interdependence between geometry and electronic structure in modulating Si–P bonding, offering design principles for future silicon-phosphine architectures relevant to catalysis and materials development.

**Key words:** Sillyl cations, Lewis bases, Density Functional Theory, Natural Bond Orbital analysis.

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# Structure-Guided Crystallisation of Phosphotungstate Keggin Anions with Guanidinium: A Multitechnique Characterisation and Photoredox Study

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A simple and scalable reflux protocol was developed to grow colourless cubic single crystals of $(CH_6N_3)_3[PW_{12}O_{40}]\cdot 4H_2O$ from $H_3PW_{12}O_{40}$ and guanidinium carbonate in a water/acetonitrile mixture at 100 °C for 3 hours. The resulting crystals, with edges up to 0.35 mm, were fully characterised using a combination of techniques including single-crystal X-ray diffraction, FT-IR, solid-state NMR, UV-Vis spectroscopy, and thermogravimetric analysis.

Single-crystal XRD at 150 K revealed a cubic unit cell (Pm-3m, a = 11.9652(2) Å) with the Keggin cluster located on a crystallographic three-fold axis, surrounded by hydrogen-bonded guanidinium cations and four well-ordered water molecules. FT-IR spectroscopy showed a shift in the $\nu(W–O_t)$ band from 968 to 975 $cm^{-1}$ upon incorporation of guanidinium, while the $\nu(P–O_a)$ band at 1081 $cm^{-1}$ remained sharp, confirming the integrity of the Keggin structure.

Solid-state $^{31}P$ MAS-NMR exhibited a single resonance at −14.8 ppm, consistent with an intact cluster, and $^{1}H$ MAS-NMR identified two guanidinium proton environments at 6.8 and 7.2 ppm, along with a broad water signal at 4.1 ppm. UV-Vis spectroscopy (diffuse reflectance) indicated a band-gap of 2.41 eV, which is 0.3 eV narrower than the parent acid, suggesting ligand-to-metal charge transfer involving the guanidinium counter-ion. Solution UV-Vis (258 nm, $\varepsilon = 1.8 \times 10^4\ M^{-1}\ cm^{-1}$) confirmed cluster stability in aqueous media.

Thermogravimetric analysis showed a 5.9 % mass loss between 25 and 150 °C, corresponding to the loss of four lattice water molecules (calc. 6.0 %), with organic decomposition occurring above 285 °C.

Under visible-light irradiation ($\lambda \geq 420$ nm) and in the presence of oxygen, the hybrid material catalysed the aerobic oxidation of benzyl alcohol to benzaldehyde with 88 % conversion and 95 % selectivity after 4 hours (TOF = 11 $h^{-1}$), outperforming the pristine HPOM by a factor of four.

These findings demonstrate that guanidinium carbonate acts as an efficient and eco-friendly structure-directing agent, enabling the rapid formation of cubic hybrid POM crystals with tailored electronic properties for selective photoredox applications.

**Keywords:** Polyoxometalate; Keggin; guanidinium; cubic single crystal; FT-IR; solid-state NMR; UV-Vis; single-crystal XRD; photoredox catalysis

# Hydrogen storage studies of nanocomposites derived from O-ethyl-S-((5-methoxy-1H-benzo[d]imidazol-2-yl)carbonothioate (OESMBIC) with ZnO

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5-Methoxy-2-mercaptobenzimidazole was used to synthesize O-ethyl-S-((5-methoxy-1H-benzo[d]imidazol-2-yl)carbonothioate) (OESMBIC) via reaction with ethyl chloroacetate in a KOH solution. Zinc oxide (ZnO) nanoparticles were prepared by a chemical route under highly alkaline conditions and subsequently employed to form a novel nanocomposite, OESMBIC–ZnO. The obtained ZnO in the nanocomposite appeared as nanorods with varying lengths and diameters between 40–65 nm, decorated with OESMBIC molecules, as confirmed by morphological characterization. Hydrogen storage studies revealed a significant enhancement in storage capacity upon the incorporation of ZnO nanoparticles. Pure OESMBIC exhibited a storage capacity of 0.50 wt.% at an equilibrium pressure of 40 bar, whereas the OESMBIC–ZnO nanocomposite achieved 2.40 wt.% at 60 bar. These findings demonstrate that ZnO incorporation markedly improves hydrogen uptake, suggesting the promising potential of OESMBIC–ZnO nanocomposites for hydrogen storage and sustainable energy applications.

# In silico investigation of the anti-scabies activity of Tea tree essential oil

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**Introduction:** Tea tree oil is known for its medicinal properties, including a promising but underexplored acaricidal activity. With increasing resistance of *Sarcoptes scabiei* to conventional treatments like permethrin and ivermectin, alternative therapy options are urgently needed [1]. **Aim:** This study aims to investigate the molecular mechanisms underlying the acaricidal effects of Tea tree oil by identifying compounds with strong interactions with key parasite proteins and to study their pharmacotoxicological profiles. **Methods:** Using molecular docking and homology modelling, we assessed interactions between Tea tree oil compounds and Scabies Mite Inactivated Protease Paralogs, linked to immune evasion, as well as voltage-gated sodium channels, associated with acaricidal effects. Pharmacokinetic and toxicological profiles were also evaluated.
**Results:** Our findings revealed that most Tea tree oil compounds displayed moderate to good affinity for SMIPP-S-I1, with globulol showing the strongest interaction (-7.6 kcal/mol), while δ-cadinene had the highest affinity for SMIPP-S-D1 (-7 kcal/mol). Viridiflorene, globulol, and viridiflorol exhibited the strongest binding affinity to the sodium channels. All compounds showed good physichochemical properties and favorable tolerability profiles. **Conclusion:** These findings suggest that Tea tree oil contains compounds with potential acaricidal and immunomodulatory effects, supporting its further evaluation through molecular dynamics and experimental validation as a therapeutic option for scabies.

**Key words:** Tea tree oil, Sarcoptes scabiei, molecular docking simulation

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# Characterization and synthesis of a nanocarbon nanomaterial based electrodes for use in an electrochemical process in water treatment

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This research study focuses on the detailed characterisation of a nanocarbon material using eight different methods. These techniques include Fourier transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), Raman spectroscopy, the Brunauer, Emmett and Teller model (measured by BET), transmission electron microscopy (TEM), scanning electron microscopy (SEM), contact angle and physicochemical technique (electrical conductivity of electrodes), and electrochemical measurements (cyclic voltammetry, charge-discharge, electrochemical impedance spectroscopy (EIS), specific capacitance).

All characterizations carried out on the nanocarbon material revealed the exceptional attributes of this material: a considerable specific surface area, an exceptional electrical conductivity and an advanced porous structure. These attributes make it ideal for the production of high-performance electrodes in the context of electrochemical process application.

The manufacture of graphite substrate electrodes using the studied nanocarbon material has been improved to optimize their ion storage capacity. Various parameters such as the type of binder and drying conditions were analyzed to ensure consistent and stable electrode manufacture.

**Keywords:** Electrochemical process, nanocarbon material, electrodes fabrication, water treatment.

# Hydrothermal Synthesis of Monoclinic $WO_3$ Nanorods on FTO Substrates

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Monoclinic tungsten trioxide ($WO_3$) nanorods were directly grown on fluorine-doped tin oxide (FTO) substrates via a simple hydrothermal process. XRD analysis confirmed the monoclinic phase of $WO_3$ on FTO, while $WO_3$ formed in solution exhibited an orthorhombic phase, highlighting the substrate's role in directing nucleation and growth. The crystallite size was estimated at ~38 nm for $WO_3$/FTO and ~42 nm for bulk $WO_3$. SEM images showed dense, vertically aligned nanorods (length: 200–900 nm; width: 90–280 nm), and EDX confirmed the presence of tungsten and oxygen.

This work demonstrates that FTO substrates promote phase control and uniform nanorod formation, making $WO_3$/FTO a promising platform for electrochemical energy storage and related applications.

**Key words:** $WO_3$ nanorods, FTO substrate, hydrothermal synthesis, electrochemical energy storage.

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# Effect of $Lu^{3+}$ ion content on the garnet phase stability and photoluminescence properties of GAG:Ce

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Cerium-activated mixed garnet, with the chemical formula $(Gd,Lu)_3Al_5O_{12}$: Ce, is widely studied due to its broad range of applications, including medical imaging techniques, X-ray computed tomography, and positron emission tomography. Recently, increased attention has been directed toward gadolinium aluminium garnet (GAG), which has received less focus compared to the well-established YAG and LuAG compounds. The structural instability of the GAG lattice is the primary reason for the delayed interest in this material. However, advancements in doping techniques using rare-earth ions with small radii have been successful in stabilizing the garnet structure, opening new possibilities for its application in advanced scintillators. This study aims to examine the influence of Lu3+ ion substitution on the phase stability and luminescent properties of $(Gd_{1-x}Lu_x)_{2.97}$ $Al_5O_{12}$:$Ce_{0.03}$ (x =0, 0.1, 0.2, 0.3, 0.4 and 0.5) synthesized vi sol-gel method. The XRD analysis revealed that the stability of the garnet phase is significantly influenced by $Lu^{3+}$ content substitution and substituting 20% of $Lu^{3+}$ ions (x = 0.2) in the GAG host resulted in a pure garnet phase after heat treatment at 1100°C for 4 hours. A pure perovskite phase was identified in the sample prepared with $x$=0. For $x$=1, mixed phases of garnet and perovskite were observed. A more stable garnet phase was obtained for the nanopowders prepared with $x \geq 0.2$. Photoluminescence spectra exhibited a yellow emission band centered about 520 nm, attributed to 5d → 4f transitions of $Ce^{3+}$ ions. The intensity of this band is affected by the content of substituted $Lu^{3+}$ ion. Indeed, it gradually increases with the $Lu^{3+}$ content, reaching a maximum at x=0.4, and then decreases at x=0.5.

**Keywords:** GAG: $Ce^{3+}$; $Lu^{3+}$ content; phase stabilization; DRX; Photoluminescence

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# Copper-Based Magnetic Nanocomposites for Antibacterial Applications

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Copper-based nanocomposites have attracted considerable attention due to their potential in environmental applications, particularly for controlling bacterial contamination and treating wastewater. In this study, magnetic copper-based nanocomposites were successfully synthesized via a polyol-mediated chemical route. The synthesis parameters were optimized to control particle size and to adjust the composition of the metallic and oxide phases within the materials. Structural properties were characterized using X-ray diffraction (XRD), while morphological and compositional features were examined by scanning (SEM) and transmission (TEM) electron microscopy coupled with energy-dispersive X-ray (EDX) analysis. Magnetic measurements were performed to evaluate the influence of composition and microstructure on magnetic behavior. The antibacterial activity was assessed against both Gram-positive and Gram-negative bacterial strains. The results highlight the promising potential of copper-based magnetic nanocomposites as multifunctional materials with efficient antibacterial activity for environmental applications.

**Key words:** Copper-based nanocomposites, Polyol-mediated synthesis, Magnetic properties, Antibacterial activity.

# A Novel $Fe_2O_3$@DCTA-Ag Nanocomposite Sensor for Sensitive Lead ($Pb^2$) Detection: Applications in Environmental and Food Monitoring

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Lead ($Pb^{2+}$) contamination represents a significant threat to both human health and environmental integrity, underscoring the urgent need for sensitive, selective, and environmentally relevant detection strategies. In this study, we developed a novel nanocomposite, $Fe_2O_3$ nanoparticles functionalized with 4-(3,5-dimethyl-1H-pyrazol-1-yl) carboxylate (DCTA) and decorated with silver nanoparticles ($Fe_2O_3$@DCTA-Ag), through simple and efficient synthesis methods. This nanocomposite was employed to fabricate an electrochemical $Pb^{2+}$ sensor based on differential pulse voltammetry (DPV). Sensor performance was systematically optimized using response surface methodology (RSM) combined with a Box-Behnken design (BBD), assessing the influence of pH, contact time, drop volume, and drying time via a $3^4$ factorial design. A multivariate regression model linked the peak current to these parameters, allowing identification of optimal conditions. Under these optimized settings, the sensor exhibited a wide linear detection range from 0.2 nM to 10 µM, with an impressive detection limit of 0.2 nM. The sensor demonstrated high selectivity toward $Pb^{2+}$ in the presence of interfering ions and maintained consistent performance in both environmental water samples and food matrices (rice, corn, milk, honey, and tea), confirming its potential for practical environmental monitoring and food safety applications.

**Keywords**: Electrochemical sensor, Differential pulse voltammetry (DPV), $Fe_2O_3$ nanoparticles, Environmental monitoring, Food safety, Heavy metal contamination.

# Interaction of bioactive substance with algerian palygorskite

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In light of the increase in bacterial resistance and the limitations of conventional treatments, research is focusing on natural solutions that combine bioactive substances with minerals such as clays. Algerian palygorskite [1-3], due to its adsorbent properties, is an excellent candidate for the development of hybrid biomaterials for therapeutic purposes.
The study focuses on evaluating the interaction of a bioactive substance with palygorskite in order to design a hybrid biomaterial with antibacterial and antioxidant activities. Adsorption experiments were carried out by varying the reaction parameters such as clay mass, contact time, pH, initial concentration of the bioactive substance and reaction temperature. XRD, FTIR and SEM characterized the obtained biomaterial called BS-Sif Pal. The antioxidant (DPPH assay) and antibacterial activities (4 strains of *Escherichia Coli, Staphylococcus aureus, Pseudomonas aeruginosa and Staphylococcus aureus* (MRSA+)) on Muller-Hinton agar were studied.
The optimal adsorption was observed for a clay mass of 100 mg, a contact time of 20 min, a bioactive substance concentration of 1mg/mL and a basic pH at room temperature with pseudo-second order kinetics. The modeling of isotherms shows that the Langmuir model is in agreement with the reaction process. The biological study of the BS-Sif Pal biomaterial showed a significant antioxidant activity with an $IC_{50}$ equal to 2.4mg/mL, as well as a significant antibacterial effect. In conclusion, the biomaterial resulting from the association of a bioactive substance with Algerian palygorskite has promising biological properties. This work opens the door to new pharmaceutical applications.

**Key words:** Algerian Palygorskite, Bioactive Substance, Adsorption, Antibacterial, Antioxidant

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# Theoretical Investigation of New Functional Materials for Optoelectronic Devices

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This study investigates the photophysical and photovoltaic properties of newly designed thiazolic materials using UV–Visible spectroscopy and DFT calculations (Gaussian09). The work focuses on the charge-transfer process between rhodanine-based thiazolic donor structures and fullerene acceptors, analyzed through frontier orbitals, energy gap, density of states, and charge-transfer rate. Photovoltaic performance is evaluated in terms of open-circuit voltage ($V_{OC}$), exciton binding energy ($E_b$), and light-harvesting efficiency (LHE).

**Key words:** Photovoltaic, Rhodanine, DFT, Charge transfer, Energy gap.

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# Photocatalytic Zinc-Based Metal-Organic Frameworks for Selective Oxidation of Biomass-Derived Molecules

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Natural bio-based molecules, including aromatic alcohols such as eugenol, estragole and other compounds derived from plant biomass, are increasingly valued for their potential in the pharmaceutical industry, perfumery, and as chemical intermediates in sustainable processes. Their selective oxidation enables access to structurally complex motifs, highly prized in fine chemistry, such as aldehydes, acids, or functionalized aromatic compounds. Metal-Organic Frameworks (MOFs) [1], particularly as semiconductor supports, facilitate light activation to generate reactive radicals capable of initiating these transformations under mild conditions.

This study reports the hydrothermal synthesis of a zinc-based metal-organic framework (MOF-Zn) using zinc acetate and ascorbic acid in dimethylacetamide. The resulting material was thoroughly characterized by X-ray diffraction, revealing two crystalline phases, and by electron microscopy, showing a nanoscale porous structure. Thermal and spectroscopic analyses confirmed the MOF's stability and coordination environment. Optical absorption and fluorescence spectra highlighted its photocatalytic potential. Additionally, zeta potential measurements demonstrated good colloidal stability, enhancing its suitability for catalytic applications in aqueous media. The synthesized MOF-Zn exhibits promising properties for efficient selective oxidation of biomass-derived molecules under environmentally friendly conditions, contributing to the development of sustainable valorization methods for bioactive compounds.

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# From Posidonia oceanica to Cellulose Nanocrystals: Extraction, Characterization, and Perspectives for Temperature Sensor Applications

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Posidonia oceanica (P.O), a Mediterranean seagrass abundantly found on coastal beaches, is a renewable and lignocellulosic-rich biomass[1,2] with great valorization potential. This study aims to extract and characterize cellulose from P.O residues and convert it into cellulose nanocrystals (CNCs) for potential sensing applications. The biomass underwent washing, drying, grinding, and chemical pretreatments to remove extractives, hemicellulose, and lignin. Delignification was performed using hydrogen peroxide under acidic conditions, followed by alkaline purification with sodium hydroxide. The purified cellulose was analyzed by FTIR, $^{13}C$ CP/MAS NMR, and TGA, confirming cellulose enrichment. Controlled sulfuric acid hydrolysis yielded CNCs, which were neutralized, dialyzed, and sonicated for dispersion. Characterization by FTIR, TGA, and DLS confirmed nanoscale, stable, and highly crystalline CNCs with enhanced thermal stability. Future work targets surface modification of CNCs with chiral and fluorescent molecules to design biocompatible, water-based temperature sensors**.** These responsive materials are expected to react to environmental stimuli[3], offering a sustainable solution for cold-chain monitoring, smart packaging, and biosensing. This research promotes the circular bioeconomy by converting ***P.O*** waste into high-value nanostructured materials with promising technological potential.

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# Synthesis and characterisation of a new sensor for oxytetracycline detection

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The excessive and uncontrolled use of antibiotics has led to their widespread presence in the environment, contributing to the emergence of antibiotic-resistant bacteria and posing serious risks to both ecosystems and human health **[1]**. Detecting and quantifying antibiotic residues has therefore become a major environmental and public health concern. In this context, metal–organic frameworks (MOFs) have emerged as highly promising fluorescent probes for antibiotic detection. Their large surface area, tunable porosity, and chemical versatility allow strong interactions with antibiotic molecules, resulting in fluorescence enhancement or quenching through mechanisms such as electron or energy transfer. MOF-based fluorescent sensors thus provide a rapid, sensitive, and selective strategy for monitoring antibiotic contamination and mitigating its harmful impacts **[2]**.

**Key words:** MOFs, antibiotics, sensors, detection.

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# Effect of nickel and manganese oxides on properties of a carbon matrix based on pyrogallol-formaldehyde

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A carbon matrix (CM) based on pyrogallol-formaldehyde and hybrid nanocomposites (CM/NiO and CM/MnO) were synthesized using the sol-gel method by incorporating nickel oxide and manganese oxide nanoparticles into the carbon matrix. The samples underwent thermal treatment at a pyrolysis temperature of 650°C in a tubular furnace under an inert atmosphere and were characterized using various techniques. XRD analysis reveals the presence of a broad band corresponding to the nanometric structure of graphite, along with two distinct phases: metallic nickel (Ni) in the CM/NiO nanocomposite and manganese oxide (MnO) in the CM/MnO nanocomposite. XPS analysis identifies five prominent peaks in the different samples corresponding to C1s, O1s, Ni2p and Mn2p, Mn3p. The Raman spectra confirm the presence of a disordered graphitic structure in the various materials, as demonstrated by the D to G band intensity ratio, which ranges between 0.7 and 1.5. The impedance plots exhibit semi-circular arcs at different temperatures and two equivalent electrical circuits have been proposed for our materials. The frequency and temperature dependent maxima of the imaginary part of the impedance follow electrical relaxation behavior with activation energies found to be nearly identical to those obtained from dc conductance.

# Textile Dye Decolorization Using Magnetic Chitosan nanocomposite - Immobilized Manganese Peroxidase

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The enzymatic remediation of wastewater presents a promising approach for degrading organic pollutants, with manganese peroxidase (MnP) being a particularly effective biocatalyst. In this study, MnP was extracted from *Anthracophyllum discolor* fungi and immobilized onto a magnetic $Fe_3O_4$/chitosan nanocomposite, which provided a high surface area for enzyme loading. The free enzyme's activity was characterized in terms of pH, temperature, and storage stability. The successful synthesis and immobilization were confirmed through comprehensive characterization using FT-IR, SEM, XRD, and TEM. The nanocomposite demonstrated exceptional efficacy in decolorizing two model textile dyes, achieving removal rates of 98% ± 2% for Reactive Orange 16 (RO 16) and 96% ± 2% for Methylene Blue (MB), a significant enhancement over the free enzyme. Furthermore, the immobilized MnP retained high degradation efficiency over five consecutive reuse cycles, underscoring its operational stability. These results affirm the $Fe_3O_4$/chitosan-immobilized MnP as a highly efficient, durable, and promising biocatalytic platform for the bioremediation of textile wastewater.

**Key words:** nanocomposites, chitosan; enzymes, microorganisms, dye decolorization

# Treatment of textile industry wastewater using adsorption techniques through the application of biological materials

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The dyes released in liquid effluents from textile industries constitute major pollutants based on its impossible or extremely slow biodegradability. Therefore, there is a need to develop efficient methods to remove these pollutants. Adsorption by use of natural materials is among the methods currently adopted to treat contaminated water, orange peels served as newly synthesized material were considered to adsorb two dyes methylene blue and Congo red. A optimization of the production of the biomass showed that the medium that gave a value an important yield of biomass of 6.6 g/L is the medium composed as follow (Liquidize Crypto-Casein Soy Broth supplemented with (yeast (30g/L ), ammonium sulphate (30g/L), magnesium sulphate (30g/L).For powdered bacterial biomass gives a yield of 9.9 % in Congo red discoloration for a concentration in biomass of 0.016 g/L. Concerning methylene blue, an adsorption yield of 59.84% was obtained for a concentration of 0.08g/L. The adsorption kinetics of methylene blue by the biomass of the bacterial consortium gave an adsorption efficiency of 73.75% after 60 min of contact. And for Congo red an adsorption yield of 71.59% is recorded after 60 min of contact.

**Keywords**: textile industries, adsorption, Congo red, Orange peels, methylene blue.

# Electrochemical Monitoring of Ammonium in Aquaponic Systems Using Modified Hydrochar Electrode

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A sustainable aquaponic cultivation system requires rigorous monitoring of water quality, with the concentration of ammonium $NH^{4+}$ being a critical parameter due to its potential toxicity upon excessive accumulation [1]. This study presents the development of a novel electrochemical sensor for the rapid and reliable detection of $NH^{4+}$ to optimize aquaponic system operation.

The sensor is based on a Glassy Carbon Electrode (GCE) modified with magnetized hydrochar (CHT), synthesized via the hydrothermal treatment of a natural biomass mixture: pine cone and eggshell. Characterization using IR, XRD, SEM, and zeta potential confirmed the material's stability, high porosity, and possession of active functional groups suitable for sensing.

The modified GCE was successfully tested for $NH^{4+}$ detection using voltammetry. Optimization of key electrochemical parameters, including solvent choice, pH, concentration, scanning speed, and detection limit, was performed. The resulting sensor demonstrated excellent selectivity, reproducibility, and stability. These superior electrochemical performances validate the modified GCE as a sensitive, reliable, and durable platform for continuous and accurate monitoring of $NH^{4+}$ concentration, offering a promising solution for the effective management and optimization of sustainable aquaponic systems.

**Key words:** aquaponic, ammonium $NH^{4+}$, magnetized hydrochar, eggshell

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# Design a new ZnO/$ZnWO_4$ photocatalysts for high effective degradation of organic compounds under UV-light irradiation: Photocatalytic mechanisms

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In this presentation, novel ZnO/$ZnWO_4$ nanocomposites were synthesized by a two-step process. ZnO nanoparticles were first prepared by precipitation method coupled, and the resulting materials was impregnated by a tungsten chloride solution followed by calcination in air to form ZnO/$ZnWO_4$ nanocomposites. The presence of surface hydroxyl groups was confirmed by X-ray photoelectron spectroscopy, and these hydroxyl groups play a significant role in the photocatalytic activity of the compounds by catching the formed holes in the valence band under irradiation to create the hydroxyl radical, thus improving the photocatalytic property. Zn-$ZnW_{0.2}$ showed the best photodegradation of rhodamine B (RhB), with a rate constant $K_{app}$=0.095 $min^{-1}$ (98.5% degradation) and after 30 min of irradiation under UV-light. This improvement was rationalized by the effective separation of photogenerated electron-hole ($e^-/h^+$) pairs due to the formation of heterojunction structure between $ZnWO_4$ ($E_{CB}$= +0.165 eV; $E_{VB}$ =2.885 eV) and ZnO ($E_{CB}$= -0.365 eV; $E_{VB}$ =3.115 eV). In addition, results confirmed that holes ($h^+$) and $^{\bullet}OH$ radicals are the major reactive species involved in the photodegradation of RhB dye. A possible reaction mechanism was proposed for explaining the photodegradation of RhB over ZnO/$ZnWO_4$ photocatalyst. The Zn-$ZnW_{0.2}$ photocatalyst retained high photodegradation rate and good photostability over four consecutive cycles with no changes in its morphology.

**Keywords:** ZnO/$ZnWO_4$; Photogenerated; Rhodamine B; Photostability; Photodegradation.

# Ultrasound-Assisted Synthesis of Pyrandione Derivatives via p-Toluenesulfonic Acid: Ligand Properties and Metal Coordination

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A novel series of 3,3′-{alkane-α,ω-diylbis[imino-eth-1-ylidene]}bis(6-methyl-2H-pyran-2,4(3H)-dione) derivatives (3c–e) was synthesized through an efficient ultrasound-assisted condensation of diamines with dehydroacetic acid in the presence of a catalytic amount of **p**-toluenesulfonic acid. The structures of the synthesized compounds were confirmed by IR, $^{1}$H NMR, mass spectrometry, and elemental analysis. A plausible tautomeric form of these derivatives is also proposed. Furthermore, these compounds were evaluated as ligands and successfully coordinated with different metal ions, highlighting their potential in coordination chemistry.

**Keywords:** Dehydroacetic acid; Schiff base; Condensation; Catalyst; Ultrasound irradiation; Tautomerism; Metal complexes.

# The conversion of Walnut shells (Juglans regia) biomass into activated carbon

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The disposal of organic waste poses a major environmental challenge [1]. Activated carbon, which possesses highly developed pore structure, is widely used as adsorbents, catalysts and catalyst supports for the removal of pollutant [2]. Walnut shells (Juglans regia) are an agricultural waste rich in carbon, making them a suitable raw material for the production of activated carbon. In an effort to valorize natural resources and reduce pollution, these shells were used to prepare activated carbon. The preparation method involved chemical activation using phosphoric acid followed by a carbonization step. To characterize the resulting material, several properties were studied: pH, moisture content, ash content, and iodine number. A comparison with commercial activated carbon (C. Merck) was carried out regarding the removal of methylene blue using UV-Vis spectroscopy. The results showed that the carbon derived from walnut shells exhibits properties similar to industrial carbon, making it suitable for water treatment applications.

**Keywords:** activated carbon, walnut shells, Juglans regia, carbonization, chemical activation, adsorption

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# Cytotoxicity study and mechanical tests of Bioscaffolds based on Hydroxyapatite with “native” and “degraded” chitosan using a Crosslinker

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The Crosslinking had been widely used to improve the properties of hybrid materials in tissue Enginnering [1]. Hydroxyapatite/ Native and Degraded Chitosan scaffolds were prepared using Freeze Drying and were crosslinked with “glutarledehyde”. The materials were characterized by Infrared Spectroscopy (IR), X-ray Diffraction (XRD)and TGA/DSC analysis. The structure of the scaffolds were observed by Scanning Electronic Microscopy(SEM) and Transmission Electronic Microscopy (TEM).The compression tests were carried out to evaluate the strength of the scaffolds. In addition, cytotoxicity tests are studied to prove that the materials aren’t harmful with fibroblasts cells. The use of a cross linker would offer some new ideas in fabrication of porous scaffolds with enhanced Strength and good bio compatibility [1,2]

**Key words:** degraded chitosan, hydroxyapatite., Crosslinker, Cytotoxicity.

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# Molecular docking analysis on a comparison of two bioactive compounds: DMACB and DNBP.

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This study presents a comparative analysis of two bioactive compounds, 4,4′-dimethylaminocyanobiphenyl (DMACB) and 4,4′-dimethylamino-4-nitrobiphenyl (DNBP), using both experimental and theoretical approaches. The compounds were characterized experimentally by IR, $^{1}$H NMR, and $^{13}$C NMR spectroscopy, while Density Functional Theory (DFT) calculations at the B3LYP/6-311++G(d,p) level were employed to optimize molecular structures and simulate spectra. Theoretical results showed strong agreement with experimental data, confirming molecular geometries and electronic distributions.

Toxicity prediction using Protox II indicated low toxicity, suggesting that both compounds are safe for biological use. Biological activity predictions from the PASS server suggested potential taurine dehydrogenase inhibition. To explore this hypothesis, molecular docking studies were performed using the PDB: 5VN6 enzyme structure. The results revealed favorable binding affinities, with the DMACB–5VN6 complex showing the most stable interaction (binding energy ≈ –6.3 kcal/mol).

These findings demonstrate that DMACB and DNBP possess promising pharmacological potential, and their combined spectroscopic, theoretical, and docking analyses provide valuable insight into their structure–activity relationships.

**Keywords:** DFT, DMACB, DNBP, Molecular docking, Biological activity.

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# Improvement of Iron Oxyhydroxides by Ultrasound-Assisted Synthesis, Study of Phosphate Removal in Aqueous Solutions

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In the present study, ferrihydrite, goethite, and hematite were synthesized under low-frequency ultrasound (20 kHz). X-ray diffraction (XRD) spectra confirm the formation of the three iron oxyhydroxides. Compared to preparation under magnetic stirring, infrared analysis (DRIFT) shows that the amount of surface-adsorbed water is higher in all three cases. Laser granulometry indicates a significant reduction in particle size. In all three cases, the batch removal results of phosphate ions from water by the synthesized oxyhydroxides show a rapid kinetics with an equilibrium time that does not exceed 300 minutes. The pseudo-second-order and Elovich kinetic models fit the experimental data well. Goethite and hematite present similar adsorption capacities, whereas ferrihydrite shows a much higher adsorption capacity. The three adsorption isotherms are well described by the Temkin model, while the Freundlich model fits well for goethite and hematite. In all cases, the Langmuir model is not applicable. All three adsorption isotherms are well represented by the Temkin model, whereas the Freundlich model adequately fits goethite and hematite. In all cases, the Langmuir model is not applicable. Comparison of phosphate removal efficiency between oxyhydroxides prepared under ultrasound and those prepared under magnetic stirring shows improvement for goethite and hematite. The use of ultrasound in ferrihydrite preparation has no effect on its phosphate adsorption capacity.

**Keywords:** Iron oxyhydroxides, Ultrasound, Phosphate, Adsorption, Water treatment

# Élaboration et caractérisation d'un charbon actif microporeux issu de noyaux de dattes sauvages

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Ce travail porte sur la valorisation du noyau de dattes sauvages en tant que précurseur pour la fabrication d'un charbon actif à haute performance. L'élaboration du charbon actif a été réalisée par activation physique. La caractérisation du précurseur et du charbon actif obtenu a été effectuée à l'aide de différentes techniques analytiques, notamment la microscopie électronique à balayage (MEB), la spectroscopie infrarouge à transformée de Fourier (FTIR) et l'étude des propriétés texturales (BET, BJH). Les résultats montrent que le charbon actif présente une surface spécifique élevée (820,25 $m^2/g$ selon BET) et une structure majoritairement microporeuse (82,93%). La spectroscopie FTIR met en évidence la présence de divers groupes fonctionnels tels qu'hydroxyle, carboxyle, éther et ester. Les observations MEB révèlent une surface poreuse bien développée, caractéristique d'un matériau hautement structuré. Ce travail met ainsi en évidence le potentiel du noyau de dattes sauvages comme ressource naturelle locale pour la production de charbons actifs performants, contribuant à la valorisation des déchets agricoles et à la promotion de matériaux durables issus de biomasses abondantes.

**Mots clés :** Noyaux de dattes sauvages, Charbon actif, Activation physique.

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# Development and Characterization of CTS-HEC Films with Enhanced Antioxidation Properties

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Natural polymers are organic compounds derived from natural sources such as plants, animals, and microorganisms. They have been widely used in healthcare due to their biocompatibility, biodegradability, and non-toxic properties. Some common natural polymers include polysaccharides like alginate, chitosan, hyaluronic acid, cellulose and starch, as well as proteins such as collagen, silk, and fibrin.

Chitosan (CTS) and hydroxyethyl cellulose (HEC) are two biopolymers that have garnered significant attention in the field of wound care due to their exceptional biocompatibility, biodegradability, and non-toxic nature. This study investigates the preparation and characterization of CTS-HEC films, with a specific emphasis on their antioxidant activity. The unique properties of chitosan, such as its antimicrobial activity and ability to promote hemostasis, are complemented by the excellent film-forming capabilities and hydrophilicity of HEC, resulting in a synergistic blend.

In this study, CTS and HEC films are prepared through a solution casting method, and their antioxidant activity is investigated using the DPPH (2,2-diphenyl-1-picrylhydrazyl) method, a widely-used assay for measuring free radical scavenging capacity. The FTIR study demonstrated a good combination of the two polymers, confirming that the film has formed well. Additionally, the antioxidant activity of HEC increased when combined with CTS, while the antioxidant activity of CTS decreased in the films, though it did not completely lose its effectiveness. This synergy enhances the overall antioxidant efficacy of the composite material.

**Key words:** Chitosan, hydroxyethyl cellulose, biopolymers, antioxidant activity, wound care.

# Ac conductivity and modulus behavior of $K_{0.12}Na_{0.54}Ag_{0.34}Nb_4AsO_{13}$ compound

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This work investigates the electrical properties of $K_{0.12}Na_{0.54}Ag_{0.34}Nb_4AsO_{13}$ compound synthesized via a solid-state reaction at 800 °C. The crystal structure of this material **[1]** consists of infinite chains of ($Nb(1)O_6$–$Nb(1)O_6$–$As(1)O_4$) units extending along the [100] direction. These chains are interconnected through the sharing of $Nb(2)O_6$ octahedral edges forming a three-dimensional framework with large hexagonal cavities, containing $Na^+$, $K^+$ and $Ag^+$ cations. A Rietveld refinement of the powder diffraction pattern confirmed the formation of a pure phase. Complex impedance spectroscopy was used to study the compound's electrical conductivity, dielectric properties and relaxation behavior over the 240–500 °C temperature range and frequencies between 0.01 and 13000 kHz **[2]**. Similar activation energies, deduced from impedance spectra and $\sigma_{dc}$ conductivity, were found revealing that the relaxation process may be attributed to the same type of charge carriers and the same conduction mechanism based on ion hopping process. The thermal variation of both *ac* and *dc* conductivity follows an Arrhenius-type behavior.

**Keywords:** Impedance spectroscopy, ionic conductivity, dielectric properties, modulus analysis, ac conductivity.

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# Elaboration, structural study and biological activity of a new cobalt complex

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The cobalt(II) complex, diaqua-tetrakis(phosphoric acid)cobalt(II) dichloride dihydrate, $[Co(H_3PO_4)_4(H_2O)_2]Cl_2{\cdot}2H_2O$, belongs to a class of coordination compounds in which cobalt(II) ions are surrounded by neutral phosphoric acid and water ligands. Such systems are of interest due to their rich hydrogen-bonding networks and potential applications in catalysis, materials science, and bioinorganic chemistry. Investigating their structural and physicochemical properties provides insight into metal–phosphate interactions and the role of hydration in complex stability [1].

The elaboration and development of innovative multifunctional complexes represent a cross-disciplinary research area. This is not only because of their fascinating structures and diverse forms but also due to their wide-ranging uses in catalysis, magnetism, optoelectronics, biological and medical sciences [1]. In this context, we have focused our work on the synthesis of a new, unreported cobalt(II) complex with the formula $[Co(H_3PO_4)_4(H_2O)_2]Cl_2{\cdot}2H_2O$. This compound crystallizes in the monoclinic $P2_1/n$ space group with lattice parameters $a = 7.2317(2)$ Å, $b = 11.0769(2)$ Å, $c = 1.0769(3)$ Å and β= 100.197(2). The structure was solved and refined using full-matrix least-squares methods on $F^2$, leading to reliability factors R (F) = 4.41% and wR ($F^2$) = 15.58%. The central cobal(II) ion is coordinated by four O atoms from phosphoric acide ligands and two oxygen atoms from coordinated water molecules, forming a distorted octahedral environment.

The formed layers are interconnected to the framework through O-H…O hydrogen bonds between adjacent ligands. The cobalt(II) compound wast characterized using techniques such as IR spectroscopy and thermogravimetric analysis. In vitro tests were performed to evaluate the antibacterial activity of the synthesized compound against both Gram-negative and Gram-positive bacteria, confirming its biological efficacy.

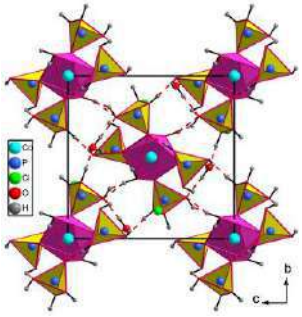


**Figure 1:** Structure of $[Co(H_3PO_4)_4(H_2O)_2]Cl_2{\cdot}2H_2O$ viewed along the a-axis, showing the succession of mixed layers parallel to the (011) plane. The red dotted lines represent hydrogen bonds.

**Key words:** Cobalt complex, structural study, TG analysis, Band gap Energy, Hirshfeld surface analysis and biological activity

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# Ecological Process for Deinking of Waste Paper and Synthesis of Carboxymethylcellulose (CMC) Using Ultrasound Treatment and Bio-based Surfactants.

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Addressing the challenge of cellulosic waste recovery, especially from used paper, is both an environmental and economic priority. This research presents a sustainable deinking method that integrates ultrasound treatment with bio-based surfactants. The proposed technique offers improved deinking efficiency while significantly reducing the environmental impact compared to conventional processes that rely on harsh chemicals [1]. After deinking, the purified cellulose serves as a precursor for synthesizing carboxymethyl cellulose (CMC), a valuable polymer with broad applications in the food, pharmaceutical, and textile sectors [1]. The study explores how variables such as ultrasonic intensity, surfactant concentration, and reaction time influence the deinking yield and the quality of the resulting CMC. Findings reveal that combining ultrasound with bio-based surfactants ensures efficient ink removal and yields CMC with desirable physicochemical characteristics [2]. This approach reflects the principles of green chemistry, providing a sustainable pathway for managing cellulosic waste and generating high-value materials.

**Key words:** Deinking, Ultrasound treatment, Bio-based surfactants, Carboxymethyl cellulose, Waste paper recycling, Green chemistry.

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# Effect of cobalt addition on the electrochemical response of copper sulfides and their application as electrode materials for supercapacitor

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This work focuses on the effect of cobalt addition on the electrochemical response of copper sulfides and their application as electrode materials for supercapacitor. The influence of the copper-to-cobalt molar ratio was investigated in order to optimize the electrode composition in regards to the electrochemical performance.

The elaborated composite materials were characterized by X-ray diffraction (XRD) to characterize the crystal structure, scanning electron microscopy (SEM) to examine the morphology, X-ray photoelectron spectroscopy (XPS) to identify surface elements and their oxidation states and the Brunauer–Emmett–Teller (BET) method was also used to evaluate the specific surface area.

The electrochemical results demonstrate that the composite with a Cu/Co molar ratio of 1:1 exhibits a remarkable specific capacitance of 570 F/g at a current density of 2 A/g, along with excellent cycling stability, retaining 104% of its capacitance after 2000 cycles. These promising results highlight the strong potential of these materials for applications in supercapacitors.

**Keywords :** Advanced materials ; Renewable energy ; Supecapacitors.

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# Grafting of β-cyclodextrin polymers onto lignocellulosic materials for simultaneous removal of Triclosan and Paracetamol from water

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Pharmaceutical and personal care products (PPCPs), including paracetamol (PCM) and triclosan (TCS), are emerging contaminants frequently detected in aquatic environments [1-2]. Their presence raises significant concerns due to their persistence and low removal efficiency in conventional wastewater treatment processes. To address this issue, this study presents the development of a sustainable bioadsorbent synthesized by grafting β-cyclodextrin (β-CD) polymers onto Posidonia oceanica, a Mediterranean seagrass rich in lignocellulosic components. The grafting process utilized citric acid as an eco-friendly crosslinking agent and potassium dihydrogen phosphate as a catalyst. The resulting material (POS-βCD) has been engineered to selectively adsorb polar molecules like paracetamol through a combination of hydrophilic interactions and inclusion complexation. Various formulations were synthesized and extensively characterized by multiple analytical techniques, confirming surface chemical modification and enhanced thermal stability. These bioadsorbents demonstrate promising potential for the simultaneous removal of PCM and TCS from contaminated water, providing an environmentally friendly and cost-effective alternative to conventional adsorbents, while promoting marine biomass valorization within a circular economy framework.

**Key words**: Posidonia, biomaterials, adsorption, Triclosan and Paracetamol

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# Degradation of Acid Orange in Contaminated Water Using Mechanically Alloyed FeCoNi Catalyst and Organic Matter Removal by Coffee Grounds

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A FeCoNi trimetallic powder was synthesized by high-energy ball milling and evaluated for its catalytic efficiency in degrading Acid Orange, an azo dye widely used in textile industries. Structural characterization by X-ray diffraction (XRD) confirmed the formation of a single-phase solid solution with a face-centered cubic (FCC) structure, while scanning electron microscopy (SEM) revealed fine, homogeneously distributed particles with high surface reactivity. The catalytic activity of the FeCoNi powder was tested in aqueous solutions of Acid Orange, and UV–Visible spectrophotometric analysis showed a marked decrease in the absorption band at around 485 nm, corresponding to the cleavage of the azo (–N=N–) bond. To complement the catalytic degradation, waste coffee grounds were employed as a low-cost biosorbent for the adsorption of residual organic matter. The combined use of FeCoNi catalyst and coffee-ground adsorption demonstrated an efficient and sustainable approach for the treatment of dye-contaminated wastewater.

**Keywords:** FeCoNi, high-energy ball milling, XRD, SEM, UV–Vis, azo bond cleavage, coffee grounds, wastewater treatment

# Efficient Cadmium Removal by Bioadsorbents

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Cadmium (Cd(II)) is a toxic priority pollutant that requires efficient and affordable remediation strategies. This study evaluates the performance of four low-cost bio adsorbents: prickly-pear seeds (PPS), Concount shell (CS), and two natural clays (C1, C2) for the removal of Cd(II) from aqueous solutions. The equilibrium data were fitted using equilibrium isotherm models (Langmuir, Freundlich, Temkin and Dubinin–Radushkevich) and kinetic models. Kinetic data were best described by the pseudo-second-order model. Equilibrium analysis showed that CS conformed best to the Langmuir model, whereas PPS, C1 and C2 were better described by the Dubinin–Radushkevich model. These results identify PPS as the most promising adsorbent among those tested.

**Keywords:** cadmium, biosorption, prickly-pear seed, clay, concount shell, isotherms, pseudo-second-order.

# Synthesis, X-ray Crystallography, Spectroscopic Characterization of a New Hybrid Compound: Tris(2,2'-bipyridine) Chloride Manganese(I)

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A new manganese(I) hybrid compound with 2,2'-bipyridine was synthesized and characterized using UV-vis, IR spectroscopies, and single crystal X-rays. Crystals suitable for X-ray analysis were obtained by slow evaporation at room temperature. The structure was determined by single crystal X-rays diffraction at 153 K. It crystallizes in the hexagonal space group P6/mcc with the following unit cell parameters: a = 13.1501(3) Å, b = 13.1501(3) Å, c = 20.9629(6) Å, Z = 2 and V = 3139.35(17) $Å^3$. The structure was solved by direct methods and refined with a final R = 0.0689 for 1355 independent reflections.

The molecular structure of the title complex $[Mn(bipy)_3]Cl$ (**I**) shows that the divalent ion $Mn^+$ is coordinated by six nitrogen atoms from three 2,2′-bipyridine ligands. The average equatorial manganese-pyridine nitrogen bond length (Mn-Np = 2.090(2) Å) and the distance from the manganese and to the six-atom mean plane of the pyridine ring (Mn-Pc = 0.1306(4) Å) are consistent with those observed in other hexacoordinated manganese(I) low-spin complexes. The crystal packing is stabilized by weak non-covalent interactions, particularly C-H··N and C-H··Cl hydrogen bonds to form an expanded supramolecular device.

**Keywords:** Manganese; X-ray; Crystal structure; 2,2′-bipyridine; UV/Visible; Hirshfeld surface.

# The adsorption of nitrophenol in fixed-bed columns and in batches using cheap activated carbon

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This paper describes the synthesis of environmentally friendly, low-cost adsorbents and examines their adsorption capabilities in the removal of 4-nitrophenol from wastewater. Simple analysis, FTIR, and SEM were used to characterize unmodified date palm fibers biochar.

The maximum adsorbed quantities for date palm fibers biochar were determined to be 81.076 mg/g, after isotherm experiments in the batch system were examined. Strong coefficient correlation (R2), low RMSE, and $\chi 2$ in the measurements of isotherms were well-suited for the Langmuir equation.

To assess the column's functionality, fixed bed adsorption was investigated under operational settings, including bed height, 4-nitrophenol flow rate, and 2-nitrophenol inlet concentration.

As the rate flow decreases and bed height increases, breaktime and breakthrough curves both increases.

With 4 cm (0.5 g) of bed height, 160 mg/L of intake 2-nitrophenol concentration, and 2 mL/min rate flow, the highest percentage of 4-nitrophenol solution treated (65.46%) and highest bed capacity of 31.42 mg/g were achieved.

Nelson, the breakthrough curves were fitted using the Yoon and Thomas models. The models exhibit strong behavior of the breakthrough and an R2 that is higher than 0.99, indicating their good applicability.

**Keywords:** 4-nitrophenol, Fixed bed adsorption, batch adsorption, biochar.

# Theoretical Study of the Optical Properties of material $BaTiO_3$

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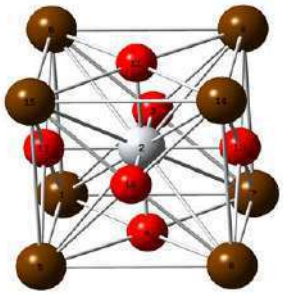
The spectroscopic and photophysical behavior of barium titanate ($BaTiO_3$) and polymer/$BaTiO_3$ composites have been highlighted by a large number of reports in last three decades, due to their luminescence properties. In an attempt to understand these properties, we undertook a theoretical study of polymer/$BaTiO_3$ composites using the density functional method (DFT) and time-dependent (TD-DFT) to determine their geometries and electronic structures DFT method, and also to study their first electronic excitations (energy, nature, transition probability)[1-2].

TD-DFT calculations with the use of hybrid functionals are shown to provide an excellent cost-effective computational approach for the treatment of the excited states of these composites. The present paper can provide the experimentalists with data to develop a working device using this system.



*Barium titanate ($BaTiO_3$)*

**Key words:** Barium titanate; TD-DFT; Absorption spectrum; Charge transfer; electronic; excitations.

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# Herbicidal activity of Eucalyptus aqueous extracts against *Leucaena leucocephala*

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Plant extracts can act as herbicides and represent valuable alternatives to conventional biocontrol products, as they are biodegradable and safe for humans and the environment. In this study, we investigated the allelopathic potential of aqueous leaf extracts from two Eucalyptus species: *E. oleosa and E. socialis,* grown in the Gabès region. This work evaluated both their effect on the germination of *Leucaena leucocephala* seeds, an invasive species, and their impact on seedling root growth.We compared two Eucalyptus species (*E. socialis and E. oleosa*) and two subspecies within each species (*E. socialis subsp. socialis and subsp. viridans; E. oleosa subsp. oleosa and subsp. cylindroidea*), as well as two extract concentrations (5 % and 10 %). Herbicidal activity was generally stronger with *E. oleosa*. Both concentrations caused a significant slowdown in the germination kinetics of *L. leucocephala* seeds and resulted in low final germination rates. The control exhibited a high germination rate (86.65 %), which decreased to 50 % and 45 % with 5 % extracts of *E. socialis subsp. socialis and subsp. viridans*, and dropped further with 5 % extracts of *E. oleosa subsp. oleosa and subsp. cylindroidea* (18.3 % and 11.65 %). At the 10 % concentration, only seeds treated with *E. socialis subsp. socialis* extract germinated, with a final germination rate of 16.65 %.

These preliminary results will be followed by an analysis of the chemical composition of all aqueous extracts.

**Keywords :** *Eucalyptus socialis, Eucalyptus oleosa*, allelopathic activities.

# Carvacrol-Based Antioxidant Cream Formulated with *Thymus vulgaris* Essential Oil

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This study aimed to formulate and evaluate a cosmetic cream containing thyme (*Thymus vulgaris*) essential oil, rich in carvacrol, with a focus on its antioxidant potential. The cream was developed as an oil-in-water (O/W) emulsion using the hot emulsification method. The oily phase consisted of almond oil, beeswax, and emulsifying agents, while the aqueous phase contained distilled water and glycerin. Both phases were heated separately to approximately 70 °C and emulsified under continuous stirring. Once the temperature decreased to around 40 °C, thyme essential oil was incorporated to preserve its volatile and thermolabile compounds. The resulting formulation exhibited a smooth, homogeneous texture and stable physicochemical characteristics, including a pH of approximately 5.5-6.0 and no phase separation upon storage.

The antioxidant activity of the thyme essential oil and the formulated cream was determined using the DPPH free radical scavenging assay. Results showed that thyme essential oil, mainly composed of carvacrol, possessed strong antioxidant activity, while the cream retained about 70-80% of this capacity, indicating partial preservation of its bioactive potential after formulation.

In conclusion, the thyme essential oil-based cream demonstrated notable antioxidant properties, good physicochemical stability, and desirable cosmetic attributes. These findings suggest that thyme essential oil, particularly due to its carvacrol content, could serve as a natural and effective ingredient in antioxidant skincare formulations.

**Keywords:** *Thymus vulgaris*, carvacrol, antioxidant activity, DPPH assay, cosmetic formulation, natural skincare

# Solid State experimental and theoretical studies of a new Nickel based Material properties

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Organic–inorganic framework materials have emerged as a fascinating area of research in the last decades. Since these materials are composed of metal ions or clusters that are connected through molecular bridges, properties inherent to both the inorganic and organic components may be manifested. Their interest may be due to their diversities in structural features and their potential applications in the field of molecular sieves, optical luminescence, non-linear optics, electrical conductivity and magnetic materials.

In this work, we report on structural, vibrational and optical properties of a new member of the family of Nickel based crystals. A new structure consisting of tow octahedral forms was detected by X-Ray diffraction technique. Vibrational properties were studied by performing a room temperature IR and Raman spectra. The optical properties were also investigated using UV-Visible absorption spectroscopy and Photoluminescent measurements on a spin-coated film of the grown crystals. In addition, theoretical calculations performed on an appropriate cluster are done for more suitable discussions of all properties.

# Green Approach to Catechol Detection via CuO@PANI-Based Electrochemical Sensor

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A CuO@polyaniline (CuO@PANI) nanocomposite was synthesized via in situ oxidative polymerization and used to modify a glassy carbon electrode (GCE) for developing a novel electrochemical sensor **[1,2]**. The composite was thoroughly characterized using FT-IR, XRD, TGA, BET surface area analysis, and SEM-EDX with elemental mapping, confirming enhanced structural stability, increased surface area, and improved electrical conductivity due to the synergistic interaction between CuO nanoparticles and polyaniline **[3]**. Electrochemical performance was evaluated by EIS, CV, and DPV, revealing significantly enhanced electron transfer kinetics and excellent electrochemical responsiveness **[4]**. Sensor parameters were systematically Box-Behnken development (BBD) optimization, establishing ideal conditions of pH 7.18, an accumulation time of 4.49 min, a deposition 13 µL of content and the drying period of 3.25 h. In these ideal conditions, DPV measurements exhibited remarkable sensitivity (17.823 µA/µM), a broad linear range of motion (0.001–10 µM) and an extremely low limits of detection of 1 nM. DPV measurements showed high sensitivity (17.823 µA/µM) a wide linear range (0.001–10 µM), and an ultralow detection limit of 1 nM **[5]**. The sensor also demonstrated excellent selectivity against common interfering species and achieved recovery rates of 98–103% in real water sample analysis **[6]**.

**Keywords**: Catechol detection, CuO@PANI nanocomposite, Electrochemical sensor, Box-Behnken Design, Differential pulse voltammetry, Environmental monitoring.

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# Sol-gel synthesis and characterization of $Na_4Co_7(AsO_4)_6$ for visible-light photocatalytic hydrogen production

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$Na_4Co_7(AsO_4)_6$ was synthesized via a sol–gel method to investigate its structural, morphological, and functional properties. X-ray diffraction (XRD) confirmed the formation of a single-phase crystalline material crystallizing in the monoclinic space group C2/m with lattice parameters a = 10.696 Å, b = 14.766 Å, c = 6.677 Å, β = 105.579°. Raman and infrared (IR) spectroscopy identified the characteristic vibrational modes of $AsO_4^{3-}$ groups, confirming well-defined arsenate tetrahedra. Thermal analyses (TG–DSC) and spectroscopy complemented the structural and functional characterization. Scanning electron microscopy (SEM) revealed a homogeneous morphology with well-crystallized and uniformly distributed particles. Photocatalytic hydrogen production under light irradiation demonstrated the compound's promising potential for clean energy applications.

# Conception de nouveaux inhibiteurs anticancéreux du VEGFR2 à l'aide de la modélisation pharmacophorique et 3D-QSAR : Pertinence pour la chimie de coordination

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Les protéines kinases constituent une vaste famille d'enzymes impliquées dans la régulation de la croissance et de la division cellulaires. Parmi elles, les récepteurs à activité tyrosine kinase, tels que le VEGFR2, représentent des cibles thérapeutiques majeures pour le développement d'agents anticancéreux.

Dans ce travail, une approche combinée de modélisation pharmacophorique et de modélisation QSAR tridimensionnelle (3D-QSAR) a été utilisée pour concevoir et cribler virtuellement de nouveaux inhibiteurs du VEGFR2. Quarante modèles pharmacophoriques et 1 440 modèles QSAR 3D ont été générés à partir de 101 inhibiteurs connus du VEGFR2 répertoriés dans la base de données ChEMBL. Les meilleurs modèles ont été sélectionnés sur la base d'une validation statistique rigoureuse, incluant l'analyse des courbes ROC. Ces modèles ont ensuite été appliqués au criblage virtuel de 399 analogues du sorafénib, une molécule de référence. Deux composés ont présenté des valeurs d'$IC_{50}$ prédites inférieures à celle du sorafénib (0,16 nM), et l'un d'eux a révélé des propriétés pharmacocinétiques et de drug-likeness favorables.

Ce cadre computationnel illustre la puissance de la modélisation mathématique et de l'analyse structure–activité dans la conception rationnelle de médicaments. Au-delà des inhibiteurs organiques, cette approche peut également être appliquée à l'étude de composés de coordination à base de métaux présentant un potentiel anticancéreux, ouvrant ainsi de nouvelles perspectives pour la découverte de métallodrogues innovantes.

**Mots clés** : Inhibiteurs du VEGFR2, Modélisation pharmacophorique, 3D-QSAR, Agents anticancéreux à base de métaux, Chimie computationnelle

# Influence of ceria addition in $TiO_2$ and $TiO_2$-$ZrO_2$ aerogel materials on the textural, structural and catalytic properties of supported vanadia in chlorobenzene oxidation

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Vanadia based $TiO_2$ materials constitute a very important class of catalytic materials resistant against chlorinated volatile organic compounds (Cl-VOCs). Besides, the direct incorporation of zirconium species in the $TiO_2$ aerogel support prepared by the sol gel route has generated great interest in the catalytic performances of $V_2O_5/TiO_2$ catalyst in the total oxidation of chlorobenzene. Besides, the combined $TiO_2$–$CeO_2$ mixed oxide has also attracted considerable attention recently as active catalyst as well as support. Therefore, the aim of this work is to study the effect of the direct incorporation of $CeO_2$ in $TiO_2$ –$ZrO_2$ and $V_2O_5/TiO_2$ – $ZrO_2$ aerogel materials prepared by sol–gel route on the physico–chemical and catalytic properties in the total oxidation of chlorobenzene.

$TiO_2$-$ZrO_2$ and $TiO_2$-$CeO_2$-$ZrO_2$ materials were prepared via sol-gel method. To obtain mixed oxides, cerium nitrate and zirconium acetylacetonate were added to titanium isopropoxide according to molar ratios Ce/Ti=0.1 and Zr/Ti =0.1. The gels were transformed into aerogels using supercritical drying process. $V_2O_5/TiO_2$ –$ZrO_2$-$CeO_2$ with 2 wt.% of $V_2O_5$ were prepared using impregnation method. They were calcined for 3h at 500°C under $O_2$ flow and characterized by means of $N_2$ physisorption, XRD, $H_2$-TPR and $NH_3$-TPD.

According to $N_2$physisorption, all catalysts exhibit high surface areas (>110 $m^2/g$) with homogeneous mesoporous distributions. XRD patterns show, in addition to the prominent $TiO_2$ anatase lines, a few peaks belonging to cubic $CeO_2$. Moreover, no vanadia and zirconia pattern was observed. The incorporation of $CeO_2$ increases the surface global acidity of the catalysts ($NH_3$-TPD). TPR results suggest that the doping with $CeO_2$ affects the reduction behavior of vanadium species. Catalytic test results reveal that ceria doped materials is beneficial for the improvement of catalytic properties in chlorobenzene total oxidation. In particular, ceria containing titania-zirconia support had improved catalytic properties at high temperature (400°C). However, when vanadia is present, an enhancement in catalytic performanceis observed in the range 350°C -400°C.

**Key words:** $TiO_2$-$ZrO_2$, $TiO_2$-$CeO_2$-$ZrO_2$, $V_2O_5/TiO_2$ –$ZrO_2$-$CeO_2$**,** cholobenzene oxidation

# Towards Designing a Sandwich-based Lateral Flow Immunoassay to Detect F17-Positive Escherichia coli

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Escherichia coli (*E. coli*) is a common bacterium, with certain pathogenic strains posing serious risks to both human and animal health [1]. Among its virulence factors, F17 fimbriae play a critical role in adhesion and colonization, particularly in calves [2]. This study focuses on the development of a lateral flow immunoassay for the rapid and specific detection of F17-positive *E. coli* strains. This rapid test relies on the capillary migration of the sample along a nitrocellulose membrane, where specific antibodies or antigens are immobilized on the test and control lines to enable capture and visual detection of the target analyte. It represents a simple, rapid, and sensitive approach suitable for point-of-care diagnostics.

Given that the test is composed of four layers; the sample, conjugate, detection and adsorbent pads; optimization of key assay parameters was carried out. These parameters included: (*i*) the choice of specific biomolecules (proteins and/or nanobodies) to be immobilized onto the test and control lines in the detection pad, (ii) the type of nitrocellulose membrane to be used as the detection pad, (*iii*) optimization of the concentration of the blue latex nanoparticle-conjugates to be added to the conjugate pad, and (*iv*) the pretreatment steps for each pad to form the desired test.

Preliminary results indicated that color development at the test line indicates formation of a sandwich complex between the mobilized anti-F17A nanobody conjugates, target F17 fimbriae, and immobilized bispecific nanobodies, confirming the presence of F17-positive *E. coli* and active infection in the animal. Conversely, absence of test line color with control line color development indicates binding of nanobody conjugates with immobilized F17A protein at the control line, confirming the absence of target F17-positive fimbriae of *E. coli* in the sample.

**Key words:** *E. coli*, virulence factors, F17 fimbriae, lateral flow immunoassay.

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# Synthesis and computational studies of the homonuclear complex $[Co_2(\mu-Benz)_2(Benz)_2(Pyr)_4]$ and biological evaluation

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Coordination chemistry of transition metals based on Co has attained importance for its ability to bind dioxygen reversibly. According to their interest structures, some of these complexes displayed interesting pharmacological effects such as antimicrobial, anti-inflammatory, anticancer, antidiabetic, antimalaria and antioxidant activities. In this study, a binuclear cobalt (II) benzoate complex having pyridine as auxiliary ligands was synthesized and characterized by UV–Vis, IR spectroscopy and TG-DTA analysis. The molecular structure of the complex was determined by single X-ray diffraction. Furthermore, by using the density functional theory (DFT) method, all the calculations have been carried out in gas phase with GGA-BLYP method at TZP level. Good consistency was obtained between the calculated and the experimental findings. Moreover, the antimicrobial activity was assessed by agar disk diffusion assay against seven pathogenic strains and the antioxidant activity was established using four different assays. In addition, the *in vitro* anti-inflammatory activity was evaluated by albumin denaturation method.

**Key words:** Binuclear cobalt complex, X-ray, DFT, UV-Vis, Biological activities

# Imidazole-based ionic liquid: Synthesis and study of its performance as an electrolyte.

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Ionic liquids have experienced rapid growth in recent decades thanks to their compelling physicochemical properties [1] notably their strong thermal [2] and electrochemical [3] stability which enable their deployment across many sectors, especially energy storage. Imidazolium salts $[Imim]^+A^-$ comprise the largest family of ionic liquids currently known. Their modular nature makes them amenable to tailored design for a wide range of applications [4], such as enhancing supercapacitor performance.

In this work, we report the synthesis and characterization of allylmethyl-imidazole, and evaluate its reactivity as an alternative electrolyte in conjunction with selected transition-metal sulfides.

**Key words:** Ionic liquids, electrolyte, Imidazolium salts


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# Natural Iron Oxides as Sustainable Adsorbents for Phenol Removal and Regeneration via Photo-Fenton Process

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Industrial wastewater frequently contains phenol, a toxic and persistent organic pollutant widely employed in pharmaceutical, cosmetic, and petrochemical industries. Its effective removal remains a major environmental challenge, requiring low-cost and sustainable treatment approaches. In this work, the adsorption performance of two iron oxides—a natural iron ore (MFnat) and a commercial hematite (OXF)—was evaluated to assess their potential as eco-efficient adsorbents for phenol removal.

Structural and textural characterizations using XRD, BET, FTIR, TEM, and EDX confirmed the amorphous nature and higher specific surface area of MFnat compared to OXF. Batch adsorption experiments revealed that MFnat exhibited nearly three times higher adsorption capacity than the commercial oxide. Kinetic studies fitted both pseudo-first-order and pseudo-second-order models, while equilibrium data correlated with both Langmuir and Freundlich isotherms, indicating the coexistence of mono- and multilayer adsorption. Thermodynamic parameters ($\Delta H°$ and $\Delta G°$) suggested that the process is endothermic and spontaneous.

The regeneration of saturated MFnat was successfully achieved through a Photo-Fenton advanced oxidation process, reaching a phenol degradation efficiency of up to 93%, thus maintaining excellent adsorption recovery.

These findings highlight the potential of natural iron ore as a low-cost, abundant, and sustainable adsorbent for phenol-contaminated wastewater, especially when coupled with efficient regeneration via UV/Fenton treatment.

**Keywords:** Phenol removal, adsorption, iron oxides, natural ore, Photo-Fenton regeneration, wastewater treatment

# Synthesis and Characterization of PMMA-Based Nanocomposites Reinforced with SDS-Modified MgAl-Layered Double Hydroxide (LDH)

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Polymethyl methacrylate (PMMA) is widely used in applications requiring optical transparency; however, its limited thermal and mechanical properties restrict its use in demanding environments [1]. To overcome these limitations, layered double hydroxides (LDH) can be employed as reinforcing agents [2]. In this study, SDS-modified MgAl-LDH nanomaterials, were incorporated into the PMMA matrix at various loadings (0, 3, and 5 wt.%) using a solvent blending technique.

Structural and physico-chemical characterizations were performed using Fourier-transform infrared spectroscopy (FTIR), differential scanning calorimetry (DSC), dynamic mechanical analysis (DMA), and thermogravimetric analysis (TGA-DTG). FTIR spectra indicated successful SDS intercalation and interactions between the LDH and polymer chains. DSC analyses revealed a slight increase in the glass transition temperature (Tg), suggesting restricted polymer chain mobility due to the presence of LDH. DMA results showed an improvement in storage moduli, indicating enhanced mechanical performance. TGA-DTG analyses demonstrated a modest improvement in thermal stability for the nanocomposites compared to neat PMMA.

**Key words:** PMMA, MgAl-LDH, Nanocomposites.

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# Synergistic adsorption–photocatalysis for phenol degradation using S-g-$C_3N_4$/$MnO_2$ ternary composites

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The significant threat posed to environmental health by the presence of toxic and persistent phenolic pollutants in water is widely recognized. To address this challenge, novel nanocomposites were developed through the combination of sulfur-doped graphitic carbon nitride (S-g-$C_3N_4$) with metal oxide nanomaterials based on cobalt and manganese. Two distinct systems were engineered: a binary composite ($C_3N_4$-$MnO_2$) and ternary composites that were further modified with doped graphene quantum dots (GQDs).

The successful formation and strong interfacial interaction within these materials were confirmed by advanced characterization techniques, including SEM, EDS, FTIR, and UV-Vis analyses. The effectiveness of the composites in phenol removal was then evaluated through both adsorption and UV-Visible-light photocatalysis.

The ternary composites were demonstrated to significantly outperform their individual components. This enhanced performance is attributed to superior light absorption, more efficient separation of electrical charges, and faster electron transfer. The overall degradation rates were found to be markedly higher, underscoring the potential of these composites to be utilized as effective and sustainable photocatalysts for advanced wastewater treatment.

**Keywords:** Phenolic pollutants, Sulfur-doped $C_3N_4$, Metal oxide nanocomposites, Heterojunction, Photocatalysis, Water remediation.

# Simple, Low-cost, Ultra-sensitive Electrochemical Platform For clinical monitoring of kidney molecules

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The organic–inorganic hybrid compound [Cu2I2(μ-pyrazine)] was synthesized via a hydrothermal method and characterized using X-ray diffraction (XRD), infrared (IR) and UV–visible. The compound crystallizes in a triclinic system and forms a 2D staircase-like framework. Optical measurements indicate a direct bandgap of 0.95 eV, suggesting semiconducting behavior and potential applicability as a biological sensor. Furthermore, electrodes modified with [Cu2I2(μ-pyrazine)] were evaluated for creatinine detection, exhibiting high sensitivity and selectivity, with a detection limit as low as 1 × 10−8 M. The sensor also demonstrated excellent stability and reproducibility in real sample analyses, achieving recovery rates between 90.3% and 103.9%. These findings highlight the multifunctionality and potential of this hybrid material for applications in both clinical diagnostics and environmental monitoring.

**Key words:** Cu, Semi-conductor, Creatinine

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# Role of long-chain carboxylate ligands in glycerol dehydrogenation catalyzed by Co decorated nanoparticles

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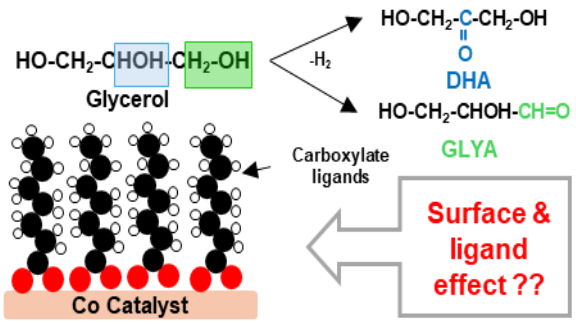


Acceptorless dehydrogenation of alcohol is a green process to obtain several added-value products such aldehydes and ketones and $H_2$. Decorated Co nanoparticles have shown great catalytic activity in this reaction. In this catalytic system, long-chain carboxylate ligands are present to protect the Co nanoparticles from aggregation and oxidation and to stabilize their shape [1-2]. The most active shape is as a nanorod, exposing mainly the Co(0001) and Co(11−20) surfaces. We propose here the combination of classical molecular dynamics and DFT to better understand the role of carboxylate ligands when decorated Co nanorods are used as catalysts in glycerol dehydrogenation. Classical molecular dynamics simulations provided the free energy of adsorption at the interface as a function of the ligand surface coverage on the two mainly exposed facets Co(0001) and Co(11−20). This allows us to determine the possible organization of carboxylate ligands around the active site using DFT to investigate the activity and selectivity of glycerol dehydrogenation into dihydroxyacetone (DHA) or glyceraldehyde (GLYA) on the two exposed facets. We found that DHA, which is the thermodynamic product, is predicted to be the dominant product. Pristine Co(11−20) and decorated Co(0001) are the most active surfaces, showing that the presence of ligands can alter the structure sensitivity of a reaction, an effect that needs to be considered in the design of shaped decorated metallic nanoparticles to be used as catalysts.

**Key words:** Co NPs, ligands, Density functional theory, dehydrogenation of glycerol.

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# Excel Template for Measurement Uncertainty Evaluation Using the GUM Approach: Average Mass and Uniformity Tests for Solid Dosage Forms

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The mass of solid dosage forms directly affects dosage accuracy and product safety. Reliable results require compliance with pharmacopoeial tests for average mass and mass uniformity, as well as adherence to metrological standards, including calibration corrections and measurement uncertainty estimation. This study presents an automated Excel template that calculates average mass, mass uniformity, and Type B measurement uncertainty. The tool applies calibration corrections, evaluates the impact of measurement uncertainty on compliance, and provides traceable, reproducible, and error-reduced documentation suitable for laboratory audits and quality assurance.

**Keywords:** Automated Excel spreadsheet, Mass correction, Measurement uncertainty, Mass uniformity

# Design of a fluorescent chitosan-derived biomaterial incorporating triazole moieties for the selective sensing of aluminum ions in aqueous environments

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The fluorescent biomaterial based on chitosan, ***Cs-Tri-Carb***, has been studied as a selective sensor for metal cations, with a particular focus on the detection of aluminum ($Al^{3+}$) in aqueous media. This material combines triazole units, which act as chelating agents, and carbazole units, which are responsible for its fluorescent properties.

Photophysical characterizations, performed by UV-Vis and photoluminescence spectroscopy, reveal that ***Cs-Tri-Carb*** emits blue fluorescence in dilute solution. Among all the metal ions tested, ***Cs-Tri-Carb*** demonstrates high selectivity and sensitivity towards $Al^{3+}$, with a detection limit of 6.31 µM, well below the maximum value recommended by the World Health Organization for drinking water. These results demonstrate the potential of Cs-Tri-Carb as a selective, sensitive, and reliable fluorescent sensor for the detection of $Al^{3+}$, paving the way for promising applications in the field of environmental monitoring.

**Key words:** Chitosan, click chemistry, triazole, $Al^{3+}$ detection

# Photocatalytic Degradation of Methylene Blue Using a $TiO_2$–Ferrite–Graphene Oxide Nanocomposite

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The textile industry is a major contributor to water pollution due to dye-contaminated effluents, which are resistant to conventional treatment. Among advanced oxidation processes (AOPs), photocatalysis is an effective method for removing such pollutants, owing to the generation of hydroxyl radicals (HO•) that oxidize organic contaminants [1-2].

In this work, a nanocomposite (CMFT/GO) based on titanium dioxide ($TiO_2$), ferrite, and graphene oxide (GO) was synthesized for the photocatalytic degradation of methylene blue (MB). The materials were characterized by XRD, FTIR, and Raman spectroscopy, confirming successful synthesis. Photocatalytic tests showed that the CMFT/GO composite, particularly at 10% loading, achieved high degradation efficiency of MB under visible light irradiation. These findings highlight CMFT/GO as a promising material for wastewater treatment applications.

**Keywords:** $TiO_2$, graphene oxide, ferrite, photocatalysis, dye degradation, wastewater treatment.

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# Advanced Zinc Ferrite Thin Films: From Development to Applications

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The low-cost, solution-based synthesis of advanced zinc ferrite ($ZnFe_2O_4$) thin films by chemical bath deposition (CBD) is a key enabler for their large-scale application. This work presents a detailed investigation of porous $ZnFe_2O_4$ nanoarchitectures directly grown on stainless steel substrates via this facile method. A suite of characterization techniques was employed to fully elucidate the material's properties. X-ray diffraction (XRD) confirmed the formation of a pure, crystalline spinel phase, while profilometry verified the uniform thickness and strong adhesion of the film. Morphological analysis via scanning electron microscopy (SEM) revealed a highly porous, interconnected network of nanoflakes. This porous architecture was quantitatively validated by BET surface area analysis. Furthermore, Fourier-Transform Infrared (FTIR) and Raman spectroscopy analyses unequivocally confirmed the spinel structure through the identification of characteristic metal-oxygen vibrational modes, ensuring phase purity. The combination of the porous, high-surface-area morphology, confirmed crystallinity, and robust substrate integration establishes this CBD-synthesized $ZnFe_2O_4$/SS system as a versatile and promising platform. The detailed structural-property relationships outlined in this study provide a foundational blueprint for its potential exploitation in a wide range of applications.

**Key words:** $ZnFe_2O_4$/SS, Thin films, Chemical Bath Deposition, Porous Nanoarchitectures.

# Comparative Study of Pure and Multi-Cation Lithium Phosphates with Carbon Coating: Structure, Morphology, and Electrochemical Properties

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In this study, single-component ($LiMnPO_4$, $LiFePO_4$, $LiCoPO_4$, $LiNiPO_4$) and multi-component high-entropy phosphate $LiMn_{0.25}Fe_{0.25}Co_{0.25}Ni_{0.25}PO_4$, with and without carbon coating, were synthesized and systematically investigated as potential cathode materials for lithium-ion batteries. X-ray diffraction (XRD) confirmed the formation of a pure olivine-type orthorhombic phase, while FTIR and Raman spectroscopy provided insights into the structural and surface properties. Electron microscopy (SEM, TEM, HRTEM) revealed homogeneous particle morphology and confirmed the presence of an amorphous graphitic carbon coating. Electron paramagnetic resonance (EPR) highlighted the presence of paramagnetic defects associated with transition-metal ions, contributing to electronic conduction. Thermogravimetric analysis (DTA/TGA) quantified the carbon content and demonstrated good thermal stability of the composites. Electrochemical impedance spectroscopy (EIS) showed that the carbon-coated multi-component phosphate exhibited the lowest charge-transfer resistance and enhanced ionic/electronic conductivity, directly correlated with improved electrochemical performance. These findings underline the synergistic effect of high-entropy mixing and conductive carbon coating in optimizing the structural stability and charge transport properties of olivine-type $LiMPO_4$ cathodes.

**Keywords:** Conventional solid-state reaction; Lithium phosphates ($LiMPO_4$); Raman / FTIR spectroscopy; Carbon coating; Electrochemical Impedance Spectroscopy.

# Chitosan with π-conjugated units based on Triazole in the side chain As a fluorescence sensor for $Cd^{2+}$ cations in aqueous media.

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This study contributes to biomass valorization via the design of a novel functional fluorescent biomaterial based on chitosan, developed as a fluorescence probe for the detection of cadmium ions ($Cd^{2+}$) in aqueous media. Indeed, the design of our biomaterial is based on a macromolecular architecture strategy, incorporating a triazole complexing agent and a conjugated fluorescent system onto the chitosan side chain. The synthesis was achieved using click chemistry and Wittig reactions, yielding a water-soluble polymer with good thermal stability up to 290 °C.

Photophysical characterization by UV-Vis and fluorescence spectroscopy confirmed that **Cs-tri-Van-Naph** is an organic semiconducting biomaterial, exhibiting blue fluorescence in dilute solution. The sensing assays demonstrated a highly selective and sensitive "turn-on" fluorescence response toward $Cd^{2+}$ ions over competing metal cations. A detection limit of 3.48 µM was determined, underscoring the probe's capability to detect trace levels of cadmium in environmental samples. These findings establish **Cs-tri-Van-Naph** as a promising, biosourced fluorescent sensor for monitoring $Cd^{2+}$ contamination in water.

**Key words:** Chitosan, chemical modification, fluorescent bio-sourced material, fluorescent sensor, DFT studies.

# One-Step Electrodeposition of $MFe_2O_4$/TMD Heterostructures as Bifunctional Electrodes for Overall Water Splitting

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The urgent demand for clean and renewable energy has positioned water electrolysis as a pivotal technology for efficient hydrogen generation. To address this, we developed a series of bimetallic $MFe_2O_4$ nanocomposites directly fabricated on electrode substrates via a facile one-step electrodeposition method. This innovative synthesis ensures excellent electrical contact and integrates the advantageous properties of $MFe_2O_4$-inspired nanocomposites. The resultant $MFe_2O_4$ nanostructures, characterized by their cubic spinel configuration, form numerous interconnected nanosheets. To further enhance the catalytic activity and stability, these $MFe_2O_4$-modified electrodes were functionalized with a layer of transition metal dichalcogenides (TMDs). This synergistic coupling creates a hierarchical heterostructure that provides a vast surface area, promotes exceptional interfacial activity, and facilitates charge transfer, significantly enhancing the electrocatalytic redox reactions for water splitting. Electrochemical findings confirms that the TMD-functionalized $MFe_2O_4$ nanocomposites serve as exceptional dual-functional catalysts for both the hydrogen evolution reaction (HER) and the oxygen evolution reaction (OER). This is demonstrated by their low overpotentials and small Tafel slopes, which indicate fast reaction kinetics and high electrical conductivity. When configured in a two-electrode system for overall water splitting, with the functionalized electrode serving simultaneously as both the cathode and anode, the device achieves a low cell voltage and demonstrates remarkable long-term durability.

**Keywords:** Electrodeposition of $MFe_2O_4$, Electrocatalytic water splitting, Overall water splitting**,** Hydrogen Evolution Reaction (HER), Oxygen Evolution Reaction (OER).

# Modified Pectin from Mespilus germanica Leaves as a High-Efficiency, Eco-Friendly Corrosion Inhibitor for Mild Steel

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The development of sustainable corrosion inhibitors derived from renewable agro-resources has gained significant interest due to environmental and safety concerns associated with traditional synthetic compounds. In this study, a pectin-rich biopolymer extracted from Mespilus germanica leaves was examined as an eco-friendly corrosion inhibitor for mild steel in 1 M HCl solution. Structural characterization using FTIR, GC–MS, and SEC confirmed the presence of a highmolecular-weight pectic polysaccharide mainly composed of galacturonic acid. Both native pectin (NPS) and its chemically modified derivative (MPS) were tested using weight-loss measurements, potentiodynamic polarization (PDP), and electrochemical impedance spectroscopy (EIS). Results showed that inhibition efficiency increased with higher inhibitor concentration, reaching 82.62% for NPS at 1 g/L and 92.46% for MPS at 3 g/L. Electrochemical studies indicated a significant rise in charge-transfer resistance and a decrease in double-layer capacitance, suggesting the formation of a stable, compact protective film on the steel surface. Adsorption behavior followed the Langmuir isotherm, with calculated $\Delta G°_{ads}$ values ranging from −23 to −26 kJ $mol^{-1}$, indicating spontaneous and mainly physical adsorption enhanced by structural modification. Surface protection provided by MPS was improved due to stronger polymer-metal interactions and greater film compactness. These results demonstrate that Mespilus germanica–derived modified pectin is a promising green corrosion inhibitor for industrial use, aligning with recent advances in natural polysaccharide-based anticorrosion materials.

**Key words:** Green Corrosion Inhibitor, Mespilus germanica Pectin, Adsorption, Mild Steel, Electrochemical measurements, Chemical Modification

# Multifunctional Cellulose Composite Adsorbent for High-Efficiency Congo Red Removal

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Industrial activities, particularly those related to textiles, plastics, paper manufacturing, cosmetics, and food processing, generate large quantities of wastewater containing synthetic organic dyes. These dyes are known for their toxic, carcinogenic, mutagenic, and teratogenic effects, making their discharge into natural ecosystems extremely hazardous for both plant and animal life **[1]**. Various physical and chemical treatment methods have been proposed for dye removal, including catalytic degradation, membrane filtration, advanced oxidation, flocculation, and adsorption **[2]**. Among them, adsorption remains one of the most attractive due to its simplicity, high efficiency, low energy requirements, versatility, and cost-effectiveness.

Considering this, the present work focused on removing Congo Red from water using a multifunctional cellulose composite adsorbent prepared from cress seed powder.

The physicochemical properties of the developed material were characterized using $N_2$ physisorption, FTIR spectroscopy, $pH_{PZC}$ measurements, Boehm's titration method and XRD analysis. Furthermore, the influence of key operational parameters, including the initial dye concentration, solution pH, temperature, contact time, and adsorbent dosage, was systematically evaluated under batch conditions to optimize the adsorption performance. The synthesized composite exhibited remarkable removal efficiency toward Congo Red, achieving up to 96% elimination.

**Key words:** Water treatment, Adsorption, Congo red, Cress seed, Composite

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# Green Synthesis of Iron Oxide Nanoparticles from Orange Peel Extract

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The objective of this research was to develop a simple, effective, and environmentally-friendly method for synthesizing iron oxide nanoparticles (FeONPs) using a green synthesis approach based on vegetal waste derived from *orange* peels. The primary goal was to produce FeONPs with potential antioxidant properties. Ferrous sulfate was used as the precursor for nanoparticles synthesis. The resulting FeONPs which were analyzed and characterized using XRD, SEM, FT-IR, and TGA techniques.

**Highlight**: Orange peels, nanoparticles, extract, iron oxide

# Computational and Biochemical Investigation of IDO1 Inhibition by Synthetic and Natural Compounds

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Indoleamine 2,3-dioxygenase 1 (IDO1) is an immunoregulatory enzyme involved in the catabolism of tryptophan along the kynurenine pathway. Recent studies have highlighted its crucial role in chronic inflammation, particularly in obesity-related metabolic disorders. The overexpression of IDO1 in adipose tissue contributes to local and systemic inflammation by modulating immune responses and promoting insulin resistance. In this study, we investigate the potential of IDO1 as a therapeutic target in obesity-induced inflammation. Through molecular modeling and literature analysis, we explore known inhibitors of IDO1 and evaluate their capacity to reduce inflammatory signals. Our findings suggest that selective IDO1 inhibition could represent a promising strategy to alleviate inflammation and improve metabolic outcomes in obese individuals.

# Optimization of $MgAl_2O_4$ spinel synthesis from dissolution solutions of waste aluminum dross and dolomite

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Magnesium aluminate spinel ($MgAl_2O_4$) is an excellent structural ceramic of great technological importance. It has many attractive properties such as: high melting point (2135°C), very high hardness (16 GPa), relatively low density (3.58 g/cm3), high resistance against chemical corrosion, high thermal shock resistance, and low thermal expansion coefficient. These features make the use of $MgAl_2O_4$ spinel very desired in several technical and industrial applications such as refractory material, high temperature and erosion resistant windows, optical windows for pressure vessels.

Conventionally, $MgAl_2O_4$ spinel can be prepared by solid phase reaction of magnesium oxide (MgO) and alumina ($Al_2O_3$). Unfortunately, the involved costs are high due to the raw materials price and the very high temperature required for the achievement of the reaction (T>1600°C).

Aluminum industries generate large quantities of aluminum dross that are harmful for health and environment. Aluminum dross contain a significant amount of alumina ($Al_2O_3$) associated to other chemicals such as metal oxides (CaO, MgO, and $SiO_2$). Over the last few decades, several research studies have been conducted on the use of aluminum dross in the production of high purity α-alumina, γ-alumina, aluminum sulfate, calcium aluminates, to manufacture refractory materials and active catalyst, to make spinel composites, and only few research works were devoted to the synthesis of $MgAl_2O_4$ spinel.

In this work, we were interested to the study of the synthesis of $MgAl_2O_4$ spinel from local aluminum dross (AMR company, El-Eulma, Setif, Algeria) and local dolomite ore (Djebel Teioualt, Ain M'lila, Algeria). Aluminum dross serves as alumina ($Al_2O_3$) source and dolomite serves as MgO source. The process adopted is based on chemical dissolution in sulfuric acid ($H_2SO_4$) followed by precipitation by $NH_4OH$ and completed by thermal calcination. First, we prepared the two dissolution solutions of the two starting materials, aluminum dross and dolomite. We then made several mixtures of these two dissolution solutions with different volume ratios. We then led the precipitation tests, at different temperatures, by adding $NH_4OH$ to the prepared mixture solution. The precipitated species were calcined at different calcination temperatures and subjected to characterization to identify the formed phases. The obtained results are promising and have highlighted the possibility of synthesizing spinel ($MgAl_2O_4$) as principal phase by precipitation at 40°C of the $M_3$ mixture ($V_{dolomite\ solution}$ /$V_{Al\text{-}dross\ solution}$ = 14) and calcination at relatively low temperature (1100°C).

**Key words:** Aluminum dross, alumina, dissolution, precipitation, spinel.

# Photocatalytic Activity of Gd-Doped ZnS Multifunctional Nanomaterials

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In the present study, rare earth gadolinium elements doped high-active ZnS semiconductor nanoparticles (NPs) were developed [1]. The nanomaterial was prepared via a facile aqueous route using zinc acetate as Zn source and cetyltrimethylammonium bromide (CTAB) as ligand and stabilizer agent. The microstructure of the obtained NPs was characterized using XRD and TEM techniques. Elemental analysis was performed to prove the purity of the sample using EDX measurement. The optical response of the Gd-doped ZnS NPs was performed via a UV–visible spectrophotometer to further characterize the gap energy of the nanomaterials [2]. A photocatalytic test was also performed to evaluate the photodegradation activity of the doped semiconductor. According to the preliminary results, we found that Gd-doped ZnS NPs exhibited high photocatalytic activity after the doping process compared to bare ZnS.

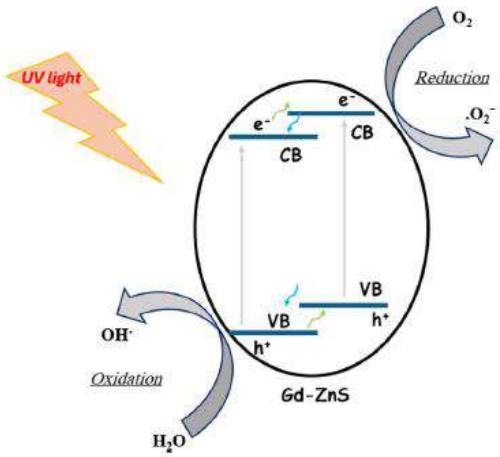


**Figure.** Proposed photodegradation mechanism using Gd-doped ZnS NPs.

**Key words:** Synthesis, Nanomaterial, Semi-conductor, photocatalytic.

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# Facile synthesis of a novel $FeS_2/BC/TiO_2$ composites for enhanced RhB removal from aqueous solution

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In this study, a novel $FeS_2/BC/TiO_2$ composite was synthesized through a simple and environmentally friendly hydrothermal method, enabling the simultaneous valorization of agricultural waste (biomass-derived biochar, BC) and mining waste (natural pyrite, $FeS_2$). This sustainable strategy transforms low-cost and abundant resources into a high-value functional material for the treatment of contaminated water.

The combination of BC, natural pyrite and $TiO_2$ yielded a promising photocatalyst capable of efficiently degrading Rhodamine B (RhB) under light irradiation. This work revealed that the photocatalytic removal of RhB was significantly improved when using $FeS_2/BC/TiO_2$ composite as a catalyst.

The as-prepared composite integrates the synergistic properties of biochar, which enhances adsorption and electron transfer, pyrite, which provides strong redox activity, and $TiO_2$, renowned for its photocatalytic efficiency.

Preliminary results demonstrate rapid degradation of RhB, confirming the high potential of the $FeS_2/BC/TiO_2$ composite as a multifunctional material for sustainable wastewater treatment. This work introduces an innovative approach to the valorization of agricultural and mining wastes, contributing to the development of promising hybrid materials with high environmental performance.

**Key words:** $FeS_2/BC/TiO_2$ composites; Heterogeneous photocatalysis; RhB; Water purification.

# Synthesis, characterization, DFT and molecular docking study of a potential antiviral drug, the 6-methoxylated derivative of favipiravir

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Favipiravir has recently attracted considerable attention as an effective antiviral against RNA-based viruses, like SARS-CoV-2 virus. Here, the 6-methoxy-3-hydroxypyrazine-2-carboxamide, a favipiravir's derivative was synthetized for the first time in presence of $Fe^{3+}$. The reaction product was successfully separated, washed and fully characterized using various analytical techniques including single-XRay, IR, UV and $^{1}H/^{13}C$ NMR. The crystal structure and IR data exhibit the exclusive existence of enolic form in the solid state. UV and NMR data highlighted that the tautomeric equilibrium of the molecule in solution depends on the proton donor effect of the solvent. Consequently, the enol tautomer is exclusively present in aprotic solution. The DFT theoretical data confirm that the enol form of the methoxylated derivative is more stable comparing to favipiravir due to the change in electronic distribution. Moreover, basing to DFT, a smaller energy gap and a higher value of chemical potential (μ) for the synthetized derivative, designate a propensity for increased chemical reactivity. Additionally, the studied compound was docked on SARS-CoV-2 main protease (6LU7) and spike receptor-binding domain (7BZ5) to evaluate the binding affinity. The docking simulation predict that the two forms of the molecule had high binding affinity to the critical amino acids residues of the receptors thanks to several hydrogen bonds and hydrophobic interactions with the enol form. Finally, the druglikness prediction estimated promising pharmacologic properties including adequate bioavailability, favorable tissue distribution, predictable metabolic pathways, manageable elimination routes, and a low probability of causing significant toxicity. These results collectively conduct to conclude that the synthetized product could present a promising potential drug against inflection diseases caused by RNA-based viruses.

**Key words**: COVID-19, Favipiravir derivatives, single-XRay, DFT, Molecular docking.

# A New Nickel(II) Iminopyridine Complex: Synthesis, Characterization, and Computational Exploration for Catalytic and Drug Design Potential

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The structural organization of redox-active ligands plays a crucial role in organometallic chemistry because it influences the reactivity and stability of transition metal complexes. This research deals with the synthesis and characterization of a novel series of nickel(II) complexes, including an additional newly synthesized complex, with iminopyridine-based ligands.

The ligands were synthesized by a condensation reaction between pyridine-2-carboxaldehyde and primary aromatic amines, and subsequently, the nickel (II) complexes were derived by the reaction of the ligands with $NiCl_2{\cdot}6H_2O$.

Box-Behnken Design (BBD) was employed to optimize the synthesis conditions, with priority given to reaction time, temperature, and ligand equivalents.

The complexes were characterized by various techniques, including infrared spectroscopy, UV-visible spectroscopy, X-ray diffraction, and electrochemical studies. In addition, DFT calculations and ADMET predictions were used to investigate their molecular structure, reactivity, and potential drug-like properties. The results show that the complexes, including the new complex, exhibit significant redox activity, stable chelation with nickel(II), and favorable electronic properties, demonstrating their potential for further applications in catalysis and drug design.

**Keywords:** α-iminopyridine ; Nickel complexes; Box-Behnken Design (BBD) ; DFT calculations; ADMET predictions.

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# Comparaison des performances du chitosane et du chitosane modifié dans l'adsorption d'un colorant textile

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Cette étude porte sur l'élimination d'un colorant textile synthétique, complexe ferrique trisodique du N-methyl-1,8-naphtalimide-4-sulfonate, à partir d'eaux contaminées en utilisant deux biosorbants : le chitosane industriel et une forme modifiée par le fer. Les matériaux ont été caractérisés par FTIR, DRX et pHpzc, révélant des modifications structurales liées à l'incorporation du fer.

Les essais en mode discontinu ont montré que le chitosane enrichi en fer présente une capacité d'adsorption nettement supérieure, atteignant 96 % d'élimination du colorant, avec un équilibre établi en 120 minutes pour les deux adsorbants. L'étude cinétique a confirmé l'adéquation du modèle pseudo-second ordre, tandis que les isothermes se rapprochent du modèle de Freundlich, traduisant une adsorption multilayer sur surface hétérogène.

Le comportement vis-à-vis du pH s'est révélé déterminant : le chitosane brut est plus efficace en milieu basique, alors que la version modifiée conserve une performance optimale en milieu acide. De plus, une agitation modérée a été identifiée comme condition idéale, assurant à la fois une diffusion adéquate et une meilleure efficacité d'adsorption.

Dans l'ensemble, ces résultats démontrent le potentiel du chitosane, et plus particulièrement de sa version fonctionnalisée au fer, comme alternative durable, économique et respectueuse de l'environnement pour le traitement des eaux usées chargées en colorants textiles.

**Key words:** adsorption, colorants textiles, chitosane, chitosane modifié.

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# Thorough DFT design of 2D single and multilayers and 1D zigzag (n,0) single walled nanotube platinum disulfide ($PtS_2$)

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In this contribution, we focus on studying dimensionality quantum confinement effect for designing stable 1D and 2D low dimensional platinum disulfide $PtS_2$ layered materials. Their structural and dynamic properties are obtained by employing density functional theory (DFT) at the B3LYP level of theory. Geometry optimizations combined with the calculation of the elastic tensor elements reveal that the 2D monolayer, multi-layers and the 1D rolled up (n,0) zigzag single walled nanotube family of $PtS_2$ are mechanically stable. Then, IR and Raman spectra were simulated by using the coupled perturbed Hartree-Fock/Kohn-Sham CPHF/KS approach which confirms dynamic stability of all forms. Quantum confinement from 3D bulk to 2D single and multi-layers breaks the symmetry and affects the lattice dynamics. Two groups of phonon modes are present in the IR and Raman spectra of (n,0) zigzag nanotube family in the frequency range from 200 to 400 $cm^{-1}$ tend to the active modes of the 1T $PtS_2$ single layer. Our simulation offers a pathway for the design of dynamic stable low dimensional transition metal dichalcogenides, and will pave the way to broad investigation on such class of 2D and 1D nanomaterials.

**Keywords:** DFT, monolayer, multilayers, single walled nanotube, lattice dynamic.

# Impact of Saccharin and SDS Additives on the Microstructural and Surface Characteristics of Ni–Fe Alloy Coatings

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This study systematically investigates the synergistic effects of saccharin and sodium dodecyl sulfate (SDS) additives on the structural and morphological properties of electrodeposited Ni-Fe coatings. Copper substrates were electroplated in a sulfate-chloride electrolyte under controlled conditions (pH 5.5, 1 A/dm², 10 min), with saccharin (0-0.5 g/L) and SDS (0-0.9 g/L) concentrations varied to optimize coating performance. Comprehensive characterization via SEM, XRD, and crystallite size analysis revealed that saccharin significantly refines grain structure, achieving minimal crystallite size (25 nm) and optimal surface homogeneity at 0.33 g/L. Conversely, SDS (0.4-0.6 g/L) reduced grain size to 18 nm but induced porosity and roughness at higher concentrations (0.9 g/L) due to hydrogen evolution. XRD analysis further demonstrated that SDS modulates phase homogeneity, suppressing secondary Ni-Fe alloy formation at elevated concentrations. The combined additives promoted (111)-oriented face-centered cubic (FCC) growth, enhancing microstructural integrity. Optimal parameters 0.33 g/L saccharin and 0.4-0.6 g/L SDS yielded coatings with refined grains, reduced internal stresses, and improved corrosion resistance. These results provide critical insights for tailoring high-performance Ni-Fe coatings in magnetic and anti-corrosion applications.

**Key words:** Electrodeposition, Ni-Fe coatings, Saccharin, Sodium Dodecyl Sulfate (SDS), Morphology, Grain refinement, Phase orientation.;

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# Synthesis and Biological application of New Pyrazolo-Triazaphophosphorin-2-Oxide Derivatives

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A new series of pyrazolo-triazaphosphorine derivatives was synthesized and characterized using NMR, IR, LC-MS, and elemental analysis. The series of phosphorus products were screened for their antifungal activities and for their antibacterial activities. Finally, the antioxidant activity was tested for one of them (**2a**). The results were compared with biological activities of some drugs and demonstrate that the antibacterial and antifungal activities of **2 a–f**, are influenced by the variation of the group R, R' and the donor or attractor effects of the group R'. Likewise, the donor effect of the group in compound 2 e has a positive influence on the antifungal activity and **2e** reacts against *Alternaria alternata* with the lowest IC50= 0.795 µg mL 1 than drug. The phosphorus products can be used as some antibacterial and antifungal agents and one of the compounds (2a) have an excellent antioxidant power.

# Characterization and Functional Evaluation of a Polysaccharide Extracted from Illicium verum as a Sustainable Bio-based Material

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The growing interest in bio-based materials has promoted the exploration of natural polysaccharides for environmental and cosmetic applications [1] [2]. In this study, a water-soluble polysaccharide was extracted from *Illicium verum* (star anise) and characterized using FTIR, UV–Vis, and SEC analyses. The results revealed the presence of typical carbohydrate functional groups and a homogeneous molecular weight distribution, indicating good structural stability. The polysaccharide exhibited promising emulsifying and rheological properties, suggesting its potential use as a natural stabilizer in oil-in-water emulsions. Moreover, its biodegradability and non-toxicity highlight its potential as a sustainable alternative to synthetic polymers in cosmetic and pharmaceutical formulations. These findings contribute to the development of functional bio-based materials derived from renewable resources, in line with current trends in green chemistry and sustainable materials design.

**Keywords:** *Illicium verum*, polysaccharide, bio-based materials, emulsions, sustainability

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# Green Synthesis and Characterization of Metal Oxide Nanoparticles Using Medicinal Plant Extracts: A Sustainable Approach for Functional Nanomaterials

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**Purpose:** This study explores an eco-friendly approach for the synthesis of metallic nanoparticles using plant-based extracts as natural reducing and stabilizing agents. The objective was to combine the bioactive potential of local medicinal plants with the advantages of nanotechnology to produce metal oxide nanoparticles via green synthesis. This work aimed to establish sustainable protocols that maintain reproducibility, purity, and the physicochemical performance of the resulting nanomaterials.
**Methods:** Plant decoctions and hydrodistillates were prepared under controlled conditions of pH, temperature, and agitation. These aqueous extracts were used as reducing agents to synthesize nanoparticles of $Fe_3O_4$, ZnO, MgO, and NiO from corresponding metal salts. The reactions were optimized through controlled addition of NaOH, moderate heating, and magnetic stirring. The synthesized nanoparticles were purified, dried, and characterized using X-ray Diffraction (XRD), Laser Granulometry, Scanning Electron Microscopy (SEM), and Vibrating Sample Magnetometry (VSM). Structural, morphological, and magnetic analyses were performed to confirm nanoparticle formation, crystallinity, and magnetic response.
**Results:** XRD analysis confirmed the crystalline structure of $Fe_3O_4$, MgO, ZnO, and NiO nanoparticles, with crystallite sizes ranging between 5 and 20 nm as estimated by the Scherrer equation. Laser granulometry revealed overall particle sizes from 129 nm up to 2700 nm, depending on the plant extract, reflecting varying degrees of agglomeration. SEM images of NiO nanoparticles showed predominantly spherical morphology with notable polydispersity, consistent with granulometric data. Magnetic characterization of $Fe_3O_4$ nanoparticles exhibited soft magnetic behavior with a saturation magnetization (Ms) of 45.358 emu/g, coercivity (Hc) of 25.75 Oe, and very low remanence (Mr = –1.646 emu/g), indicating excellent reversibility and suitability for biomedical or environmental applications.
**Conclusion:** The successful green synthesis of $Fe_3O_4$, MgO, ZnO, and NiO nanoparticles using plant decoctions demonstrates an efficient, sustainable alternative to conventional chemical methods. The natural polyphenols and flavonoids of plants acted as effective reducing and stabilizing agents. The obtained nanoparticles display desirable crystalline, morphological, and magnetic properties, highlighting their potential for biomedical, pharmaceutical, and environmental applications. This work confirms the promise of green nanotechnology as a bridge between phytotherapy and materials science.

**Keywords:** Green synthesis, Metal oxide nanoparticles, Plant extracts, Characterization, Eco-friendly nanotechnology

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# Characterization of Powders Properties for Optimizing Tablet Compression and Performance

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Recent advances in the characterization of solid-state materials have significantly improved understanding of powder behavior during tableting. This study explores how comprehensive characterization of powder and excipient properties can guide the rational design of robust solid oral formulations. Conducted within the framework of a neuroprotective BCS Class II drug development, the work integrates classical and modeling-based approaches to elucidate the relationships between material properties, compression behavior, and tablet performance.

Key solid-state parameters - including particle size distribution, density, flowability, and moisture content - were systematically characterized to assess their influence on compressibility and compaction. Quantitative evaluation using the Heckel and Kawakita models provided insight into plastic deformation, packing behavior, and densification mechanisms, offering a deeper understanding of the mechanical properties of the excipients. The combination of these models enabled a refined assessment of compressibility and tool–material interactions, revealing that theoretical suitability for direct compression does not always translate to industrial feasibility.

By coupling advanced characterization methods with experimental formulation design, a series of optimized formulations (F1–F6) was developed using direct compression and wet granulation. The results highlight the value of solid-state characterization in predicting and resolving practical manufacturing challenges such as sticking and poor compressibility. This study demonstrates how integrating mechanistic modeling and material science characterization can advance the development of high-quality, robust solid dosage forms.

**Key words:** Compression, Powder compressibility, Heckel model, Kawakita model, solid state

# Valorization of Citrus Waste : Green Synthesis of $SmFeO_3$ Nanoparticles for Water Remediation and Crop Development

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This study presents an innovative and eco-friendly approach for the synthesis of samarium ferrite ($SmFeO_3$) using lemon juice as a natural chelating agent. The formation of a pure perovskite phase upon calcination at 800 °C was confirmed by X-ray diffraction and infrared spectroscopy. The functional properties of the green-synthesized material were evaluated for water treatment applications, where it demonstrated a significant efficacy in reducing water salinity. Furthermore, the use of water treated with this $SmFeO_3$ powder exhibited a remarkable beneficial impact on barley seed germination and seedling development, promoting a high germination rate and enhancing the growth of roots and shoots. These findings underscore the potential of this sustainably synthesized perovskite material for environmental remediation and for enhancing agricultural productivity.

# Theoretical Investigation of the Vibrational Spectroscopic Signatures of Glyphosate Dimers: Unified Assignment method of IR spectra in Gas and Condensed Phase

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A Theoretical study of the vibrational spectra of glyphosate (N-phosphonomethylglycine) [1,2] in the gas phase and condensed media is reported. Band assignments are given in the 1800-850 $cm^{-1}$ range based on the analysis of the spectral changes from low to high pH values (2-11). The infrared region 4000-1800 $cm^{-1}$ is found to be different for gas, liquid and crystal phases of glyphosate. Our vibrational analysis reveals the presence of bands at 3500-3400 $cm^{-1}$ assigned to specific (OP)-O-H….O=(COH) intermolecular H-bonds, characterizing either zwitterionic-zwitterionic or anion-cation paired structure of ionized glyphosate dimers in aqueous solution. There is no evidence of any absorption band(s) in 3200-3500 $cm^{-1}$ in the observed IR spectrum of glyphosate in crystal phase. This underscores the tendency of glyphosate to form stable H-bonded glyphosate dimers via the self-association of phosphonate and carboxylate zwitterionic structures of monomers in aqueous solution and gas phase. These results highlight the importance of phase-dependent analysis in understanding the full IR spectroscopic profile and molecular interactions of glyphosate.

**Key words:** Quantum Calculation, DFT, Solvation, SMD, Empirical dispersion correction Glyphosate, IR vibrational analysis.

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# Functionalized Cobalt based Metal-Organic Framework as an Efficient Electrocatalyst for Water Splitting

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The urgent demand for efficient hydrogen generation is a major force behind the search for clean and renewable energy. In this search, water electrolysis is commonly seen as a very promising technique. A particular class of materials, known as metal-organic frameworks (MOFs), has shown great potential for the water-splitting reactions at the heart of this process. This promise comes from their exceptional qualities, such as a vast surface area, a high density of metal sites, and electronic structures that can be finely tuned.

In this study, a specific MOF based on cobalt, named Co-BDC, was created using a solvothermal method. To understand its properties, the material was carefully analyzed with a suite of characterization techniques, including X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), and scanning electron microscopy (SEM). Its surface area was measured, and its structure was found to be uniformly porous, a feature that aids in the efficient movement of electrical charge.

The material's performance was then tested in electrochemical reactions. The results showed that Co-BDC is an excellent catalyst for both producing hydrogen (the Hydrogen Evolution Reaction, HER) and oxygen (the Oxygen Evolution Reaction, OER). This was confirmed by its low overpotentials and small Tafel slopes, key metrics that indicate fast reaction speeds and good conductivity, underscoring its practical potential for efficient water electrolysis.

**Keywords:** Bimetallic Metal organic framework, electrocatalysis, green hydrogen, Water splitting**.**

# Eco-designed hydroxyapatite–magnetite nanocomposites mediated by carbohydrates: Biofunctional characterization and potential for biomedical applications

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The eco-designed synthesis and biofunctional evaluation of hydroxyapatite–magnetite (HAp–$Fe_3O_4$) nanocomposites were performed using natural carbohydrate-based agents—fructose, galactose, and pectin—as reducing and stabilizing agents, to investigate the influence of saccharide type on structural organization and biological activity for biomedical applications. Nanocomposites were prepared via aqueous co-precipitation followed by mild thermal treatment. Their structural and morphological properties were characterized by X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), scanning electron microscopy coupled with energy-dispersive spectroscopy (SEM–EDS), and vibrating sample magnetometry (VSM) [1-2]. Antimicrobial activity was evaluated against representative Gram-positive and Gram-negative strains using agar diffusion and minimum inhibitory concentration assays, and molecular docking simulations were performed to explore interactions between the nanocomposite surfaces and bioactive molecules. The nature of the carbohydrate significantly influenced both crystallinity and magnetic behavior: fructose promoted the formation of highly crystalline hydroxyapatite, while galactose and pectin produced partially carbonated apatites incorporating quasi-superparamagnetic $Fe_3O_4$ domains. Antimicrobial effects were observed against *Bacillus subtilis* and *Candida albicans* with MIC values of 512 µg/mL and 1024 µg/mL, respectively, while other strains were unaffected. Molecular docking indicated strong binding with 5-fluorouracil, suggesting efficient adsorption and sustained release. These results demonstrate that eco-designed HAp– $Fe_3O_4$ nanocomposites combine biocompatibility, magnetic responsiveness, and selective biological activity, highlighting their potential as multifunctional platforms for drug delivery, antimicrobial coatings, and regenerative medicine.

**Key words:** Hydroxyapatite, Magnetite, Nanocomposites, Green Synthesis.

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# Analyse chimique de la composition de l'extrait de l'alaterne *Rhamnus alaternus* famille de Rhamanaceae

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En Algérie, les hépatopathies constituent un problème de santé publique majeur et le recours à la phytothérapie en général et à la consommation de l'alaterne en particulier s'avère propice. Cette étude met en lumière la composition chimique de cette plante utilisée pour le traitement des affections hépatiques en Algérie.

L'analyse phytochimique a confirmé la présence de nombreux métabolites secondaires dans l'extrait aqueux de la plante, tels que les polyphénols, flavonoïdes, tanins, et alcaloïdes, contribuant à l'activité antioxydante et hépatoprotectrice. L'extrait de l'alaterne révèle une teneur importante voire satisfaisante en polyphénols. L'identification des polyphénols par HPLC a permis de détecter plusieurs substances actives et l'analyse des spectres Infrarouge révèle l'existence des trois groupes avec des propriétés phytochimiques en commun.

**Mots clés :** Alaterne, Phytochimie, HPLC, Infra Rouge, Hépatopatoproctrice.

# Enhanced properties of semiconducting ZnO nanorods for potential energy applications

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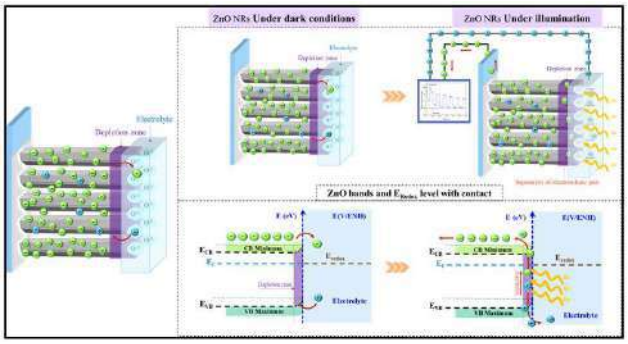
Nanostructured materials have attracted significant attention in several applications owing to their exceptional and tunable properties. The advancement of nanocrystalline semiconductor materials properties enables their exploitation in a wide range of technologies, their elaboration in nanoscale plays a crucial role in determining the properties and functionalities of nanostructured materials and directly influencing their performance. Consequently, nanocrystalline systems have emerged as key materials in recent years for solar energy and environmental applications. ZnO based devices find use in diverse areas such as photovoltaic cells for electrical power generation, photo(electro)catalysts for solar fuel production, degradation of organic pollutants, and energy storage devices, including batteries, capacitors, and supercapacitors. In particular, the crystalline structure plays a crucial role in determining the properties and functionalities of nanostructured materials, directly influencing their performance. The effect of ZnO seed layer thickness on the ZnO nanorods (NRs) properties was investigated. Different characterization and analysis were conducted using X-ray diffraction, atomic force microscopy (AFM; MFP-3D; Asylum Research) and scanning electron microscopy (SEM) for the crystal structures and morphologies, respectively. All samples exhibited a highly Würtzite-type with a preferential growth along (002) planes. The crystallite size (D) increases while micro-strain (δ) decreases with the increase in ZnO seed layer thickness. Atomic force microscopy (AFM) and scanning electron microscopy (SEM) measurements point out the surface topography, roughness, verticality, density and diameter of the nanorods with the change of the thickness of seed layer. Optical characteristics were investigated through transmission measurements; the optical band gap energy (Eg) was found to correlate inversely with Urbach energy and surface roughness as a function of ZnO seed layer thickness. Photocurrent measurements confirm the n-type conductivity excepted from Mott-schotky plots for all the samples. The photocurrent response and the charge transfer resistance were dependent on ZnO seed layer thickness. The improvement of structural and morphological properties, combined with high transparency in the visible spectral region and the enhancement of electrical performance of electrodeposited ZnO NRs, enable their integration into a wide range of nanostructured-based devices. The improvement in transparency and carrier density, with increasing ZnO seed layer thickness, coupled with the enhancement of crystallinity and morphology, helps to overcome existing limitations and boost the performance of ZnO-based devices. The obtained results helps to understand and correlate between structural characteristics and the electrical and optical properties of ZnO NRs and highlight on ZnO NRs as a non-toxic material synthesized through a low-cost growth technique.




**Key words:** photovoltaic, energy, ZnO, nanostructures

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# Synthesis and Photophysical Characterization of a Novel Triazole-Based *p*-phenylenevinylene Organic Material

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This abstract outlines the design of a new semiconducting polymers ***(P1BPAC2)***, which combines a highly emissive typical PPV chromophore with chelating triazole units. The synthetic strategy begins with the preparation of the dipole and dipolarophile. The dipole is obtained via azidation of 4,4′-diamino-2,2′-stilbene disulfonic acid, a PPV-derived fluorophore exhibiting strong emission and high aqueous solubility due to its sulfonic acid groups, yielding the azido-functionalized derivative ***DASS-N₃***. The dipolarophile is synthesized through propargylation of vanillin ***(VAN-TRIP)***.

The dipole ***(DASS-N₃)*** and dipolarophile ***(VAN-TRIP)*** are then coupled via a click chemistry reaction, forming the triazole-containing motif ***DASS-Tri-VAN***, known for its strong chelating properties. This motif is subsequently engaged in a Wittig reaction with a phosphonium salt ***(Bis A)***, previously prepared through sequential alkylation, chloromethylation, and phosphination ***(Bis Ph3)***.

The resulting polymer, ***P1BPAC2***, demonstrates good solubility in polar organic solvents such as DMF, DMSO, and THF. Its molecular structure was confirmed using NMR and FT-IR spectroscopies. The intrinsic optical properties of this π-conjugated polymer were characterized by UV–vis absorption spectroscopy, while the HOMO and LUMO energy levels were estimated through cyclic voltammetry, highlighting its potential for electronic and optoelectronic applications.

**Key words:** Semiconducting, organic material, Triazole, optoelectronics properties

# Non-Centrosymmetric Hybrid Selenomolybdate for Advanced Optical Applications: A Combined Crystallographic and Theoretical Study

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Hybrid materials incorporating polyoxometalates (POMs) are attracting considerable interest due to their adaptable structures and promising functional properties [1]. Our research successfully created a new hybrid material made of ethylenediamine and selenium molybdate, formulated as $(C_2H_{10}N_2)_2[Se_2Mo_5O_{21}]\cdot 2H_2O$. This was synthesized under mild aqueous conditions and evaluated through structural study and theoretical investigation. Its orthorhombic crystal structure, with non-centrosymmetric space group $P2_12_12_1$, exhibits a robust supramolecular network stabilized by extensive N–H···O and O–H···O hydrogen-bonding interactions and electrostatic interactions between the $[Se_2Mo_5O_{21}]^{4-}$ clusters and the protonated ethylenediamine units. Within this architecture, water molecules significantly influence the spatial organization of the macromolecule and enhance the network's aggregate resilience. Density functional theory (DFT) calculations complement the experimental results, providing new insights into the electronic structure, HOMO-LUMO energy gaps, and charge distribution. Analysis of the Hirshfeld surface further elucidates the dominant non-covalent interactions governing crystal packing. This comprehensive study highlights the pivotal role of ethylenediamine in fine-tuning both the structural framework and the electronic landscape of the selenomolybdate network. The chirality of the material endows it with remarkable nonlinear optical (NLO) properties [2], making this hybrid an excellent candidate for next-generation optical devices and paving the way for innovative optical technologies.

**Keywords:** Hybrid-selenomolybdate material • Crystal structure • Hydrogen bonds • Theoretical investigation • Nonlinear optical properties.

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# $Bi_2WO_6/WO_3/g\text{-}C_3N_4$ ternary nanocomposite-modified glassy carbon electrode for sensitive photo-electrochemical detection of dopamine

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Dopamine is an essential neurotransmitter involved in critical physiological processes, and its sensitive and selective detection is of great importance. In this work, we developed a novel photoelectrochemical (PEC) sensor based on a triphasic $Bi_2WO_6/WO_3/g\text{-}C_3N_4$ (BWWCN) composite. The synergistic interaction among the three components enhances light absorption, charge separation, and electron transfer. BWWCN was synthesized via a hydrothermal method and deposited onto a glassy carbon electrode (GCE). XRD, TEM, and UV-Vis characterizations confirmed the successful formation of the composite. The band gap of BWWCN (2.65 eV) is lower than those of the individual components. Photoluminescence (PL) analysis revealed significantly reduced electron–hole recombination, following the order $Bi_2WO_6$>$WO_3$>g-$C_3N_4$>BWWCN. The sensor exhibited superior PEC activity and was evaluated using cyclic voltammetry and differential pulse voltammetry. It showed a wide linear detection range (0.01–110 µM), a low detection limit (0.01 µM), and excellent stability and reproducibility. Its effectiveness was demonstrated in saliva samples, confirming its potential for real-world dopamine monitoring.

# Synthesis of Chromium Doped g-$C_3N_4$/$CeO_2$ with Enhanced Visible-Light Photocatalytic Levofloxacin Degradation

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In this work, a novel binary g-$C_3N_4$/$CeO_2$ nanocomposite doped with chromium by different doping percentages (1%, 3%, 5%) is used for the photocatalytic degradation of levofloxacin under visible light irradiation. The prepared photocatalysts by the hydrothermal method were characterized by XRD, SEM, HTEM and studied by UV, PL and CV. The UV-visible reflectance spectra showed a shift of the absorption edge to a longer visible region upon loading $CeO_2$ with Cr thus forming new dopant energy levels that facilitate the interfacial charge transfer of both electrons ($e^-$) and holes ($h^+$) implying an enhanced photocatalytic activity of the nanocomposites in the visible region. The experimental photodegradation results reveal that the g-$C_3N_4$/$CeO_2$(Cr3%) photocatalyst exhibits the highest photocatalytic activity, with 100% degradation efficiency after 90 min under visible light irradiation. Recycling tests suggest a high photostability and reusability of the photocatalyst. Schematic diagram for the possible photocatalytic mechanism of the Cr doped g-$C_3N_4$/$CeO_2$ composite under visible light irradiation.

# Synthesis and characterization of binary and ternary composites based on organic polymers/transition metals. Study of electrochemical behavior

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This work aims to enhance the electrical properties of polyaniline (PAni) through the synthesis of binary and ternary composites with PEG and various inorganic fillers (ZnO, $Fe_2O_3$) [1-2]. Oxidative polymerization was followed by physicochemical (FTIR/ATR, SEM, XRD) and electrochemical (CV, EIS) characterizations. FTIR analysis revealed intermolecular interactions within the hybrid systems. SEM showed good dispersion of metal oxides (notably ZnO) in the polymer matrix. XRD confirmed the crystallinity of the composites. CV and EIS analyses demonstrated enhanced electrochemical performance, especially with ternary blends PAni/PEG/5%ZnO/5%$Fe_2O_3$ and PAni/PEG/10%ZnO/10%$Fe_2O_3$. These systems exhibited high specific capacitance, low resistance, and good reversibility. The synergistic effect of the fillers is crucial to optimize conductivity, stability, and capacitance. The results highlight the strong potential of these composites for applications in super capacitors and electrochemical sensors.

**Keywords**: Supercapacitor, Polyaniline, Impedance spectroscopy, Cyclicvoltammetry.

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# Computational Design of an Amino-Functionalized MOF for the Mitigation of Greenhouse and Toxic Gas Emissions

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The increasing atmospheric concentrations of pollutant gases such as carbon dioxide ($CO_2$), sulfur dioxide ($SO_2$), and hydrogen sulfide ($H_2S$) pose serious environmental and health threats, contributing to climate change, acidification, and air toxicity. These emissions, largely derived from fossil fuel combustion and industrial processes, underscore the urgent need for efficient gas capture and mitigation strategies. In this study, we design and investigate ZTF-1, a novel zinc-based metal–organic framework (MOF) constructed from 3,5-amino-1,2,4-triazolate linkers. ZTF-1 is developed through the structural modification of MAF-66 by substituting a hydrogen atom with an amino group ($–NH_2$), thereby enhancing the framework's chemical functionality and gas affinity. Using Grand Canonical Monte Carlo (GCMC) simulations, we systematically evaluate the adsorption performance of ZTF-1 toward $CO_2$, $SO_2$, and $H_2S$ under both dry and humid conditions. Particular attention is devoted to competitive $CO_2/H_2O$ adsorption and to the distinct interaction mechanisms governing $SO_2$ and $H_2S$ uptake. The results highlight ZTF-1 as a promising candidate for selective gas capture and environmental remediation applications.

# Oilfield produced water treatment using the microalgae *Chlorella pyrenoidosa* and biofuel production

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Oilfield-produced wastewater (OPW) supplied by the local petroleum industry was directly employed, without prior treatment, as a growth medium for the outdoor cultivation of the microalga *Chlorella pyrenoidosa*. The study aimed to assess both algal biomass production and its effectiveness in wastewater purification. Cultivation was performed in open raceway ponds exposed to natural sunlight in a desert environment. After 21 days of culture, the maximum biomass concentration reached 1.15 ± 0.07 g/L. FTIR analysis was applied to evaluate the lipid content of *C. pyrenoidosa* cultivated in both OPW and BG11 media. Environmental conditions during the experiment included daytime temperatures ranging between 26–31 °C and solar irradiation peaking at 1036 ± 30 W/m² around midday, with an average of no less than 10 hours of sunlight daily. The results demonstrated notable pollutant removal, with reductions in COD, $NH_4^+$-N, TN, and TP of 89.67%, 100%, 57.14%, and 75.51%, respectively. In addition, significant biosorption of heavy metals was observed, achieving removal efficiencies of 73.39% for Cu, 72.80% for Pb, and 48.42% for Cd. The oil content extracted from this microalgae was approximately 37.35%. Chemical analyses also revealed the presence of fatty acid methyl esters (FAME), compounds considered suitable for biodiesel production.When compared with conventional activated carbon treatment, the *C. pyrenoidosa*-based system proved to be a promising and eco-friendly alternative for simultaneous wastewater treatment and biomass production.

**Keywords:** Microalgae, Produced water, Wastewater bioremediation, Biomass production, Open raceway pond, biodiesel.

# Effect of flame retardants on the Thermal and Mechanical properties of PVC

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Plastics, particularly polyvinyl chloride (PVC), are widely used in various industrial applications due to their low cost, lightweight nature, corrosion resistance, and ease of processing. However, their inherent thermal and mechanical limitations restrict their performance under demanding conditions. In this communication, we present the study's results of the effect of mineral additives incorporation: aluminum hydroxide (ATH) and magnesium hydroxide (MDH), in the presence of calcium carbonate ($CaCO_3$), on the thermal and mechanical properties of the polyvinyl chloride (PVC) properties—used specifically for electrical cables.

PVC compounds were prepared with different amounts of ATH and MDH, along with $CaCO_3$, which increases stiffness without greatly reducing flexibility. Thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC) revealed notable improvements in thermal stability with the addition of hydroxides. Fire resistance also increased, as confirmed by UL-94 flammability tests and higher oxygen index values. These results confirm that reinforcing PVC cables with ATH and MDH significantly improves both thermal stability and mechanical performance.

# Optical Properties of Thue-Morse Quasi-Periodic One-Dimensional Photonic Crystals

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Quasi-periodic one-dimensional Thue-Morse [1] photonic crystals were fabricated by depositing alternating layers of silicon and silica using radiofrequency magnetron sputtering with cold plasma [2]. The reflectance spectra of these quasi-crystals reveal a broad photonic band gap that spans the key optical telecommunication wavelengths of 1.33 µm and 1.55 µm in the infrared region at normal incidence. The experimental results show excellent agreement with theoretical predictions obtained using the transfer matrix method. To further optimize the optical performance of these filters for telecommunication applications, we propose a hybrid multilayer system that integrates two types of photonic arrangements: periodic and Thue-Morse quasi-periodic. The proposed structure exhibits a significantly higher maximum slowing-down factor compared to the conventional Thue–Morse multilayer. This enhanced configuration demonstrates precise control over light propagation [3], enabling functionalities such as bending, switching, and reflection, which are crucial for advanced photonic and optoelectronic devices.

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# Mechanism and Selectivity of Synthesis Nanometallic with Pd-Ni@2-Mercaptoethanol as Effective Catalyst for Suzuki-Miyaura Reactions

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Finding new strategies that are clean, economical and more environmentally friendly involves the development of certain catalytic processes for chemical reactions. The palladium-catalyzed Suzuki coupling reaction is one of the most efficient strategies for constructing a carbon–carbon bond. In recent years, bimetallic catalysts have become candidates for the Suzuki coupling reaction. Nowadays, interest is focused on the synthesis of new compounds with potential applications, such as in cancer diagnosis and tumor therapy. In this work, Pd-Ni@2-Mercaptoethanol nanoparticles were synthesized for the Suzuki-Miyaura cross-coupling of arylboronic acids with aryl bromides, in the N,N-dimethylformamide/water mixture catalyzed by Pd-Ni: A simple and efficient reaction performed in a solvent, without a ligand, and in open air. We found that the Suzuki-Miyaura reactions are remarkably fast (5 min), with high yields and the products are highly pure. The Pd-Ni@2-Mercaptoetanol nanoparticles have a narrow size distribution with a mean crystallite size of 10 nm. Radical scavenging activities of the complexes have been evaluated by using DPPH, DMPD+ and ABTS+ assays. IC50 values (µg/ml) of the complexes and standards on DPPH, DMPD+ and ABTS+ respectively following the sequences.

**Keywords:** Nanoparticles, Suzuki C-C Coupling, ROS scavenging activities, Ultrasound, Arylboronic acids, Biaryls.

# Improvement of dielectric properties of nickel-doped calcium and copper titanate ceramics

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In this work, the effect of $CaCu_3Ti_4O_{12}$ ceramic substitution and sintering conditions (temperature and time) on resistivity, dielectric constant, morphological evolution and grain growth are analyzed and discussed. Specifically, the effects of Ni addition on the dielectric characteristics, microstructure and crystal structure of CCNTO ceramics are established. The traditional solid-state reaction approach was used to synthesize compositions with the formula $CaCu_{3-x}Ni_xTi_4O_{12}$ ($0 \leq x \leq 0.6$). Scanning electron microscopy (SEM) and X-ray diffraction (XRD) were used to examine the samples. Dielectric measurements were performed in the frequency range of $10^2$ Hz to $10^7$ Hz at room temperature. XRD analysis revealed the presence of secondary phases such as CuO, $CaTiO_3$ and $TiO_3$ in the samples with $x \leq 0.6$ and validated the production of a single-phase material in the samples calcined at 1000 °C for 12 hours with $x \leq 0.6$. The structure remained cubic in all compositions. The permittivity, resistivity, loss factor and dielectric characteristics of these ceramics were improved and explained.

**Key words:** $CaCu_3Ti_4O_{12}$, dielectric properties, colossal dielectric, CCNTO, Microstructures.

# Study of the structural and dielectric properties of $CaCu_3Ti_4O_{12}$-based Oxides

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This work aims at the development of a new CCTO-based dielectric material, suitable for many applications, especially as a capacitor. This is a simple approach to achieve practical dielectric characteristics when designing electronic materials. $CaCu_3Ti_4O_{12}$ (CCTO) is a double perovskite that exhibits a stable cubic structure at high temperatures. It is known to be a highly dielectric material and could play an important role in energy storage potential. This colossal dielectric has attracted considerable attention due to its potential applications in capacitors and memory devices. In this study, we explored the impact of Ni and/or Co substitutions on the microstructure and dielectric characteristics of a material that is highly sensitive to its dielectric properties, namely a colossal dielectric permittivity. $CaCu_{2.9}Ni_{0.1}Ti_{4-x}Co_xO_{12}$ (x = 0.1, 0.2, 0.3). Its CCTO-based ceramics were prepared by solid-state method. The influence of the presence of cobalt in the studied compositions on the dielectric properties is highlighted. The presence of nickel in the ceramic significantly improves the dielectric response. The evolution of the dielectric permittivity (Ɛr) of the cobalt-doped compositions followed the internal barrier layer capacitor model. The results obtained confirm that doping with an appropriate amount of cobalt affects the microstructure of the $CaCu_3Ti_4O_{12}$ compound and improves its electrical properties.

**Keywords:** Colossal permittivity, electrical characterizations, capacitors, ceramics, $CaCu_3Ti_4O_{12}$.

# Promising multifunctional doped $BiFeO_3$ nanoparticles: impact of partial multi-substitution on structural transformation

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This work explores the multifunctional applications of the multi-doped $Bi_{0.7}Ba_{0.2}Ce_{0.1}Fe_{0.9}Ni_{0.1}O_3$ (BBCFN10%) nanoparticles which were synthesized via the Sol-Gel method exhibiting a particle size of around 66 nm. X-ray diffraction (XRD) results confirmed the formation of a majoritarian tetragonal structure (*P4/mmm* space group) as it was validated by the Rietveld refinement. Our findings indicate that the structural transformation affected the magnetic, optical, and dielectric properties. The insertion of $Ba^{2+}$, $Ce^{4+}$, and $Ni^{2+}$ ions into the $BiFeO_3$ structure raised the remanent magnetization ($M_R$), and coercive field ($H_C$), and a 39 times enhancement of the saturation magnetization ($M_S$ = *13.96 emu/g*). Moreover, the title compound exhibited an interesting value of the maximum energy product $(B.H)_{max}$ of 6.716 MG.Oe (53.446 kJ/m³) at room temperature allowing its uses for permanent magnetic applications. Notably, this study presents the first report on the energy product of Bismuth ferrite. Additionally, the material featured a colossal giant dielectric constant ($\varepsilon' = 10^5$) with very low dielectric tangent loss making it a good candidate for energy storage applications. Optical absorption specifies an interesting band gap of 1.74 eV correlated with the PLE spectrum peak at 712 nm, suggesting band structure modification due to the substitution. Photoluminescence spectroscopy also revealed a defect-related blue emission peak at 475 nm.

These results highlight the investigated compound's substantial potential for a range of multifunctional uses.

# Application of Eco-Friendly Plant-Based Flocculants for Sustainable Sludge Dewatering

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Dewatering process is a necessary step in sludge treatment aiming to reduce its volume. Although the efficacy of this process to facilitate sludge handling, transport and disposal, the commonly used chemical flocculants are questioned to pose secondary pollution and adversely affect ecosystem and human health. Therefore, their substitution by natural ones derived from plant extracts is highly needed. Within this frame, the present study investigates the efficiency of six plants namely *Opuntia ficus indica, Phragmites australis, Solanum tuberosum, Moringa Oleifera, Trigonella foenum-graecum, Aloe vera* to dewater a sewage sludge from the urban wastewater treatment plant (WWTP) of Santiago de Compostela, Galicia (NW Spain)[1-3]. The dewatering activities of the plant-based flocculants were evaluated with reference to the measurement of specific resistance to filtration and dry solids. Compared between the tested plants, the best dewatering performance was obtained using 2000 mg/L of Moringa oleifera which allow a significant SRF decrease from 8.90 $\times 10^{14}$ m/Kg to 1.50 $\times 10^{14}$ m/Kg. Therefore, the six tested plants as flocculants mainly the Moringa are efficient and eco-friendly materials for dewatering. The interesting results obtained in this study affirms the possibility to apply these bio-flocculants instead of the chemical ones to ensure safe and cost-effective sludge handling and disposal [4-5].

**Key words:** Bioflocculant, Chemical flocculant, Conditioning, Dewatering potential; Sewage sludge

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# Structural, morphological and dielectric properties of $Ba_2(Mn,Re)_2O_6$ double perovskite for thermoelectric applications

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Investigating the electrical and structural properties of the $Ba_2(Mn,Re)_2O_6$ (BMRO) ceramic composite is the aim of this work. The traditional solid-state approach was used to prepare the BMRO. X-ray diffraction (XRD) analysis shows that the sample is neatly crystallized in the cubic structure with the Fm3m space group. The morphology and elemental content were examined using scanning electron microscopy (SEM) and energy-dispersive X-ray spectroscopy (EDX). The electrical measurements were examined in the temperature range of 373–453 K and the frequency range of 0.1 Hz–1 MHz. BMRO's AC conductivity is displayed using the correlated barrier hopping (CBH) model. The activation energy obtained from the DC conductivity and modulus spectra is rather close, confirming that the relaxation process and electrical conductivity are related to the same phenomenon. Furthermore, a thorough examination of Nyquist plots shows how sensitive the electrical properties of the material are to changes in temperature and frequency.

**Key words:** Double Perovskites, X-ray diffraction, Conductivity, Impedance Spectroscopy.

# Amino functionalization of tin(IV)-porphyrinic complex for the adsorption process

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In the field of catalysis, various metallo-porphyrins, particularly transition metal-porphyrin complexes, have emerged as powerful tools for enhancing a wide array of chemical transformations. Such complexes exhibit remarkable reactivity and efficiency, which facilitate reactions that may otherwise proceed slowly or inefficiently **[1,2]**.

The aim of the work, presented in this communication, is the description of the synthesis, characterization and anionic dye adsorption application of a polyethyleneimine (PEI) functionalized (5,10,15,20 tetraphenyl porphyrinato) tin(IV) dichloride [Sn(TPP)($Cl_2$)]. The adsorbent [Sn(TPP)($Cl_2$)]-PEI was prepared via a swift protocol and characterized extensively using multinuclear spectroscopic techniques including the 1H NMR, FT-IR and UV–Vis spectroscopic techniques.

X-ray diffraction (XRD) data confirmed that the addition of PEI to the Sn-porphyrin complex did not affect its crystallinity. On the other hand, scanning electron microscopy (SEM) analysis indicated that the morphological characteristics of [Sn(TPP)$Cl_2$] and [Sn(TPP)($Cl_2$)]-PEI were different. The prepared material was tested for its ability to adsorb Acid Blue 25, an anionic dye, from water.

**Key words:** Polyethyleneimine, Metalloporphyrin, Adsorption, Dyes, Water treatment

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# Oxidative degradation of dyes using manganese porphyrinic complex

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The porphyrins and metallo-porphyrins have been extensively applied for more than two decades in drug delivery, biosensing, bio-imaging, industrial, photocatalytic, nonlinear optics, molecular photovoltaics, industrial, and analytical fields **[1-3]**. Moreover, it has been demonstrated that their photophysical and biological properties are altered when a transition metal like manganese (Mn). Motivated by this, In the current work we present in this work the oxidative degradation of calmagite in water using $H_2O_2$ and chloro(meso tetrakis(phenyl) porphyrin) manganese(III). Calmagite has azo groups as chromophore groups, which can be easily degraded using metallic complexes in combination with oxidizing agents. Analytical techniques including FT-IR, SEM, XRD, UV, and TGA/DTA were used to characterize the prepared compounds. Different experimental parameters were investigated, including temperature, time of reaction, starting dye concentration, and $H_2O_2$ dose.

**Key words:** chloro(meso-tetrakis(phenyl)porphyrin) manganese(III); meso tetraphenyl-porphyrin ; calmagite; degradation; $H_2O_2$

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# Extraction des métaux lourds des eaux polluées par d'un nouveau composé PVC 4000 M – amine aliphatique primaire

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Le polychlorure de vinyle (PVC) est aujourd'hui l'un des polymères les plus utilisés dans les secteurs industriels, domestique et environnemental. Cette large adoption s'explique par ses remarquables propriétés mécaniques, chimiques et thermiques, ainsi que par la possibilité de le modifier chimiquement pour obtenir des matériaux aux fonctionnalités ciblées.

Dans le cadre de ce travail, nous avons procédé à la modification chimique de la matrice du PVC 4000 M par réaction avec une amine aliphatique primaire. Cette fonctionnalisation a pour objectif d'introduire des groupes amines actifs capables de complexer et d'adsorber les ions métalliques lourds présents dans les eaux contaminées.

Le produit obtenu, un nouveau polymère composite PVC–amine aliphatique primaire, a été synthétisé, caractérisé et évalué quant à son efficacité dans le traitement et la dépollution des eaux usées. La caractérisation structurale du polymère modifié a été réalisée par des techniques spectroscopiques, notamment la spectroscopie UV-Visible, la spectroscopie infrarouge (IR), ainsi que par la mesure de la conductivité électrique, permettant de confirmer la réussite de la modification et d'estimer sa capacité d'adsorption des métaux lourds.

Cette démarche s'inscrit dans une perspective de développement de matériaux polymériques éco-responsables, susceptibles de contribuer efficacement à la protection de l'environnement et à la gestion durable des ressources en eau.

**Mots-clés :** Polychlorure de vinyle (PVC 4000 M), amine aliphatique primaire, métaux lourds, adsorption, traitement des eaux, polymère fonctionnalis.

# Synthesis and Structural Characterization of Isoreticular Cu-MOFs Constructed from NDI and PDI Linkers

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Metal–organic frameworks (MOFs) represent an exciting class of porous materials, valued for their high surface area, tunable functionalities, and remarkable thermal stability. In this study, we report the synthesis of an isoreticular series of copper-based MOFs constructed from dipyrazole-terminated naphthalene diimide ($H_2$NDI-H) and perylene diimide ($H_2$PDI-H) linkers [1]. Due to their electron deficiency, planar structures, strong visible-light absorption, and redox activity, NDI and PDI linkers impart distinct optoelectronic and electrochromic properties to the resulting frameworks [2]. Comprehensive structural, morphological, and physicochemical characterization was performed using powder X-ray diffraction (PXRD), infrared spectra (FTIR), Raman spectra (RAMAN), scanning electron microscopy (SEM), energy-dispersive spectroscopy (EDS), thermogravimetric analysis (TGA), and $N_2$ adsorption (BET).

**Key words:** MOF, NDI, PDI, ligand, XRD, SEM, TGA, BET

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# Structural Analysis and Biological Assessment of a Novel Zwitterionic Cadmium Complex with Antioxidant, Antidiabetic, and Anti-inflammatory Activities

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A new hybrid material combining organic and inorganic components, $[CdBr_3(\eta^1\text{-}C_5H_{13}N_2)]$ (1), was synthesized, and its structure was determined at room temperature. The material crystallizes in the orthorombic space group $P2_12_12_1$, with the following parameters: a = 8.8493 (5) Å, b = 10.5402 (9) Å, c = 12.8960 (12) Å and Z = 4. The crystal structure of this compound is composed solely of distorted $CdBr_3N$ tetrahedra, with the negative charges of the bromide ions balanced by the positive charges from the $Cd^{2+}$ ion and the protonated amine. These cadmium tetrahedra are predominantly interconnected by N-H···Br hydrogen bonds. To explore the various intermolecular interactions, Hirshfeld surface analysis was conducted. Infrared spectroscopy was used to verify the structural composition of the complex and to assess its vibrational properties. Tauc's formula was applied to determine the optical band gap, with direct and indirect band gap values found to be 4.58 eV and 4.44 eV, respectively. Compound (1) exhibits notable antioxidant, antibacterial, and enzyme inhibition properties. Additionally, (1) showed moderate inhibition of alpha-amylase activity and anti-inflammatory effects, making it a promising candidate for further medicinal chemistry research.

**Keywords**: Cadmium, Crystal arrangement, Antimicrobial assays, Antidiabetic, Anti-inflammatory activity.

# Eco-Friendly Electrochemical Detection of Catechol Using CuO@Polyaniline Nanocomposite : Performance Study

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A CuO@polyaniline (CuO@PANI) nanocomposite was synthesized via in situ oxidative polymerization and used to modify a glassy carbon electrode (GCE) for developing a novel electrochemical sensor **[1,2]**. The composite was thoroughly characterized using FT-IR, XRD, TGA, BET surface area analysis, and SEM-EDX with elemental mapping, confirming enhanced structural stability, increased surface area, and improved electrical conductivity due to the synergistic interaction between CuO nanoparticles and polyaniline **[3]**. Electrochemical performance was evaluated by EIS, CV, and DPV, revealing significantly enhanced electron transfer kinetics and excellent electrochemical responsiveness **[4]**. DPV measurements showed high sensitivity (17.823 µA/µM) a wide linear range (0.001–10 µM), and an ultralow detection limit of 1 nM **[5]**. The sensor also demonstrated excellent selectivity against common interfering species and achieved recovery rates of 98–103% in real water sample analysis **[6]**.

**Keywords**: Catechol detection, CuO@PANI nanocomposite, Electrochemical sensor, Box-Behnken Design, Differential pulse voltammetry, Environmental monitoring.

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# Catalytic Degradation of Triclosan Using $Fe/ZrO_2$ and $Fe-Co/ZrO_2$ Systems

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The objective of this work was to study the catalyzed wet oxidation reaction with metal catalysts based on iron supported on Zirconia oxide and bimetallic catalysts based on cobalt and iron deposited on ZrO2, in order to degrade one of the endocrine disruptors: Triclosan.

In this study, we used the sol-gel route for the development of airgel supports. These supports are then used to prepare a series of catalysts based on iron alone or on iron and cobalt with fixed percentages by dry impregnation.

All these catalysts are reduced under hydrogen flow at 300°C.

The study of the textural and structural properties of the solids was carried out by measuring the specific surface by the BET method and by TPR. The N2 adsorption-desorption analysis of the different solids shows similar isotherms with the ZrO2 support, with varied hysteresis loops which reflects different textures and porous distributions.

The TPR-H2 profiles show the non-reducibility of ZrO2. The TPR analysis of the catalysts shows characteristic peaks of the reduction of iron and cobalt. The results of the catalytic tests show that the monometallic catalyst based on Iron supported on ZrO2 and the bimetallic catalyst impregnated simultaneously on the ZrO2 support exhibit significant catalytic activity in the degradation of Triclosan. This seems to be due to an increase in the average pore diameter and the pore volume, which results in a better iron-support interaction and therefore a good dispersion of the metallic phase at the ZrO2 surface.

**Key words:** Triclosan, Oxidation, Catalysts, Environment.

# Chemical Analysis and Evalution of Biological Activities of a Flavonioid - Enriched Fractions

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This work focused on extracting flavonoids from the two-phase olive pomace of the Tunisian Chemlali variety using an ethanol–water solvent system to yield a flavonoid-rich extract. The identification and measurement of flavonoids were carried out using HPLC with a diode array detector, then confirmed by LC–MS analysis. Five flavonoids were isolated and purified using HPLC apparatus. The antioxidant activity of purified flavonoids was evaluated by measuring the radical scavenging effect on DPPH and by using ferric reducing antioxidant power assays [1], [2].The ethyl acetate extract from two-phase Chemlali olive pomace showed minimal cidal concentrations ranging from 1.825 to 14.6 mg/ml against the tested pathogenic and phytopathogenic microbes. This antimicrobial activity is mainly attributed to the high flavonoid content of the extract, particularly quercetin-3-O-arabinoglucoside and hesperidin.

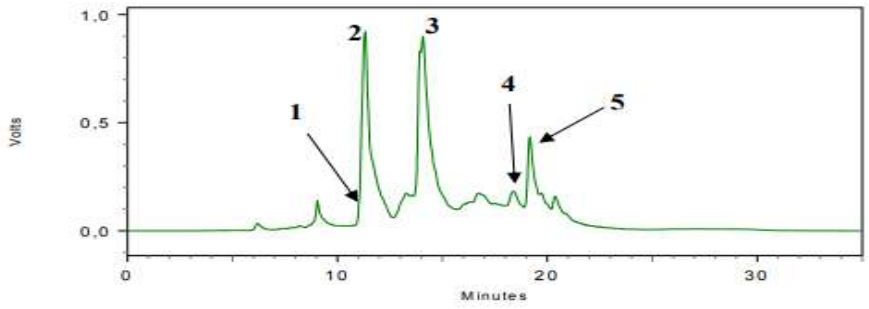


**Figure.** HPLC chromatogram of ethyl acetate extract: 1: Esculetin, 2: Hesperindin, 3: Quercetin-3-O-arabinoglucoside, 4: Quercetin, 5: Luteolin

**Keywords**: flavonoids, Chemlali, hesperidin, olive pomace, antioxidant activity.

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# Green Approach to Water Purification: Development of a Bio-Based Adsorbent

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Eucalyptus is increasingly recognized as a promising natural adsorbent for water treatment due to its lignocellulosic composition rich in hydroxyl, carboxyl, and carbonyl functional groups, which enable efficient binding of mineral and organic pollutants. Its leaves, bark, and sawdust residues are abundant, renewable, and environmentally friendly, making eucalyptus a sustainable material for low-cost water purification. This natural approach aligns with the growing need for ecological solutions to address declining freshwater resources and increasing water pollution linked to industrialization and agriculture. This study investigates the removal of nitrates and phosphates through biosorption using eucalyptus leaves as a cost-effective adsorbent. A preliminary analysis was performed to identify the optimal conditions for removing these micropollutants with eucalyptus leaves. Isotherm models were applied to understand the adsorption process, followed by a kinetic study. Thermodynamic parameters were also assessed to determine the nature of the adsorption process. Finally, the study aims to demonstrate the effectiveness of eucalyptus leaves as a low-cost and sustainable biosorbent for the removal of nitrates and phosphates; water from a well was treated.

**Keywords:** Biosorbent, kinetic study, Thermodynamic, eucalyptus leaves.

# Eco-compatible biocatalytic synthesis of (*R*)-linalyl acetate: Application of Response Surface Methodology and Box-Behnken Design

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Linalool (3, 7- dimethylocta−1,6- dien- 3- ol) is an acyclic tertiary monoterpene alcohol that is present naturally in almost all essen tial oils in varying concentration degrees[1]. It is utilized generally in perfumery and many flowery fragrance compositions for fruity- fresh odours such as neroli, lavender, and lily of the valley. Linalool was included in the list of class “A” substances due to its usefulness as primal matter for the synthesis of high- value added compounds, such as their ester derivatives, especially the acetate form. Herein, we report the production of linalyl acetate using the free lipase PPL as a catalyst in a solvent- free medium.We have study our optimization by Response surface method ology (RSM), which is a statistical model approach for empirical model ling which evaluates the effect of individual and interaction effects of the process parameters on the corresponding response value. Parametric studies referring response surface methodology (RSM) were applied to optimize the conversion. The ef fect of the variables temperature, catalyst amount, volume of acyl donor, and reaction time was studied by using the experimental design technique. The optimum conditions for the pure linalool conversion were achieved at temperature at 60°C, amount PPL at 150 mg, volume of AC2O at 1 mL, and reaction time at 5 days. The best reaction conversion was obtained at conv = 24.94%. It is to be underlined that the acylation of this tertiary alcohol using enzyme catalysis represent a challenging task [2].

**Key words:** Hydrolases, (R)-Linalool, (R)-Linalyl acetate, Acylation, Box–Behnken Design, Eco-friendly conditions

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# Development of a novel design of solar furnace supplied by optical fibers

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This paper reports on a theoretical realization of a recently proposed solar optical fiber mini dish light concentrator connected to a conical solar furnace. The prototype dish is 21.8 cm in diameter. We present the daily power obtained at the output of the optical fiber, the power supply is estimated to be 25W at the end. Then we show that the energy transported is diffused until the enclosure then disperse inside it, the receiver absorbs this energy. Temperatures higher than 1600°K may be reached while maintaining very good efficiency.

Some solar furnaces can reach very high temperatures for industrial applications such as sintering or melting metals, which could be used in some biofuel manufacturing or waste recovery processes. Biomass drying and pyrolysis: Concentrated solar energy can be used to dry organic materials or to carry out biomass pyrolysis, a key step in the production of biochar or bio-oils. Green hydrogen production: Projects are exploring the production of green hydrogen ($H_2$) by solar furnaces, which does not emit $CO_2$ or pollution.

**Key words:** concentrated solar energy, optical fibre, solar lighting, solar furnace.

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# Étude électrochimique des propriétés électrocatalytiques d'un complexe de manganèse-base de Schiff pentadentée

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Ce travail s'inscrit dans le cadre du développement de nouveaux complexes de métaux de transition à visée électrocatalytique. Il concerne la synthèse, la caractérisation structurale et l'étude électrochimique d'un complexe de manganèse(II) dérivé d'une base de Schiff pentadentée, obtenue à partir de l'amine bis(3-aminopropylamine).

L'objectif principal est d'explorer la réactivité électrochimique de ce complexe ainsi que son activité catalytique dans l'époxydation du cyclooctène, réaction modèle pour l'oxydation sélective des alcènes. Cette étude permet de mieux comprendre le rôle du centre métallique de manganèse dans l'activation de l'oxygène moléculaire et d'évaluer l'influence du groupe fonctionnel NH de la base de Schiff, susceptible de jouer le rôle de base axiale favorisant la coordination et l'activation de l'oxygène au niveau du site métallique.

Les investigations électrochimiques ont été réalisées par voltamétrie cyclique, technique permettant de suivre les processus rédox et de déterminer les conditions optimales pour la catalyse homogène. Le complexe [Mn(II)-Cl-L] a été étudié sous atmosphères d'azote et d'oxygène, sur électrode de carbone vitreux, et dans différents solvants organiques - diméthylsulfoxyde (DMSO), diméthylformamide (DMF) et acétonitrile (AN) - afin d'évaluer l'influence du milieu sur ses propriétés électrochimiques.

**Mots-clés :** Complexes à base de Schiff, manganèse(II), métaux de transition, électrocatalyse, voltamétrie cyclique, époxydation, polymétallation, oxydation sélective.

# Bioactive profiling of Urtica dioica L. and development of a stable anti-inflammatory topical formulation

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This work highlights the valorization of *Urtica dioica* L. (nettle) from northern Algeria through the development of a therapeutic topical formulation. Nettle harvested in February 2025 was subjected to detailed phytochemical characterization and, in vitro biological assessments. Phytochemical analysis revealed a polyphenol content of 36.26 mg GAE/g and a flavonoid content of 0.0647 mg/mL, confirming its strong antioxidant potential. The DPPH assay showed a maximum inhibition of approximately 60% at a concentration of 2 µg/mL, indicating significant free radical scavenging activity, comparable to that of ascorbic acid ($IC_{50}$ = 3.80 µg/mL). Anti-inflammatory activity, assessed through protein denaturation inhibition, reached 64.25%, slightly exceeding that of salicylic acid (63.53%). Antibacterial tests demonstrated strong inhibition of *Staphylococcus aureus* and moderate inhibition of *Pseudomonas aeruginosa*, while *Escherichia coli*, *Bacillus spizizenii* and *Salmonella enterica* exhibited resistance.

The developed cream showed a homogeneous texture, pleasant sensory characteristics, and maintained physical stability over 30 days under varying storage temperatures. These findings highlight the therapeutic relevance of *Urtica dioica* L. and its potential application in the development of innovative natural formulations based on local bioresources.

**Keywords**: *Urtica dioica* L., antioxidant activity, antibacterial activity, anti-inflammatory effect, polyphenols, flavonoids, topical formulation, natural products, Algeria.

# Determination of diuretics in dietary supplements for weight loss and physical fitness by GC/MS

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The increasing consumption of dietary supplements for weight management raises concerns about the presence of undeclared pharmaceutical substances, particularly diuretics. These compounds are sometimes added illegally to accelerate water loss and provide misleading weight-loss effects, but their uncontrolled use may lead to dehydration, electrolyte imbalance, kidney impairment, and potential doping violations. In this work, we developed and validated a simple, rapid, and sensitive gas chromatography–mass spectrometry (GC–MS) method for the simultaneous determination of 14 diuretics, including thiazide, loop, carbonic anhydrase inhibitors, potassium-sparing diuretics, and masking agents, in dietary supplements. The method was optimized using selected ion monitoring (SIM) for screening and SCAN mode for confirmation. Validation parameters followed international laboratory standards. Limits of detection ranged from 50 to 300 ng/g in solid matrices and from 10 to 100 ng/mL in liquid matrices. Average recoveries were between 65.13% and 95.23% with good precision. Total analysis time was 13 minutes, with sharp peaks and baseline resolution of all analytes. The validated method was applied to ten dietary supplement samples (capsules, tablets, powders, liquids) collected from the Tunisian market. None of the tested products contained the investigated diuretics. This method is reliable for routine screening of adulterated supplements, contributing to consumer safety and public health monitoring.

**Keywords:** GC-MS. Diuretics, Dietary supplements, Adulteration, Weight-loss, Food control.

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