Fourth Edition

nanoMAT

Association Tunisienne
des Nanomatériaux et Applications

nano MAT 2024

4th International Conference on Nanomaterials and Applications

01 –03 November 2024, Hammamet, Tunisia

Book of Abstracts

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Foreword

It is with great pleasure that we welcome you to the fourth edition of the International Conference on Nanomaterials and Applications (nanoMAT2024) organized by the Tunisian Society of Nanomaterials and Applications (nanoMAT). This exciting event will take place at the Hotel Laico, located in the scenic seaside town Hammamet, Tunisia, from 01 to 03 November 2024.

nanoMAT2024 is designed to be a vibrant forum for the exchange of cutting-edge ideas and development in the field of nanomaterials. The conference will bring together leading researchers, academics, and industry professionals to present and discuss the latest advancements and emerging trends in nanomaterials and their wide-ranging applications in chemistry, physics, biology and beyond.

The event will contain plenary lectures by distinguished experts, oral presentations, and poster sessions, providing ample opportunity for participants to share knowledge, foster collaboration and engage in stimulating discussions about the future of nanomaterials.

The major topics of the conference included:

1. **Nanomaterials: Synthesis, Characterization and Modeling.**
2. **Nanomaterials for Energy, Environment and Catalysis.**
3. **Nanomaterials for Electronics, Photonics and Magnetism.**
4. **Nanomaterials for Bio-sensing and Applications.**

We would like to extend our heartfelt thanks to our academic partners and sponsors for their generous financial and technical support, which has been instrumental in making this event possible. Moreover, we are deeply grateful to our keynote speakers, presenters, and participants for their invaluable contributions. Your presence and active engagement are what will ensure the success of this conference.

Finally, we hope that you will find the conference program inspiring and thought-provoking, and that you will take full advantage of the opportunities for fruitful scientific exchange.

On behalf of the Organizing Committee
The Conference Chairman
Dr. Lassaad BEN HAMMOUDA

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Organizing Committee

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Scientific Program

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SCIENTIFIC PROGRAM

Thur. 31 Oct. 2024		
14.30–18.00	**REGISTRATION**	
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08.00–09.30	**REGISTRATION**	
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10.00–10.30	**WELCOME RECEPTION**	
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11.05–11.40	Plenary lecture #2: **Prof. Frederic Favier** (Session chairman: Prof.Ouassim Ghodbane) Title: **Nano-engineered 2D Materials for Electrochemical Energy Storage**	
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11.55–12.10	OA2: Boosting of CZTS-Based Solar Cells with Cu_2S as a Buffer Layer: A Combined Experimental and Simulation Approach A. Akkari, O. kamoun, A. Akkari	OB2: Graphitization of olive mill waste biomass by pyrolysis for H_2, CH_4 and CO_2 gas detection A. Siai, M. Ben Abdallah, G.Conte, H. Nsir , A. Policicchio

10.10–12.25	OA3: Design and Computational Analysis of Nitrobenzofurazan-Based Non-Fullerene Acceptors for Organic Solar Cells B. Abdelaziz, S. Patane, S. Ayachi	12.10–12.25	OB3: Synthesis and caracterisations of nanocomposites PB@$NiFe_2O_4$ Y. Sabri, N. Hosni, H. Maghraoui-Meherzi
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14.35–15.05	**LEDlab Presentation – Pedro Hurdato**		
15.05–15.40	Plenary lecture #4: **Prof. Dongyuan Zhao** (Session chairman: Prof. Noureddine Raouafi) Title: **Molecular super-assembly for functional mesoporous materials and their future**		
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17.10–17.25	OA6: Properties of mesoporous and microporous materials modified by iron nanoparticles as potential catalysts for water purification R. Ouargli Saker, A. K. Lachachi, K. N. Sekkal	17.10–17.25	OB6: Advanced Screening of Autoimmune Diseases: A Machine Learning Approach to Spectroscopic Analysis S. Ben Brik, I. Cherni, S. Hamzaoui
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10.55 – 11.10	OA10: Synthesis and Application of 2D Mono-element Materials in an Energy Harvesting Device N. Ben Brahim Aouani, N. Rachid, O. Bel Hadj Ali, M. Jouini, A. Bali, W. Ouerghi, G. Jemai, L. Linoubli, L. Marty	10.55–11.10	OB10: Computational investigation of structural, elastic, electronic, and optical properties of predicted Alkali Metal-Based Ternary chalcogenides LiNaX (X = S_e,T_e) for optoelectronics and storage devices applications: DFT study Ly. Benbahouche, S. Boucetta, A. Khelefhoum
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P61: Optimization of batch and electrosorption of Cr(VI) from wastewater using Al_2O_3 nanoparticles | W. Sassi, N. Mnasri, R. Msaadi, S. Ammar
P62: Cost-Effective Ceratonia Siliqua for Paracetamol Removal: Equilibrium, Regeneration Studies, and Modeling via Box-Behnken Design | H. Chemingui, W. Ben Salem, N. Bensacia, A. Hannechi, H. Dbouba, R. Riahi
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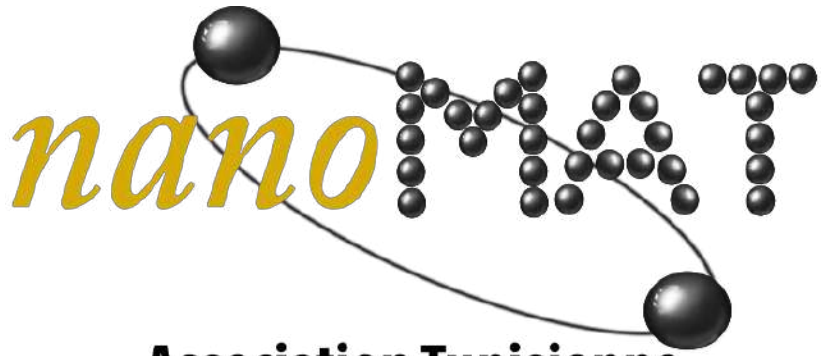
P64: Growth and Characterization of Cadmium Carbonate Nanowires | M. Ouassini Bensaid, R. Miloua,
P65: Synthesis of a new cement from waste glass powder and hydrated cement | R. Ouargli Saker, N. Kouadri,L. Saker
P66: Structural, morphological, optical and dielectric properties of $ZnAl_2O_4$ nanoparticles prepared by sol gel auto-combustion technique | Mohsen Elain Hajlaoui, Mohamed Amghar, E. Dhahri.



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Speakers' Abstracts

Short biography:

Dr. Mihai Irimia-Vladu has been since 2019 Assistant Professor in the Institute of Physical Chemistry and Linz Institute of Organic Solar Cells of Johannes Kepler University in Linz, Austria, Austria. He was born in Craiova, Romania and obtained his B.S. in Mechanical Engineering from the University of Craiova in 1997, followed by a short employment of two years as car components testing engineer at Daewoo Automobiles Romania. He completed his Ph.D. under the guidance of Prof. Jeffrey W. Fergus in the field of solid-state ensing, at the Materials Engineering Department of Auburn University, Alabama, in May 2006. He moved in July 2006 to Johannes Kepler University in Linz, Austria as post-doctoral fellow, working within the research groups of Prof. Serdar Sariciftci and late Prof. Siegfried Bauer. In Linz, he was the initiator and principal investigator of "green" materials for organic electronics. From 2012 to 2019, Dr. Irimia-Vladu was Senior Scientist at Johanneum Research, Department of Materials in Graz, Austria where he continued his unusual research directions on biomaterials for sustainable circuits, energy conversion and storage, and bio-integrated electronics. Dr. Irimia-Vladu raised in excess of 2 million Euros in external funding, edited 1 book and authored 44 publications in peer reviewed journals, with 10 front cover highlights that received more than 4500 citations for an h-index of 27. He presented his group work through 9 tutorial/keynote, 23 invited presentations at international conferences and 21 seminars at various universities or research centers worldwide. Dr. Irimia-Vladu participated as an external member (opponent) of 4 Ph.D. defenses. For his first worldwide demonstration of "edible electronics", he was awarded in 2011 the "1st prize of Austrian Society for Environment and Technology" and was named "Austrian of the day" by the regional newspaper in the Upper Austria region. Among scientific discoveries that can be credited to Dr. Irimia-Vladu, is also the first report of semiconducting properties of the historic dye indigo, which helped open a new research field on hydrogen-bonded semiconductors. Dr. Mihai Irimia-Vladu is an active member of American Chemical Society and Materials Research Society and coalesced the emerging field of bioelectronics by co-organizing 5 international meetings, among them 4 Materials Research Society symposia. Dr. Irimia Vladu's hobbies include history, literature, hiking, soccer and American football.

The Road to "Green" in Organic Bioelectronics

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Through its appealing avenues of processing the component devices at room temperature and from low-cost precursor materials, organic electronics has a tremendous potential for the development of products able to achieve the goals of production sustainability as well as environmental and human friendliness for electronics.

In an effort to stave off the e-waste growth, the presenter and his research group went further down the path opened by organic electronics research and investigated a large number of biomaterials as substrates, dielectrics, semiconductors and smoothening layers for the fabrication of organic field effect transistors, integrated circuits and organic solar cells. The presentation will focus on the highlights of our recent research, especially with respect to materials investigated, devices fabricated and the immense potential for follow up research:

- Flexible natural and biodegradable substrates
- Natural dielectrics
- Bio-origin, H-bonded semiconductors in the families of indigos, anthraquinones and acridones
- Bio-degradation protocols for organic semiconductors

These highlights will be placed in the context of the mountain that one has to climb in order to reach the coveted "green" connotation for electronics, sensors and integrated circuits:

- Biocompatibility issue
- Biodegradability issue
- Compostability issue
- Cost of production / energy expanded in production issue
- Materials choice issue (carbon foot print)
- Toxicity and the environmental impact of the synthetic avenue for component materials

The potential of follow-up research in the green electronics field is immense, with large area electronics fabrication, biomedical implants, bio-sensing and smart labeling, representing only the tip of the iceberg of many more immediate possibilities of high interest for our group. Natural and nature-inspired materials have the unrivalled capability to create "safe-first" electronic markets for human and environment, with minimal or even neutral carbon footprint.

Short biography:

Frédéric Favier is a Research Director at the National Center for Scientific Research (CNRS) within the Charles Gerhardt Institute Montpellier (ICGM). He has been a visiting researcher at UC Irvine (USA), EPFL (Switzerland), and NTU (Taiwan). His research activities focus on the synthesis and characterization of nanostructured materials for electrochemical applications, including supercapacitors, gas sensors, and electrocatalysis. He is interested in the formulation and design of new materials, as well as the elucidation of interfacial mechanisms involved in these applications. He develops his activities in strong collaboration with industry through numerous direct partnerships and within the framework of national and international collaborative projects. Since 2018, he has co-directed the joint laboratory MATELHO on alkaline electrolysis for H2/O2 production. For the last four years, he has also been the head of the "Materials Chemistry, Nanostructures, Energy Materials" department at ICGM.

Nano-engineered 2D Materials for Electrochemical Energy Storage

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As for graphene, the main issue about 2D materials is re-stacking. This is especially true for supercapacitor electrode materials as electrode/electrolyte interface and ion transport/diffusion should be both maximized to get the greatest storage capabilities. Many synthetic approaches have been explored to address this issue. Starting from exfoliated materials, including graphene, MXenes, oxydes, hydroxydes… we have developed various strategies to modify the composition, structure or morphology of the layers before re-assembling them in materials with enhanced electrochemical performances [1-4]. To illustrate our progresses in the field, three different approaches will be presented in this paper.
The first approach is on the synthesis of graphene-like carbide derived carbons produced by chlorination of SiC nanosheets obtained by the magnesio-thermal reduction of a silica/graphene oxide nanocomposite. The resulting microporosity in the graphene sheets was shown to strongly improve the rate capability of the prepared electrode material.
Electrostatic stacking of layers of opposite surface charges could also be used to associate a Faradaic layered double hydroxides (LDHs), for energy density, to a more stable and powerful pseudocapacitive MnO2. The electrochemical performances of the resulting electrode material were assigned to synergistic effects from distinct but complementary intrinsic behaviors together with the specific morphology of the composite material.
Expanded Ti3C2MXene obtained by using MgO nanoparticles as hard templates displayed an open morphology based on crumpled layers. The corresponding electrode material delivered up to 180 F.g-1of capacitance at 1 A.g-1over five thousand charge-discharge cycles in KOH electrolyte. On the other hand, an MXene foam prepared by decomposing an MXene-urea composite at 550°C, showed numerous macroporeson the surface layer and a complex open 3D inner-architecture. Thanks to this foamy structure allowing in and through plane ion diffusion, a capacitance of 203 F.g-1at 5 A.g-1current density, 99 % of which was retained after five thousand cycles.

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Short biography:

Sibel A. OZKAN is currently working as a Full Professor of Analytical Chemistry at Ankara University, Faculty of Pharmacy since 1986. She is an active member of the European Chemical Society-DAC member on behalf of the Turkish Chemical Society. She is a member of the European Pharmacopoeia-EDQM-Chromatography Section. COST Action Management Committee: PortASAP: - European network for the promotion of portable, affordable and simple analytical platform: Core group of Cost Action CA 16215. Working Group 4 (Completed 2022).COST Action Management Committee: WATERTOP: - Taste and Odor in early diagnosis of source and drinking Water Problems (WATERTOP) Core group of COST Action CA18225-Working Group 1 - Advances in sensory analysis of water T&O (2023-Continue).COST Action Management Committee: LUCES: - Supramolecular LUminescent Chemosensors for Environmental Security (LUCES) CA22131, (2024- Continue). (MC Cair: Rodriguez Laura). She has been involved in several analytical chemistry projects related to LC methods, separation techniques, chiral separation, drug analysis, electrochemical biosensors, nanosensors, nanobiosensors, MIP sensors, DNA biosensors, enzyme biosensors, biomarkers, environmental sensors, method development, and validation of drug assay.She has published more than 450 original and review papers, her h-index is 50 (indexed in ISI-WoS), and she is the Editor of 10 scientific books and about 55 book chapters. She has several international and national awards.She is the Editor of the Journal of Pharmaceutical and Biomedical Analysis (SCI-Elsevier) and Section Editor (Analytical & Environmental) of Essential Chem (Taylor&Francis) and Regional Editor (Europe part) of Current Pharmaceutical Analysis (SCI-Bentham).Besides, she is the Editorial Board member of Talanta (SCI), Chromatographia (SCI), Biosensors & Bioelectronics X, Critical Reviews in Analytical Chemistry, Electrochimica Acta, Analytical&Bioanalytical Chemistry, Advanced Sample Prep., Green Analytical Chemistry, and so on.

Design and Application of Nanomaterial Embedded Molecularly Imprinted Polymers for Electrochemical Sensing: Recent Developments and Future Prospects

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Molecular imprinting technology, which forms molecularly imprinted polymers (MIPs), is a creative method that enables synthetic biorecognition gaps to imitate real biological derivatives like antibodies, receptors, enzymes, etc,. After removing the target analyte, synthetic cavities enable the recognition and selective rebinding of the template. In this case, molecular imprinting technology offers biosimilar receptors with higher specific affinities and better stability than natural receptors and biomolecules [1]. Although stable and durable MIPs seem relatively easy to create to achieve maximum efficiency, some optimization parameters should be considered, such as appropriate functional monomer and crosslinker and optimal ratios between functional monomer, template, and crosslinker [2]. The optimization process can vary based on the polymerization technique (electropolymerization, photopolymerization, and thermal polymerization). It was reported that template monomer interactions are realized through non-covalent interactions such as van der Waals forces, hydrogen bonds, and dipolar interactions. Among them, MIP-based electrochemical sensors have a significant place because, with MIPs, it is possible to overcome the lack of selectivity issue in electrochemical sensors.

Nanomaterials, famous for their prominent electron transfer capacity and specific surface area, are increasingly employed in modifications of MIP sensors. Unlike traditional electrochemical sensors, nanomaterials-based MIP sensors have excellent sensing and recognition capabilities. Nanomaterial embeded MIP-based electrochemical sensors and miniature electrochemical transducers can detect target analytes in situ. Thanks to superior chemical and physical stability, low-cost manufacturing, high selectivity, and fast response, MIPs have become an interesting field recently. Moreover, without requiring time-consuming preparation procedures, these sensors have been successfully used in biological fluids and pharmaceutical samples.

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Short biography:

Professor Dongyuan Zhao, Hao-Qing Professor, Dean of School of Chemistry and Materials at Fudan University, Senior Editor for ACS Central Science. Professor Zhao was born in Northeastern of China, he received B.S. (1984), M.S. (1987) and PhD (1990) from Jilin University. He was a post-doctoral fellow in University of Houston (1995–96), University of California at Santa Barbara (1996–98). He was a member of Chinese Academy of Sciences and The World Academy of Science (TWAS). Prof. Zhao has devoted himself for more than 30 years to the interfacial assembly and synthesis of ordered functional mesoporous materials for the applications in energy, environment, and biology. Prof. Zhao received many awards including: National Natural Science Awards (1st Grade, 2020); IMMA Achievement Award in 2008; The Ho-Leung-Ho-Lee Award in 2009; TWAS-Lenovo Science Prize in 2016; Khwarizmi International Award in 2019; JCIS Darsh Wasan Award in 2018; Chemistry Contribution Award, China Chemical Societyin 2018; Nano Research Award in 2020, ACS Nano Award in 2021, Tan Kah Kee Science Awards in 2024. He published more than 900 peer-review papers and is listed as one of highly cited researchers ISI in both Chemistry and Materials Science fields (Total citation ~ 150,000, h index 194). (http://www.mesogroup.fudan.edu.cn)

Molecular super-assembly for functional mesoporous materials and their future

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The functional mesoporous materials can be synthesized by soft-templating method, surfactant assembly process, however, their morphology and mesostructures are difficult to precisely control. In this lecture, we mainly introduce the recent progress in the research of molecular aggregate super-assembly regulation, oriented assembly synthesis and the construction of hierarchically-ordered functional mesoporous materials. Based on the new idea of interfacial supra-assembly regulation, we have demonstrated some approaches for the synthesis of ordered functional mesoporous materials with hierarchical mesostructures. We focus on a method for super-assembly using single micelles as mesostructural units. Using this approach, we can precisely prepare a family of novel functional mesoporous materials with hierarchical ordered structures, including uniform nanospheres, hemispheres, polyhedra, two-dimensional (2-D) single-layer nanosheets. These functional mesoporous materials not only have unique and uniform morphology, but also have controllable mesopore structure, high specific surface area, large pore volume and open pore. Based on the interface control, we realized the orientation assembly of functional mesoporous materials, and created the asymmetric dumbbells, gourd, match, shuttlecock, double-leaf dimer (Y-type) multifunctional mesoporous materials for the first time. We will also introduce the applications of functional mesoporous materials in catalyst support (heavy crude oil hydrocracking), electrode materials for lithium-ion batteries, thermal insulation materials, dielectric materials (low-k) and other fields.

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Short biography:

Sami BOUFI, is a Professor at the Faculty of Sciences of Sfax in Tunisia. He got his PhD in Macromolecular Materials from the Institut Polytechnique de Grenoble, and Habilitation degree in 2001 from the University of Sfax. His research activities focus on the production and applications of nanoscale particles from biobased resources including celluloses, starch, chitins, and lignin. Other fields of interest include polymer,composites and nanocomposites, and valorization of biomass. He is the author or co-author of more than 200 papers in peer-reviewed journals and book chapters. and serves in the editorial board of several other journals.

BiobasedNanoparticles from Biomass: A promising platform for Advanced Ecofriendly Functional Materials

Sami Boufi

Faculty of Science of Sfax-University of Sfax-Tunisia
Laboratoire LMSE (Sciences des Matériaux et Environnement)

Abstract

Biomass, as the most abundant renewable resource on Earth, not only serves as a sustainable feedstock for producing chemicals and materials but also has tremendous potential for creating a wide range of nanoscale materials with valuable properties and applications. Merits of these nanoparticles (NPs), among others,include their environmental and human safety, sustainability, ease of production, and cost-effectiveness. This presentation will provide an overview of various classes of biobased NPs derived from biomass through green and eco-friendly methods, with a particular emphasis on nanocelluloses and nanochitins, which are among the most promising candidates for large-scale production. Additionally, we will explore how chemistry can expand the potential applications of biobased NPs in advanced flexible materials for energy storage, through hybridization with metallic NPs or functional polymers like PANI and PEDOT.

Short biography:

Mongi BOUAICHA is a full professor in physics since 2012 at the Centre of Research and Technology of Energy (CRTEn: Centre de Recherches et des Technologies de l'Energie) at Borj-Cedria Technopark, at Tunis, the capitol of Tunisia. Since 2015, he is the Director of the Photovoltaic Laboratory. He co-authored 64 regular papers, with a SCOPUS's h-index of 15 with more 1110 citations, and a GoogleScholar h-index of 17 with 1230 citations. On 2011, he published a book on physics and technology of solar cells (Physique et Technologies des Cellules Solaires, ISBN: 978-9973-37-667-1, with 230 pages). He was also a co-author in a book titled: Solar Cells / book 3 (ISBN : 979-953-307-192-2). He gives 15 international conferences as an invited speaker and participated with more than 65 oral and poster presentations. Prof. Mongi BOUAICHA supervised 12 master's degrees and 13 PhD.

Renewables energies and decarbonization facing the global warming

Mongi Bouaïcha

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Abstract

In approximately 150 years, the industrial revolution based especially on fossil energy sources, caused a spectacular rise of the amount of carbon dioxide (CO2) from 290 ppm in 1880 to 410 ppm nowadays, leading to a warming global of more than 1.5°C. The latter, like a domino effect, caused a global climate change, which in case of no action, will bring humanity towards to the climate singularity before the year 2050; Decarbonization is the sole practical alternative to avoid such scenario.

Since 1992, the United Nations Organization (UNO) set up the United Nations Framework Convention on Climate Change (UNFCCC), followed by the Kyoto Protocol in 1995, the Johannesburg Formula in 2002, and the setting up of the COP (Convention Of Parties) series of conferences on climate change, like the Paris agreement in the COP21 of 2015.

Different approaches are initiated to decarbonize the earth atmosphere, such as Renewable Energy (RE), caption of CO2 and its transformation, tree's implantation, etc. Using RE in a world energy and ecologicaltransitions can ensure an earth decarbonization at levels in the range of 72 – 75 %.

According to the IEA (International Energy Agency) as well as for near and middle futures, RE sources are and will be used as follows: 70 % photovoltaic (PV), 20 % wind, 2-3 % hydropower, 2-3 % bioenergy, and 4-6 % from all other RE sources.

Since PV plays a crucial role in the earth decarbonization actions to stop the global warming to the 1.5 °C target as fixed by the Paris' agreement, we give an overview of the international technological roadmap of PV for the next decade, where crystalline silicon is used material in 95 % of fabricated modules. In addition, we pay attention to the effect of the actual world energy transition, which will generate starting from 2050 an important waste at the end of life of PV systems being installed now in 2024, suggesting the application of the circular economy by recycling them.

Short biography:

Philippe Lang is a university professor and research director at the CNRS and works at the Université Paris Cité. He leads the OMNA2D team at ITODYS and has extensive experience of surface modification using both SAMs and porous 2D molecular networks. Many of these functional monolayers have been used to improve the morphological and mesoscopic properties of organic SCs (OFETs) or hybrid perovskites (PCs), as well as to control charge transfer at interfaces.

Grafting and Orientation of Carbazole-based Phosphonic acid Monolayers on conductive metallic oxides ; Template for the Growth of Hybrid Perovskite used in solar cells.

Yahya Hami[a], Balkis Nasraouia[b], Faiza Mameche[a], Mahamadou Seydou[a], Faycal Kouki[b], Philippe Lang[a*]

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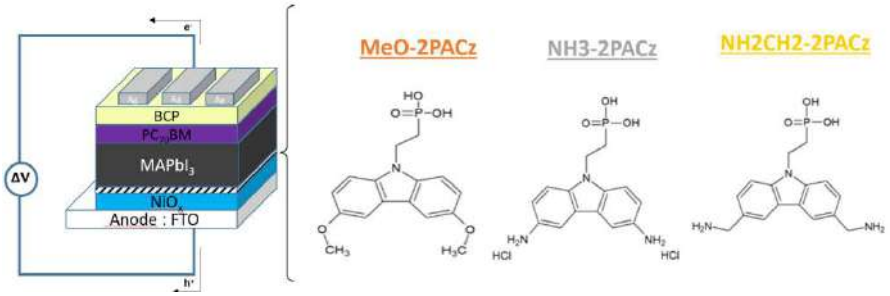
Recent advances in hybrid and organic solar cells underscore the growing importance of hybrid perovskites (HPs) in optoelectronic devices, particularly in photovoltaics, due to their superior light absorption and remarkable optoelectronic characteristics. HPs have reached impressive power conversion efficiencies (PCE) of up to 26.1% for single-junction perovskite solar cells (PSCs), positioning them among the most promising technologies in the photovoltaic sector. However, their operational instability remains a significant hurdle. To address this, recent research has focused on improving the stability and mitigating degradation of PSCs by integrating self-assembled monolayers (SAMs) at metal oxide (MOx) interfaces, particularly amino-terminated SAMs, which have shown promise in stabilizing the PSC structure and performance. Defects at the perovskite/MOx interface can result in non-radiative recombination, reducing efficiency. Careful control of the interfacial chemistry between adjacent PSC layers is crucial to overcoming these limitations. This work explores the development of amino-terminated SAMs for enhancing both the structural stability and performance of hybrid perovskites, demonstrating how interface engineering can address PSC degradation issues and improve overall device longevity and efficiency.

This study focuses on improving the structural stability and performance of hybrid perovskites (HPs) by developing a series of amino-terminated SAMs [1-3]. These SAMs, when grafted onto metal oxide (MOx) layers, include structures such as $HO_2C-(CH_2)n-PP-(CH_2)-NH_2/NH_3^+$ or $H_2PO_3-(CH_2)_2$-Cz-R_2, where P represents phenyl, Cz denotes carbazole, and R varies as CH_3O, NH_2/NH_3^+, or -CH_2NH_2/NH_3^+ (see figure) These molecules have been designed and characterized to investigate the correlation between their molecular structure, the morphology of HP films, and the overall performance and stability of PSCs.



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Short biography:

Damien Debecker is a Professor at the University of Louvain (UCLouvain), in Louvain-la-Neuve, Belgium. He is teaching physical chemistry, process engineering, bio-refining, waste treatment technologies. He is leading a research group active in the field of "catalytic processes for more sustainable chemical processes". More precisely, the group uses heterogeneous catalysts (and immobilized enzymes) to perform chemical reactions and design chemical processes in a greener way. Keywords on expertise: Heterogeneous catalysis, Hybrid catalysis, Green chemistry, sustainable chemistry, Nanomaterials synthesis, Biorefinery, CO2 capture and utilization, sol-gel chemistry, biocatalysis, enzyme immobilization, CO2 methanation, bio-based chemistry, flow chemistry, metal nanoparticles, aerosol processes, spray drying, monoliths, structured catalysts, layered double hydroxides, hydrotalcites, mesoporous mixd oxides, XPS, ToF-SIMS, catalyst deactivation, catalyst regeneration.

Nanocatalysis: a breeze of fresh air

Damien P. Debecker

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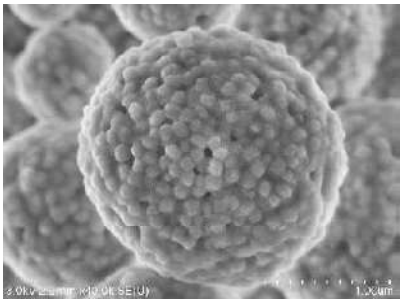
Heterogeneous catalysis relies on our ability to design, optimize, stabilize, and combine nanometric entities and features at the surface of functional materials. In this communication, we will highlight the development of continuous, air-supported processes that offer unexplored avenues for the preparation of innovative and effective solid catalysts. Aerosol processes are alluring for the continuous, large scale, and tailored production of divided nanomaterials,[1] and in particular of advanced heterogeneous (nano)catalysts.[2] Beyond the typical drying and aggregation of preformed particles via spray drying (or atomization), reactive aerosol processes allow synthesizing tailored-made catalysts in a bottom-up fashion, with tunable surface properties, textures, compositions, surface functionalities, etc. Inorganic polycondensation reactions happen in seconds, confined in “dynamic microreactors” (i.e. droplets). We explain why this peculiar mode of preparation has led to solid nanocatalysts showing high-performance in various applications including olefin metathesis, glycerol upgrading, olefin epoxidation, CO2 hydrogenation, and bioalcohol dehydrogenation and dehydration.[3] We will also demonstrate the concept of chemo-enzymatic heterogeneous catalysts obtained via spray techniques.[4] Finally, we will show the proof of concept of spark ablation as a tool to deposit metal nanoparticles on the surface of powdery catalysts supports.[5] Our objective is to illustrate the tremendous possibilities offered by airborne preparation processes, which arguably represent major routes of innovation, not only in the field of catalyst preparation, but also more broadly in the mushrooming nanotechnology field.



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Short biography:

Brahim Dkhil obtained his PhD in Physics and Materials Science in 1999 at Ecole Centrale Paris and University of Orsay, France and joined the Laboratory Structures, Properties and Modelling of Solids, at Centrale Supélec, University of Paris-Saclay to develop his research activity on ferroelectrics aiming at better understand the microscopic mechanisms at play in these materials through their structure-property relationships and better exploit their functionalities towards electronic, energy and environment applications.

Ferroelectrics: from computing devices to energy and environmental applications

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Ferroelectrics, with their intrinsic polarisation that can couple with charges, strains, spins or photons, offer a variety of properties that make them inherently multifunctional materials. Here we show how they can be used as less-energy consumption memory devices and logic elements in neuromorphic computing by exploiting their multiferroic coupling and domain states. Playing with the entropy of polarisations also provides a tool for designing efficient electrocaloric coolers that are competitive with other solid-state refrigeration technologies. This relationship between temperature and polarisation, which also exists between deformation and polarisation through piezoelectricity, is also essential not only for sensor and actuator applications, but also for energy harvesting, taking advantage of the free energy available in their immediate environment to convert it into useful electricity for mobile and autonomous devices. The above-mentioned energy conversion is also exploited in catalysis, providing other physical mechanisms for water depollution or hydrogen production that are competitive with or complementary to conventional photocatalysis. All these multiple and exciting applications, their fascinating physics and how to chemically design efficient ferroelectrics will be presented and discussed.

Short biography:

Hicham BEN YOUCEF is a professor at Mohammed VI Polytechnic University, Director of the High Throughput Multidisciplinary Research Laboratory (HTMR), and co-Director of the Applied Chemistry & Engineering Research Centre of Excellence (ACER). He obtained his Ph.D (Chemistry) in 2009 from the Swiss Federal Institute of Technology Zurich (ETHZ), Switzerland. His main interests are the development of functional and self-healing materials for different applications, such as electrochemical energy storage and conversion towards competitive targets (performance, durability, and cost). Prof. BEN YOUCEF focuses also on the implementation of automation and high-throughput solutions and workflow design for chemical processes and applied research in materials.

Functionalization of Bio-based materials for Solid Electrolyte: Towards Sustainable Energy Storage

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Lithium-ion batteries have made rapid progress as power sources in several applications including electric vehicles (EV) that require high energy density and high operating voltage [1]. However, the current technology still does not fulfill the automotive market requirements: durability, safety, autonomy, and power. In the scope of such development, the lithium-metal as anode, combined with intercalation/high-voltage-type cathodes, is one of the most viable and promising strategies towards developing high-energy-density rechargeable batteries. One of the main challenges for these next generation technologies is the uncontrolled lithium dendrite growth and consequently the poor safety due to short circuiting. Moreover, the use of liquid electrolytes is adding more concerns due to risks of leakage/volatility, limited mechanical and thermal stability, and a narrow operating voltage window (i.e., they experience pronounced electrochemical instability when exposed to voltages exceeding 4.5 V).

All-solid-state lithium batteries are experiencing strong development and are estimated to be the next marketable generation. Solid electrolytes are promising candidates for safe high energy density battery applications due to their intrinsic properties, mechanical flexibility, and scalability to the thin-film conducting configuration. Moreover, sustainable solutions for materials development are gaining more focus, helped by the establishment of constraining environmental regulations. Thus, the use of bio-based materials is a promising solution, especially, for the preparation of environmentally friendly solid polymer electrolytes [2-4]. The functionalization of cellulose, chitosan, and other biopolymers with delocalized anionic structures is an interesting approach towards the design of high performance composite electrolytes. These composites are the direction that should be prioritized for future research for developing safer, more efficient,

reliable, and cost-effective electrochemical energy storage systems (e.g., batteries, supercapacitors).

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Abstracts of Oral Communications

Session A

Exciton Fine Structure of Lead Halide Perovskite Nanocrystals $CsPbBr_3$: An interplay of Electron–Hole Exchange Interaction, Crytal Structure, Shape Anisotropy and Dielectric Mismatch

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In the present work we wish to bring a significant contribution in this still incompletely explored field by addressing the exciton fine structure (EFS) properties of $CsPbX_3$(X= Cl, Br, I) Nanocrystals. We lead a theoretical study of the excitonic band edge states applied to the more commonly studied inorganic perovskite nanocrystals: $CsPbBr_3$. We highlight the key roleplayed by the electron-hole exchange interaction, including long-range and short-range terms, in the positioning and splitting of dark and bright exciton sublevels, and discuss the influence of dielectric confinement, crystal field and shape anisotropy effects on the excitonic fine structure. The electron-hole exchange interaction splits the four excitonic states into three bright excitonic states at higher energy and a singlet dark state at lower energy. We find that, whatever the crystal phase, the bright-dark splitting is weakly sensitive to shape anisotropy. However, a strong enhancement, is obtained at the maximum of the dielectric contrast. For two crystalline symmetries (cubic and tetragonal), we particularly analyze how the bright exciton triplet energies vary, taking into account the states polarizations and considering the directions along which shape elongation/contraction applies.
The main effect of the dielectric contrast is to increase significantly the exciton energies, for all the configurations. The amplitude of bright exciton splitting are basically driven by the shape anisotropy and is almost insensitive to the dielectric contrast. On the basis of this model, we discuss recent results on $CsPbBr_3$nanocrystals photoluminescence.

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Boosting of CZTS-Based Solar Cells with Cu_2S as a Buffer Layer: A Combined Experimental and Simulation Approach

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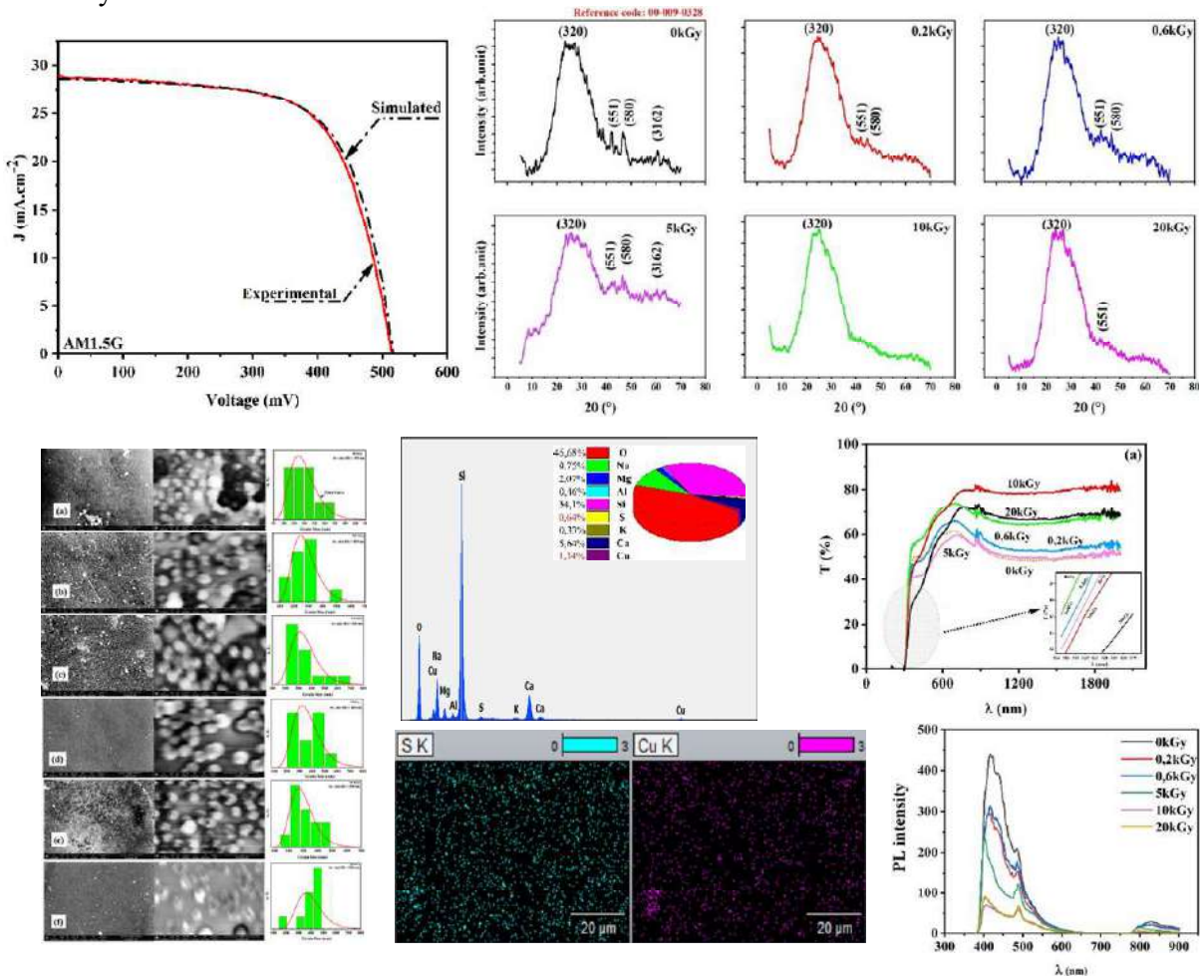
Cu_2S thin films were synthesized via chemical bath deposition and subsequently exposed to gamma radiation ranging from 0.2 to 20 kGy. The gamma ray exposure induced significant changes in film characteristics. No change in crystallinity was seen with increasing radiation exposure, according to X-ray diffraction examination. Scanning electron microscopy examination depicted variations in grain size dependent on radiation dosage. The optical band gap exhibited a reduction from 3.02 eV in the unexposed state to 2.36 eV after exposure to 10 kGy, accompanied by a decline in photoluminescence intensity with escalating radiation dosage. The proposed solar cell design uses Cu_2S as buffer layer and CZTS as the active layer. Numerous parameters such as layer thickness, doping concentration and defect density were optimized to balance and improve the device performance. A study revealed a maximum efficiency of about 30%. This work highlights the impact of gamma radiation on the properties of Cu_2S thin films and the development of solar cells based on environmentally friendly thin films.



Design and Computational Analysis of Nitrobenzofurazan-Based Non-Fullerene Acceptors for Organic Solar Cells

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This study explores the design of various nitrobenzofurazan (NBD)-based non-fullerene acceptors, labeled as Ai (i=1 to 5), using density functional theory (DFT) in acetonitrile solvent. These novel D-A type small molecules incorporate nitro (NO_2) or fluorine (F) groups into the NBD moiety with the goal of enhancing the efficiency of non-fullerene organic solar cells. The DFT and its extension time-dependent (TD-DFT) methods, using the B3LYP/6-311G(d,p), were employed to investigate the geometric, optoelectronic, optical, and charge transport characteristics of the designed molecules. These molecules exhibited narrower band gaps (2.25 to 1.67 eV) and higher maximum absorption (λ_{max} at 463 to 472 nm). Additionally, the studied compounds showed lower binding energies (E_b = 0.48-0.55 eV), indicating enhanced exciton dissociation rates due to significant charge transfer from donor to acceptor moieties, as revealed by FMOs, PDOS, MEP, and TDM analyses. These compounds also demonstrated notable photovoltaic properties, characterized by higher V_{oc} values and large FF factors. The findings suggest that all the designed molecules are highly efficiency as non-fullerene acceptors in organic solar cells (OSCs), with A4 identified as the most promising candidate due to its favorable electronic and photovoltaic properties. The blending of A4 with an NBD derivative donor strongly confirms the charge transfer dynamics between these molecules, highlighting its potential for effective application in real-world OSCs.

Impact of annealing temperature on morphological, structural, vibrational and electron paramagnetic resonance properties of spinel $CoAl_2O_4$

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Cobalt aluminate, $CoAl_2O_4$, is a special and versatile material that has attracted a lot of research attention for a wide range of applications [1,2]. It has the general formula AB_2O_4, in which A (cobalt (Co) atoms) and B (aluminum (Al) atoms) are divalent and trivalent cations that are combined in a spinel configuration to form a cubic crystal structure [3,4]. This arrangement provides to the material its distinguishing properties [5,6]. In this work, $CoAl_2O_4$ nanoparticles were effectively synthesized using a straightforward auto-combustion sol-gel method with starch as the organic fuel source. The impact of annealing temperature on their structural, vibrational, morphological, and magnetic properties was examined. The resulting spherical nanoparticles exhibited grain sizes ranging from 23.54 nm to 46.50 nm. X-ray diffraction (XRD) patterns confirmed the formation of a face-centered cubic (f_{cc}) spinel phase with the Fd-3m space group across all samples. The calculated average crystallite sizes increased from 24.65 nm to 56.27 nm, aligning with the observed grain sizes. Density Functional Theory (DFT) calculations were utilized to optimize cell parameters and confirm the structural properties of the synthesized $CoAl_2O_4$ nanoparticles. The combined experimental and DFT study revealed that higher calcination temperatures lead to an increase in unit cell volume and particle size. Fourier-transform infrared spectroscopy (FTIR) supported these findings by showing subtle shifts in characteristic $CoAl_2O_4$ absorption peaks with varying annealing temperatures, indicating a potential redistribution of Al^{3+} and Co^{2+} ions between tetrahedral and octahedral sites within the spinel structure. Electron paramagnetic resonance (EPR) spectroscopy indicated a magnetic state transition dependent on both annealing temperature and crystallite size. Fluctuations in the occupancy of Al^{3+} and Co^{2+} ions at specific sites also affected the nanoparticles' color, as the hue depends on the valence state and cationic coordination environment in the $CoAl_2O_4$ crystal lattice. Correlations between structural, vibrational, magnetic, and color properties were presented to understand how synthesis parameters influence $CoAl_2O_4$ characteristics, which is crucial for tailoring materials for specific applications.

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Optical characterization of $Si/SiO_2/HfO_2$heterostructures

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For several years, the microelectronics industry is constantly striving to enhance the efficiency of electronic components. This pursuit en compasses various aspects such as power consumption, manufacturing costs, and reliability. To achieve this objective, continuous miniaturization of electronic components (transistors, resistors, capacitors, etc.) is necessary [1]. However, the reduction in the dimensions of the transistors, in particular the thickness of the gate oxide conventionally constituted by a layer of SiO_2, is often accompanied by parasitic effects such as the appearance of leakage currents which leads to an increase in electrical consumption as well as a decrease in the reliability of the transistors.
A possible solution to this problem is to replace silicon dioxide with high-k dielectrics [2]. In effect, Hafnium dioxide HfO_2, because of its high dielectric constant (k = 16–25), its wide band-gap (5.6–5.8 eV) and its thermal stability in contact with the silicon has been considered as a promising gate material to replace SiO_2. However, It has been reported that the HfO_2 film has some intrinsic defects such as oxygen vacancies or interstitial oxygen atoms, which might lead to large trapping in the insulator, lower carrier mobility in the transistor channel, and sources of instability [3].
Therefore, a study of the optical proprieties of HfO_2 is a necessary step. Studies in the literature reveal the existence of a correlation between the trap density and the thickness of the HfO_2, as well as between the trap density and the refractive index of HfO_2[4].

In the present work, we carried out an ellipsometric study of $Si/SiO_2/HfO_2$ hetero structures, with different thicknesses of the HfO_2 layer, and determined the evolution of the refractive index of HfO_2 as a function of its layer thickness. The results obtained showed a good correlation with the results already obtained from photoluminescence measurements.

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Properties of mesoporous and microporous materials modified by iron nanoparticles as potential catalysts for water purification

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The aim of this work is to seek solutions to purify water from organic pollutants, in particular pharmaceutical residues such as Diclofenac, using the ozone degradation method catalyzed by synthetic porous materials and industrial waste such as zeolites. With this in mind, we have also deployed a new method for producing iron nanoparticles supported on these basic materials for the degradation of Diclofenac by ozone.

Firstly, we synthesized and characterized the two mesoporous materials (SBA-15 and SBA-16) with hexagonal and cubic structures respectively [1], where the results of the characterization techniques showed that these materials present very promising properties due to a higher degree of order, very large pore diameters and a very large specific surface areas.

Secondly, we used these materials as matrices in order to develop iron nanoparticles with more interesting properties than those of the parent materials using coffee and tea extract as a solvent [2] to replace the harmful reducing agent such as sodium borohydride.

Finally, these materials were tested in their purely silicic and iron nanoparticle forms for the degradation of Diclofenac using the ozonolysis method. The ozonation results showed that silicates and aluminosilicates such as SBA-15 and SBA-16 as well as type 4A zeolite are excellent catalysts for water purification with total mineralization at ambient temperature.

Keywords: Zeolite 4A, SBA-15, SBA-16, Nanoparticle, Ozonation, Diclofenac

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Elimination des micropolluants dans les effluents liquides pharmaceutiques par un bio adsorbant

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La quantité de substances pharmacologiquement actives utilisées pour traiter et prévenir les maladies et pour atténuer le stress associé à la vie moderne peut se mesurer en milliers de tonnes par an. Ces produits pharmaceutiques se retrouvent partiellement dans les effluents des stations d'épuration et par suite dans les eaux de surface. De nombreuses recherches sont actuellement menées afin de mettre en œuvre des méthodes appropriées pour l'élimination des produits pharmaceutiques des eaux usées.

Dans l'objectif de l'élimination des polluants pharmaceutiques, un substrat à base de plante (Caroube [1-3]) a été élaboré et caractérisé par : EDX, MEB, BET et FTIR. Le fruit séché est purifié et transformé en poudre selon un protocole bien déterminé. La rétention des micropolluants pharmaceutiques ont été réalisée par adsorption sur la poudre de caroube sous deux formes : brute et activée. Une optimisation des paramètres opératoires contrôlant le procédé d'élimination des polluants (pH zéro, pH, temps de contact, vitesse d'agitation, masse d'adsorbant …) a été conduite, l'étude expérimentale d'élimination des micropolluants avec les substrats élaborés a permis de déterminer une efficacité d'élimination de 80 % pour la caroube brute, cette efficacité est améliorée jusqu'à 86% pour la caroube activée. Une étude cinétique a été menée, a révélé que la réaction d'élimination suit la loi du pseudo second ordre et l'étude d'adsorption a montré et que le modèle décrivant le processus d'adsorption est celui de Langmuir. Les résultats obtenus montrent que la caroube est un bon adsorbant pour l'élimination du paracétamol cette efficacité est meilleure dans son état activé.

Mots clés : micropolluants pharmaceutiques, adsorption, caroube.

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Physical approaches of the carrier dynamics involved in the temperature dependence of the luminescence intensity for self-assembled QD systems

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Modeling of the PL intensity of nanostructures from a system of equations of standard carrier transfer rates is widely used to describe the dynamics of exciton populations in semiconductor materials outside thermodynamic equilibrium. The immense complexity of such modeling lies in the physical interpretation of the recorded appearances of the evolutions of the PL intensity as a function of the parameters of the PL experiment (excitation power and temperature). This interpretation necessarily requires knowledge of the band structure of the sample studied and especially the order of magnitude of the carrier transfer rates relative to the different processes considered in such modeling. The fitting of experimental data with the proposed models generally leads to the validation of the physical hypotheses adopted during the interpretations of the optical response of the investigated semiconductor nanostructure. The work presented here focuses on describing the physical approaches to consider in modeling temperature-dependent photoluminescence measurements from semiconductor nanostructures.

Enhanced Energy Density in Graphene-Based Supercapacitors Modified With Prussian blue and Carbonaceous Materials

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Energy storage devices are important to store energy harvested from intermittent renewable energy sources such as solar radiation and wind. Electrochemical supercapacitors are ideal for this purpose because of their high-power density still but suffer from low energy density compared to rechargeable lithium and sodium batteries. The work pertains to the design of flexible laser-induced graphene-based supercapacitors with enhanced energy storage performances. The latter was enhanced through the post-modification with carbon-based materials and redox metal-organic frameworks. First, the electrodes were prepared by direct laser scribing using an affordable carbon dioxide laser. Next, the electrode active surface was modified with carbon black or carbon nanotubes as typical carbon nanomaterials followed by the chemical deposition of iron(III) hexacyanoferrate (FeHCF) as a redox metal organic framework for faradic energy storage. The performances of the devices were studied in aqueous electrolytes by hydrodynamic electrochemical techniques such cyclic voltammetry and potential-limited potentiometry. Results showed that both materials have a synergetic effect of both materials, and the overall improvement of the specific capacitance is over 300%. This amenable approach can be generalized to other capacitive nanomaterials and redox-active inorganic nanomaterials.

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Synthesis and Application of 2D Mono-element Materials in an Energy Harvesting Device

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In this work, we present the synthesis results of 2D mono-element semiconductor materials via liquid-phase exfoliation from powder. These materials exhibit a layered crystalline structure held together by Van der Waals interactions. They have been characterized using UV-visible spectroscopy, photoluminescence, Raman spectroscopy, and optical microscopy. Image processing and numerical analysis significantly enhanced the characterization, while a theoretical study based on Density Functional Theory (DFT) was conducted to compare with experimental results. The application of these materials in energy harvesting, exploiting the triboelectric effect, enabled us to assess their electrical transport properties in a harvesting device. These materials were also ranked according to their position in the triboelectric series.

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Eigenvalues and eigenfunctions of an anharmonic oscillator perturbed with different Gaussian profiles potentials

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Many problems in physics, chemistry and biology can be modelled by a simple form of one dimensional quantum-well potentials. Trying to understand the interactions between nuclei, nuclei-particle or the structures of diatomic and poly-atomics, the scientists have created several potential models and developed many mathematical methods to study this problem. We can cite the delta function [1] and the harmonic oscillator potential [2]. However, these models cannot describe precisely the experimental values of several processes and must be corrected. In this target, other potential models have been established and discussed, like the Gaussian [3] and Morse [4] functions. In this Work, we report the numerical solutions of the time independent Schrödinger equation using the matrix Numerov's method. We used this approach to study the simple sextic anharmonic oscillator. This system has been also studied numerically with the effect of different Gaussian perturbation potentials. We have used different mathematics functions to model one simple and periodic Gaussian well perturbation. The energies and the corresponding wave functions have been also calculated.

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New phospholipase A2 enzyme inhibitor

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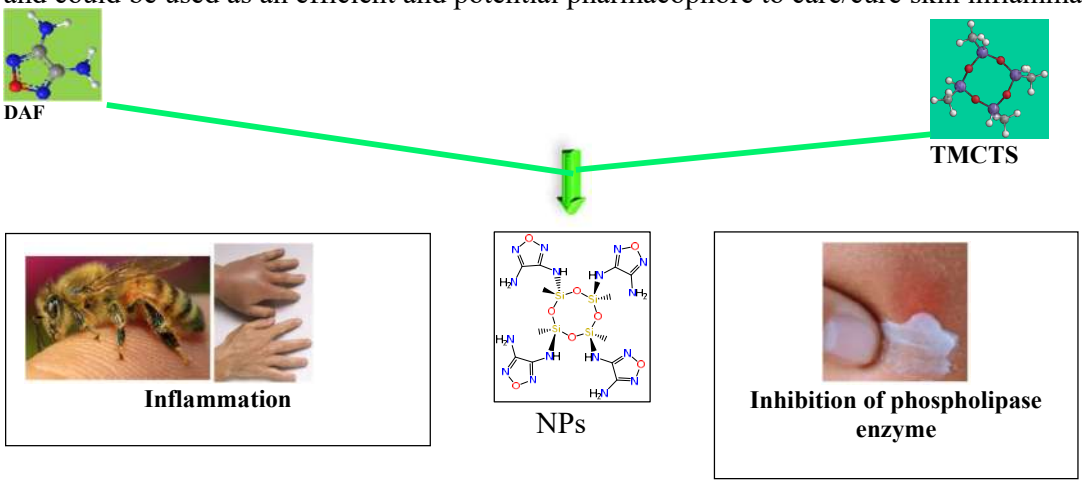
In search of new bioactive materials, novel hybrid nanomaterials (NPs) is synthesized. The main purpose of this research study is to synthesize a new hybrid nanomaterial and to investigate its anti-inflammatory activity, based on phospholipase A2 inhibition. The novel Nano material is synthesized via an hydrosilylation reaction between the Tetramehylcyclotetrasiloxane (TMCTS) used as a silicon source and the 3,4-diaminofurazane (DAF) an important component used in medicinal chemistry research. To confirm the synthesis route, the NPs chemical structure, is studied by ^{29}Si, ^{13}C CP MAS NMR and FTIR spectroscopy. According to the spectroscopic results the 3,4-diaminofurazane nuclei are attached to the silica skeleton, creating a Nano hybrid material wherein Si-N covalent bonds are established. The surface morphological shape and the size of HNPs are visualized and portrayed using the SEM technique. It is noteworthy that the sizes of the NPs are at the Nanoscale with an average size of approximately 100 nm in diameter. The NPs inhibitory activity against phospholipase A2 enzyme is studied, and based on the experimental results the new nanomaterial has a high inhibition of the phospholipaseenzyme. Safety and biocompatibility of the synthesized NPs toward normal human epithelial cells are observed. The results demonstrate that the NPs is highly effective in inhibiting phospholipase enzyme and could be used as an efficient and potential pharmacophore to care/cure skin inflammation.



Keywords: Nanomaterrial; phospholipase; enzyme; anti-inflammatory. Inhibition.

A new dipyrenylcalixazacrown chemosensor for metal cations Selectivity of Mg^{2+}

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Fluorescent chemosensors for cations composed of a cation recognition unit (ionophore) together with a fluorogenic unit (fluorophore) are usually described as fluoroionophores. An effective fluoroionophore must convert the cation recognition by the ionophore into an easily monitored and highly sensitive light signal from the fluorophore. As fluorogenic units, pyrenes (Py) are one of the most useful tools due to their relatively efficient excimer formation and emission. Host molecules with more than one pyrenyl group exhibit intramolecular excimer emission by two different mechanisms. One results from □-□ stacking of the pyrene rings in the free state, which results in a characteristic decrease of the excimer emission intensity and a concomitant increase of monomer emission intensity. The other mechanism is due to the interaction of an excited pyrene (Py^*) unit with a ground state pyrene (Py) unit.

We describe herein the synthesis and fluorescent properties of monopyrenyl-*p-tert*-butyl calix [4] tetraaza-crown-6 (**3**) and dipyrenyl-*p-tert*-butyl calix[4]tetraaza-crown-6 (**4**) (Scheme 1). Addition of various metal ions (Li^+, Na^+, K^+, Cs^+, Ag^+, Mg^{2+}, Ca^{2+}, Pb^{2+}, Zn^{2+}) to acetonitrile solutions of **3** and **4** shows that the response by the receiver **3** (one pyrene) is not significant enough, the component **4** (two pyrene) is selective for Mg^{2+}.

Keywords: Calixarene, fluorophore, Stability constant, Host-guest chemistry

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Multiferroic NanoMaterials: Synthesis, Characterization and Modelling

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Different multiferroic bismuth ferrites (BFO) with different crystalline phases and morphologies were successfully prepared using a low-cost hydrothermal method with varying reaction times [1].This led to the formation of the pure $BiFeO_3$ and $Bi_2Fe_4O_9$ powdered phases for 6 h and 18h, respectively. The structure and morphology of the as-prepared powdered samples were studied by X-ray diffraction (XRD) and Transmission Electron Microscopy (TEM). The magnetic properties were investigated by ^{57}Fe Mössbauer spectrometry and the "Physical Property Measurement System" (PPMS) [2]. The structural, electronic, and magnetic properties of bismuth ferrite BiFeO3 and Bi2Fe4O9 nanostructures were also investigated using Density Functional Theory (DFT) within Generalized Gradient Approximation (PBE-GGA) plus U calculations (Figure 1). It shows that the antiferromagnetic phase is more stable than the ferromagneticone in both structures, $BiFeO_3$ and $Bi_2Fe_4O_9$.

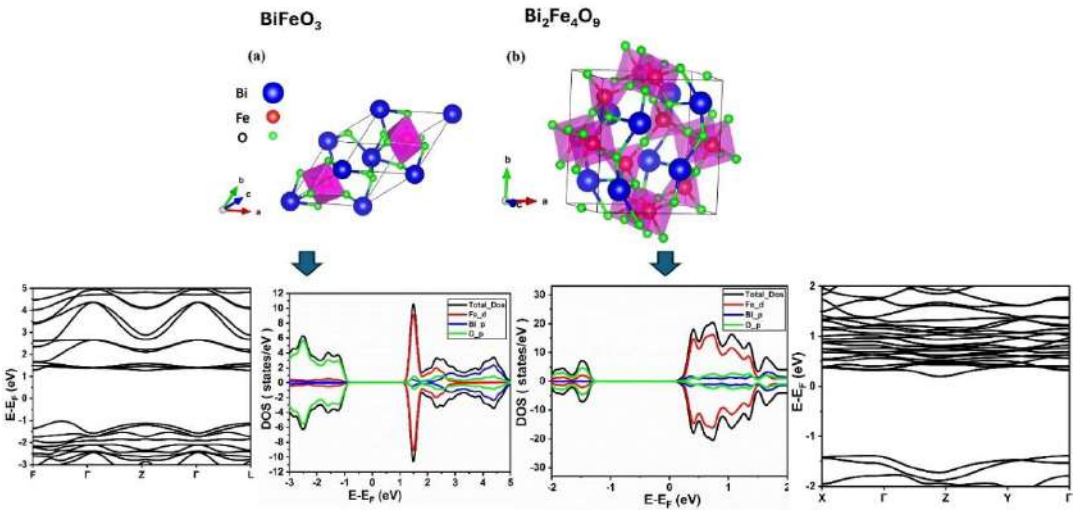

Figure 1: The PBE-GGA+U computations for $BiFeO_3$ and $Bi_2Fe_4O_9$ nanostructures.

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Computational investigation of interfacial charge transfer in dye-sensitized solar cells (DSSCs)

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Theoretical modeling plays a crucial tool in advancing the understanding of DSSCs by providing detailed insights into both individual cell components and the combined dye/semiconductor/electrolyte system, which have been the subject of a detailed experimental investigation (*Solar Energy 199 (2020) 92–99*). This approach complements experimental research by offering a deeper understanding of the fundamental chemical and physical processes that govern cell functionality and performance. Through the modeling of ground and excited state properties by using dispersion-corrected density functional theory (DFT-D3) and time-dependent DFT(TD-DFT), the present study sheds light on key mechanisms such as dye-to-semiconductor electron injection and charge transport, driving the development of more efficient DSSC technologies. Our theoretical approach has been validated via a comparison between available experimental data and obtained results. This research examines the geometries, electronic structures, absorption spectra, electron transfer, injection properties, and the overall efficacy of D-π-A dyein dye@$(TiO_2)_9$ system. The simulated absorption spectra demonstrate a redshift of the lowest optical transition of the dye upon adsorption. The interaction between dye and $(TiO_2)_9$results in an interfacial electronic charge transfer (CT) which were supported by ELF analyses by visualizing excess electrons surrounding the dye acceptor entity. Additionally, the interaction between dye and iodine before and after adsorption on $(TiO_2)_9$ surface has been also studied. Overall, this study demonstrates that the low conversion efficiency in Digital Materials Deposition "DMD" fabricated semi-transparent DSSCs can be attributed to the twisting of the dye structure, which possibly forms less compact dye layers on $(TiO_2)_9$ surface and then a significant charge recombination.

Study of the static and the dynamic correlation of the confined Rydberg dressed atoms systems

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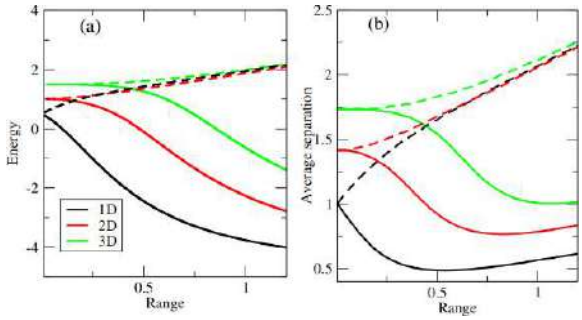
When atoms are excited to large principal numbers, these are known as Rydberg states. The interaction between such atoms is known to exhibit multipolar and long ranged proprieties as well as a very unique feature which is the excitation blockade. This kind of system has attracted a tremendous interest as a reliable candidate in the field of quantum computing [1]. This study aims at the understanding of the spatial correlation of two Rydberg atoms confined in a harmonic trap. The interaction potential in this case can be given as:

$$v(r)=\frac{g}{1+\left(\frac{r}{R_c}\right)^6}, \qquad (1)$$

where, g gives the strength and R_c is the range of the potential respectively. In order to reach an exact solution for the Schrodinger equation, this interaction is replaced by a step like potential [2]. We are proving in our calculation the fair adequacy of the step potential to replace the realistic situation. The advantage of this approach is establishing a quasi-solvable model with mathematical formulation for the eigenvalues and the eigenvectors. The previous model is then devised to characterize the spatial correlation of the two electrons. It is clearly established that the interplay between the dimensionality of the system, the available energy and the sens of the interaction whether it is attractive or repulsive (solid and dashed respectively in the figure), will dictate a whole bunch of scenarios concerning the spatial distribution of the system. The results are extensively detailed in this study [3].



The second part of this study is concerned with the temporal evolution of the previous correlation which was initially established in a static regime. To investigate this aspect different quench scenarios of the potential strength are operated on the system and then the evolution of the density alongside the electrons separation and the time is depicted. Gathering a maximum of data about these dynamical aspects and discriminating numerical artefacts could lead to a very important insight on theoretical and technological aspects of few cold particles systems.

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Hydrogen-bonded liquid crystal complexes: Thermal and dielectric properties

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A new series of hydrogen-bonded liquid crystals (HBLCs) composed of 3-flurobenzoic acid derivatives (nOBAF) and 1,4-diazabicyclo [2.2.2] octane (DABCO) has been prepared and characterized by Fourier-transform infrared spectroscopy. The thermal behavior was determinedbydifferentialscanningcalorimetryandobservedbypolarizedopticalmicroscopy (POM). All complexes were found to exhibit smectic G (SmG) and smectic B (SmB) phases over a wide temperature range. The complex dielectric permittivity was reported as a function of frequency in the range 1 Hz–10 MHz.

Impact of Miniaturization on Electrical Properties of High-k Interface Diodes

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This study explores the electrical and dielectric properties of the TiN/Al_2O_3/p-Si MIS structure within the temperature range of 380-450 K at 1 MHz. These properties were derived from experimental measurements. Results indicate that forward bias plots show a distinct peak at higher temperatures, primarily due to series resistance and interface states between Al_2O_3 and p-Si. The dependence of the dielectric constant, dielectric loss, dielectric loss tangent, and AC electrical conductivity on temperature and bias voltage was examined. Findings reveal that these values vary with changes in bias voltage and temperature. The characteristics confirm that the series resistance and interface states significantly influence the electrical parameters in the MIS device. The interface state density, dependent on temperature, was determined using the Hill-Coleman Method. An Arrhenius plot of AC conductivity at 1 MHz shows the activation energy. Additionally, electric modulus formalisms were used to understand the relaxation mechanism of the structure.

Exploring the structural, mechanical and electronic properties of Fe_2CoGa by DFT calculations

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Using the first principal study, we present and discus the structural, mechanical and electronic properties of Fe_2CoGa. The phase stability has been treated by applying the generalized gradient approximation (WC-GGA). Moreover, the calculated lattice parameters are found to be in good agreement with experimental data. Based on the structural results; the bulk modulus exhibits significantly high magnitude placing Fe_2CoGain the range of hard materials. In this case, it is best to verify this by calculating the set of elastic constants and its derivatives. For understanding the electronic properties in the studies Fe_2CoGa, band structure, total and partial density of states have also been performed and discussed thoroughly. Ending with the magnetic properties, the results show that the total magnetic moment is equal to 5.6μB making the material very useful for the spintronic applications.

Keyword: Fe_2CoGa; DFT; phase stability; mechanical properties.

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Correlation between structure, acidity and catalytic performances of tungstate catalysts for microwave assisted hemicelluloses hydrolysis

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The conversion of biomass into biofuels plays a significant role in mitigating greenhouse gas emissions, addressing the challenges associated with problematic solid waste, and reducing the health risks posed by conventional fossil fuels. It is evident that using renewable energy sources such as biomass presents a viable alternative for substituting fuels and chemicals, given their abundance as an energy resource. Depending on the specific type of biomass, catalytic processes can be employed. A variety of materials have been developed through heterogeneous catalysis, including modified zirconia. This research focuses on the development of catalysts based on zirconia, Al-SBA-15, and H-ZSM-5, which have been modified with tungsten, and aims to enhance the catalytic properties of these solids in the hydrolysis of hemicellulose.

According to the IUPAC classification, the N_2 adsorption-desorption isotherms for all synthesized samples were identified as type IV. Such isotherms are typical of mesoporous materials where capillary condensation takes place.

The examination of XRD patterns for ZrO_2 and its tungstated counterpart indicates the existence of the metastable tetragonal and the stable monoclinic phases. It is noteworthy that the incorporation of tungsten species into zirconia does not significantly alter the crystalline structure of ZrO_2 [1]. The XRD analysis of Al-SBA-15 and its tungstated counterpart samples suggests the presence of an ordered hexagonal mesoporous structure [2]. In relation to the H-ZSM-5 sample and its tungstated equivalent, the XRD patterns display peaks that are indicative of a highly crystalline orthorhombic MFI-type framework of the zeolite [3].

The NH_3-TPD results indicate that the introduction of tungsten species significantly reduces both the total quantity of desorbed NH_3 and the density of acid sites. Furthermore, the integration of tungsten species into H-ZSM-5 leads to a marked decrease in the density of acid sites on the support.

The catalytic activities of catalysts composed of ZrO_2, A1-SBA-15, and H-ZSM-5, which were doped with tungsten species, were evaluated in the hydrolysis of hemicellulose using a microwave reactor. These supports demonstrated comparable conversion rates for hemicellulose, even though they possess distinct structures, specific surface areas, pore configurations, pore dimensions, and acidity levels. Furthermore, the addition of tungsten species markedly enhances the conversion efficiency in the hemicellulose hydrolysis process.

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Effect of active layer thickness on the charge recombination and dissociation in bulk heterojunction polymer solar cells under open circuit conditions

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Bulk heterojunction organic photovoltaic cells (OPVs), which are based on anthracene-containing poly (p-phenylene-ethynylene) - alt – poly (p-phenylene-vinylene) (PPE-PPV) polymer denoted (AnE-PVstat) and phenyl C60 butyric acid methyl ester (PCBM). The active layer thickness was varied from 100 nm to 300 nm. The solar cell parameters and magnetoconductance (MC) effect were analyzed, and the results showed a positive MC effect (+MC) for active layer thickness of 100 nm, 150 nm, and 200 nm, while a negative MC effect (-MC) was observed for thickness of 250 nm and 300 nm. The Power conversion efficiency (PCE) of 4% was achieved for an active layer thickness of 200 nm. The triplet-doublet quenching (TQD) model was used to describe the MC effect, which is influenced by triplet-charge reactions on the current based on density matrix formalism using the Stochastic Liouville Equation. The dissociation and recombination rates of the T-D pairs increased with thickness of thinner layers (100, 150, 200 nm) while decreased for thicker layers (250 nm and 300 nm).

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Ab initio modeling and design of low dimensional platinum disulfide (PtS_2)

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Low dimensional2Dmonolayer and 1D single-walled zigzag platimundisulfide PtS2 nanotubes are simulated with an ab initio quantum chemical method. The (n,0) family is investigated in the range from n = 12 (72 atoms in the unit cell and tube radius R = 6.8 Å) to 32 (192 atoms in the cell and R = 18.2 Å). The trend toward the hexagonal monolayer in the limit of large nanotube is explored for a variety of properties: rolling energy, elastic modulus, vibrational infrared and Raman spectra and electronic and nuclear contributions to the polarizability tensor. Two groups of active phonon modes are found in their spectrum. Platimundisulfide PtS2 nanotubes are confirmed to be narrow band gap semiconductor with properties weakly connected to the tube radius. The attempts in this contribution may explore a new approach for design and optimization of lowdimensional PtS2 for possible use in modern nanodevices.

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

Improving Energy Density of Supercapacitors Based on Laser-Induced Graphene Electrodes by Using Cyanide-Bridged MOF nanomaterials

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Abstract

This study explores the development of high-performance supercapacitors using laser-induced graphene (LIG) electrodes modified with metal-organic frameworks (MOFs), specifically metal hexacyanoferrates (MHCF, M: Fe, Mn, Co). LIG, with its excellent conductivity and high surface area, serves as an ideal substrate for energy storage applications. By incorporating MHCF into the LIG matrix, the electrochemical performance of the supercapacitors is significantly enhanced due to the synergistic combination of the capacitive behavior of LIG and the faradaic redox activity of the metal hexacyanoferrates.

Among the tested materials, cobalt hexacyanoferrate (CoHCF) demonstrated the highest performance, with a remarkable improvement of over 300% in capacitance compared to pristine LIG. This improvement is attributed to the high redox activity and electrochemical stability of CoHCF, which facilitates fast charge-transfer kinetics and efficient ion diffusion. The CoHCF-modified LIG electrodes exhibited excellent energy storage capabilities, making them a promising candidate for next-generation supercapacitors with higher energy density and long-term cycling stability. These findings highlight the potential of combining LIG with MOFs for the development of advanced energy storage systems, particularly in applications requiring rapid charge-discharge cycles, such as portable electronics and electric vehicles.

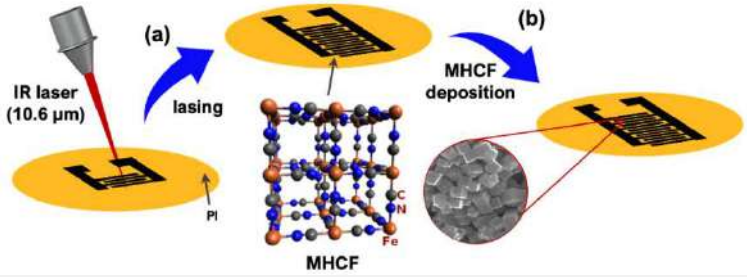

Figure:Principle of the method used to modify the laser-induced graphene electrodes with MOF for performance enhancement

Keywords

Graphene;Energy Storage; MOF; Electrochemistry; Supercapacitors

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Wurtzite InAs/InP nanowires emitting at telecommunication wavelengths monolithically grown on silicon using VLS method.

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The rapid improvement in vapor–liquid–solid (VLS) nanowire (NWs) growth by molecular beam epitaxy (MBE) has motivated the experimental investigations of 1D nano-device [1-3]. The present work combines structural, optical and theoretical investigations to study Wurtzite (WZ) InAs quantum rods (QRs) in InP nanowires (NWs) grown on silicon substrate by solid source MBE and VLS method.

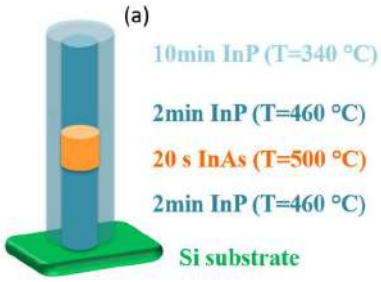

Fig.1. Schematic of the investigated sample [3].

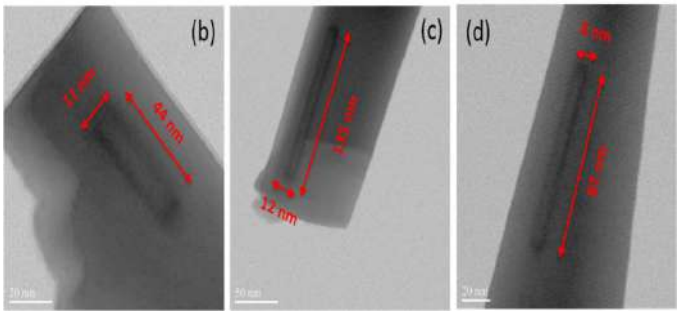

Fig.2. TEM images showing InP NWs with different dimensions of InAs QRs [3]

A theoretical model based on finite element method (FEM), considering the real shape of InAs QR revealed by transmission electron microscopy and the strain effects, has been developed to quantitatively explain the observed PL transition energies. Moreover, our results show that the room-temperature integrated PL intensity from InAs/InP QR-NWs, operating at telecommunication wavelength band, maintains over 30% of its low temperature value (14 K).

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Strain engineered InAs QDs for optoelectronic devices

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Self-assembled semiconductor quantum dots (QDs) formed by Stranski-Krastanov (SK) growth mode emerges as a key technology in ultrafast science and optoelectronic devices, induces high speed data transfer with low power conception **[1,2]**. In particular, their integration as the active layer lead to extend novel perspectives of obtaining QDs light emission in the International Telecommunication Union (ITU) window operating at room temperature **[3].** The development of a simple technology to modify the optical and dynamic properties of self-assembled QDs has been subjected to intense research. To date, various strain engineering techniques for QDs systems have been reported **[4]**. On the other hand, numerous promising post-growth techniques make also possible to increase the spectral range of detection and sensitivity of the infrared photodetector **[5]**.
In this work, we report on the first part the influence of different parameter such as size, form, composition, density, and particularly the strain on the optical properties of QDs. Time resolved photoluminescence spectroscopy was employed to demonstrate the dependence of PL decay time of InAsQDs' position within InGaAs strain reducing layer as compared to InAs QDs directly deposited on GaAs layer **[6]**. Furthermore, including the investigation of thermal induced intermixing in QDs structures could add considerable insights into carrier emission and dynamics. Due to their high uniformity and best confinement (large size), QDs with strain reducing layer may exhibit very different decay behaviors induced by RTA.
To conclude, we have investigated the effect of introducing InAsQDs within InGaAs strain reducing layer on the carrier emission and dynamics by correlation between the optical properties. We have also investigated the effects of RTA on the emission properties of uniform self-assembled InAs/GaAs QDs emitting at O-band telecommunication window at room temperature.

Key word: Quantum dot, Strain reducing layer, Time resolved photoluminescence and rapid thermal annealing.

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Abstracts of Oral Communications

Session B

Label-Free Capacitive Detection of Kanamycin Antibiotic Residues in Dairy Products

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The presence of antibiotic residues in food products poses significant risks to human health and contributes to antibiotic resistance. Kanamycin, a widely used aminoglycoside antibiotic, can persist in dairy products, necessitating sensitive, reliable, and cost-effective detection methods [1]. This study reports the development of two label-free capacitive aptasensors for detecting kanamycin residues in dairy products. The sensing platforms utilize screen-printed carbon electrodes modified with gold nanoparticles or reduced graphene oxide and polydopamine or polyaniline, which are electroactive polymers known for their excellent conductivity, biocompatibility, and functionalization capabilities.

The sensor surfaces are functionalized with a kanamycin-specific aptamer that selectively binds to kanamycin, resulting in changes in the redox capacitance of the immobilized polymer films. The capacitive response is directly correlated with kanamycin concentration, enabling quantitative analysis without complex labeling. The aptasensors exhibit a wide linear detection range with a femtomolar-level detection limit, demonstrating high sensitivity and selectivity toward kanamycin, even in the presence of other antibiotics and potential interferents.

The developed sensors were successfully applied to detect kanamycin in spiked milk samples, highlighting their potential for real-world applications. The proposed aptasensors are rapid, cost-effective, and easy to operate, offering significant advantages over conventional chromatographic methods, which are often time-consuming and require sophisticated instrumentation. This study underscores the potential of capacitive-based aptasensors for routine monitoring of antibiotic residues in food safety and quality control, supporting public health protection and regulatory compliance in the dairy industry.

Acknowledgments:
Authors acknowledge the Young Researchers Encouragement Program for financial support to PEJC2023–D1P21 project.

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Graphitization of olive mill waste biomass by pyrolysis for H_2, CH_4 and CO_2 gas detection

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Greenhouse gas (GHG) and particularly carbon dioxide (CO_2) emissions resulting from extensive burning of fossil fuels are the main actors responsible on global warming and climate changes of the last years [1]. The development of highly performant gases adsorbent materialsisseen as one of the most efficient techniques that has gained a lot of attention for carbon capture [2]. A*graphitized adsorbent of CO_2, CH_4 and H_2 gases is prepared from pre-treated olive mill waste using pyrolysis method under N_2 atmosphere. This organic adsorbent is found to have a large surface area of* 1571 m^2/g and high pore volume of 1.04 cm^3/g. The isotherms analysis by using Brunauer-Emmett-Teller (BET) method revealed that the aforementioned adsorbent exhibits mesopore structure coexisting with a microporous framework. Thanks to these textural properties, gases uptakes of this adsorbent at 298 K and 20 bars reach 5.62, 12.72 and 0.08 mmol/g for CH_4, CO_2 and H_2, respectively, which are among the highest levels compared to other solids. The adsorption-desorption cycles performed for CH_4, CO_2 and H_2 gases were found to be reversible indicating a possible regeneration of adsorbent. Considering all these advantages such as lowcostgraphitization, great uptake of various gases, good physicochemical stability and strong reversibility, this adsorbent can be a promising candidate for gases storage.

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Synthesis and caracterisations of nanocomposites PB@$NiFe_2O_4$

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Actually, PB@MFe_2O_4 nanocomposites (M = $Ni^{2+,}$ Co^{2+}, etc.) have attracted a lot of attention because of their applications in various fields such as magnetic refrigeration, magnetic resonance imaging, sensors and catalysis. A simple, inexpensive and reproducible strategy study to synthesize PB@$NiFe_2O_4$ nanocomposites was carried out as part of this work. The nanocomposites were prepared using the co-precipitation method.

The structural study by X-ray diffraction (XRD) revealed a preferential orientation according to the reticular plane (2 3 3). Surface analysis by scanning electron microscopy (SEM) confirmed the presence of elements characteristic of both Prussian blue and nickel ferrite in the samples. FT-IR spectroscopy showed characteristic bands located at 556.92 cm^{-1}, assigned to the vibration mode Ni-O, and others at 389,8 and 364,2 cm^{-1}, corresponding respectively to the complex cyanoν(Fe–C) and complex cyanoδ(Fe–C-N) vibrations. BET analysis revealed a significantly higher specific surface area for nanocomposites PB@$NiFe_2O_4$ compared to nickel ferrites $NiFe_2O_4$, which is advantageous for the proposed adsorption applications.

Keywords: PB@$NiFe_2O_4$ nanocomposites – Catalysis – Adsorption.

Effect of deposition time of cobalt oxide (Co_3O_4) nanowires into stainless-steel substrates on the supercapacitive performance and stability.

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In this study, we present the synthesis of cobalt oxide (Co_3O_4) nanowires (NWs) with varying deposition times using a hydrothermal method, aimed at designing a promising system for supercapacitor applications. The effect of deposition time, ranging from 3 to 12 hours, on the physical and electrochemical properties was investigated through several techniques. X-ray diffraction (XRD) analysis revealed the polycrystalline nature of $Co_3O_4$with a face-centered cubic phase in all samples. Scanning electronmicroscopy (SEM) demonstrated notable changes in nanowire density and surface roughness with increasing deposition time. Electrochemical characterization, including cyclicvoltammetry, galvanostatic charge-discharge, and electrochemical impedance spectroscopy (EIS), showed that the sample deposited for 6 hours (SSANWs-6h) achieved the highest specific capacitance of 824 Fg^{-1}, demonstrating excellent supercapacitive performance. EIS results also indicated superior electronic conductivity, further emphasizing the potential of SSANWs-6h for energy storage applications. To confirm this behavior, the structural stability of the electrode was tested after 1000 cycles, reinforcing its suitability for long-term energy storage applications.

New insights of the adsorption and photodegradation of textile dye using water-soluble semi-conductor nanocrystals: mechanism, interpretation and statistical physics modeling

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In this study, CdS nanocrystals capped with 3-mercaptopropionic acid (MPA) were prepared and tested as nanoadsorbents and photocatalysts for the elimination and degradation of reactive black 5 (RB5) dye in an aqueous medium[1]. Dye adsorption data were collected at 298, 308, and 318 K. The modeling of experimental data showed the best fit to the Sipsisotherm model, and the adsorption kinetics were followed for the pseudo-first order (PFO). CdS MPA was found to have a specific surface area of 140 m^2/g and 23.90 mg/g maximum adsorption capacity at 298 K, attaining a removal efficiency of 95.2% after 20 min. The steric and energetic parameters were analyzed using statistical physics models (SPM). The experimental data were predicted by an advanced single energy adsorption model. At low temperatures, dye adsorption occurred by physisorption with weak interactions to establish a monolayer adsorption process. The dye molecules can be removed in parallel and non-parallel orientations. At high temperatures, the dye adsorption was multi-molecular, indicating that the dye can be removed at a slanted position. Theoretical calculations indicated that physical interactions were involved in RB5 adsorption. Photocatalytic studies indicated that the degradation efficiency was close to 99% within 120 min, and the PFO kinetic model best matched the experimental data. RB5 adsorption on the CdS-MPA adsorbent led to three degradation-regeneration cycles. These results underline the effectiveness and sustainability of this system, reinforcing its feasibility and potential application in photocatalytic reactions[2].

Keywords: Colloidal nanocrystal synthesis; Adsorption; dye; SPM; photodegradation, regeneration

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Advanced Screening of Autoimmune Diseases: A Machine Learning Approach to Spectroscopic Analysis

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This study focuses on the development of innovative screening techniques for autoimmune diseases, particularly Systemic Lupus Erythematosus (SLE), aiming to overcome the limitations of invasive and costly analyses. By leveraging non-invasive spectroscopic methods such as the Laser Induced Breakdown Spectroscopy (LIBS) [1] and UV-Visible fluorescence [2], along with the analysis of easily acquired biological tissues like nails, hair, and skin, the research aims to enable rapid, real-time, and cost-effective disease detection on-site. The investigation involves comparing the results of tissue analyses with traditional blood analyses, encompassing patients at different disease stages. The objective is to establish criteria for disease prevention and progression through cluster analysis, drawing from extensive expertise in spectroscopic techniques and previous studies in related pathologies. Additionally, the study explores the potential of machine learning to automate screening processes, anticipating significant contributions to diagnosis prediction and classification of autoimmune diseases.

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Development of sensitive and selective electrochemical sensing platform based on AuNPs@CuNPs-supported molecularly imprinted polymer for specific recognition and determination of cefazolin

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The β-lactam antibiotic cefazolin (CFZ) is frequently administered to animals to prevent illness or stimulate growth since it works well against gram-positive bacteria. However, animal food products, including meat and milk, contain residues from the misuse or overuse of cefazolin. Furthermore, it may increase bacterial resistance, which could have detrimental effects on people's health [1].Molecular imprinted polymers (MIPs) have been used as synthetic receptors or antibody replacement materials over the past 20 years because of their great stability, quick electropolymerization time, and excellent specificity for the target analyte. However, MIPs' low conductivity and lack of electrocatalytic activity decreased the sensitivity of electrochemical sensors. To overcome this restriction, MIP-based electrochemical sensors with excellent sensitivity and specificity were created using gold nanoparticles (AuNPs), copper nanoparticles (CuNPs), silver nanoparticles (AgNPs), and their nanocomposites. This is because the high surface area, strong electrical conductivity, and simplicity of nanomaterials' functionalization increase MIP sensitivity to a specific target compound. The advantages of electrochemical techniques, such as fast response time, user-friendliness, affordable price, and miniaturization, when combined with nanomaterial-supported MIP-based electrochemical sensors, become effective tools for more selective and sensitive determination of CFZ.In the present work, the first nanomaterial-assisted MIP-based electrochemical approach with copolymerization was proposed to determine CFZ successfully using the electropolymerization method. Here, 3-thienyl boronic acid (3-TBA) and pyrrole (Py) were used as monomers. AuNPs and CuNPs were added to improve the MIP sensor's sensitivity and porosity. The MIP-based nanocomposite sensor was characterized using electrochemical (cyclic voltammetry, CV), electrochemical impedance spectroscopy, EIS), and scanning electron microscopy, SEM) techniques. The measurement of MIP parameters, such as the addition of nanoparticles, template: monomer ratio, electropolymerization number of the scan, removal solution, removal number of the scan, and the rebinding time, the monomer ratio, etc., was performed using the differential pulse voltammetry (DPV).Under the optimized conditions, CFZ/poly(Py-co-3-TBA)/AuNPs@CuNPs@MIP/GCE obtained a linear response in the concentration range between 2.5 pM and 25.0 pM. Furthermore, compounds with structural similarities to CFZ, including cefuroxime, cefdinir, cefixime, ceftazidime, and ceftriaxone, were used in the imprinting factor (IF) study. The recovery studies of CFZ were successfully applied to tablet dosage form samples, and the sensor that was designed for fast CFZ detection in tablet dosage form showed notable sensitivity and selectivity.

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Cholesteric liquid crystal as a template for nanoparticle control

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The cholesteric liquid crystal modulation texture, which may seem ordinary at first sight, is capable of microscale organization of nanoparticles that are deposited on its surface. This organization mimics the cholesteric undulations obtained by the deformation of the liquid crystal by external parameters. By controlling the organization of nanoparticles we can change their optical properties [1], and this can find technological applications. Control over the organization of nanoparticles can be obtained by understanding their self-organization at the nanoparticle scale, which is related to the elastic deformations of the cholesteric and the deformations generated by the interactions between the nanoparticles and liquid crystal [2].

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Natural Dielectrics for Bio-Organic Electronics

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Organic electronics has an immense potential for the development of products that are both sustainable and environmentally friendly. In this presentation, a large list of natural origin dielectric materials is introduced and demonstrated in the fabrication of organic field effect transistors, e.g. resins, gums, waxes, alkaloids, nucleobases, lignins and celluloses, natural clays, etc. Apart for their outstanding dielectric and film forming properties, most of the above-mentioned natural dielectrics are inherently, biocompatible (even edible) and have well known medical properties. Thus, this class of dielectrics may find suitable applications in the branches of science where dielectric materials are part of bio-integrated electronics.

Computational investigation of structural, elastic, electronic, and optical properties of predicted Alkali Metal-Based Ternary chalcogenides LiNaX (X = S_e,T_e) for optoelectronics and storage devices applications: DFT study

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Abstract

This work is one of the efficient ways to explore the structural, electronic, optical and elastic properties of inter-alkali metal chalcogenide compounds LiNaX (X = Se, Te) leading to provide data for further experimental and theoretical studies. Motivated by the high successfully GGA-PBE functional calculation and inspired by the experimental study presented by W. BRONGER and all, the main objective of this paper is to report the deeper insights of LiNaX (X = S_e, T_e) compounds by exploring their predicting properties and their potentiality in energy conversion and storage devices applications. Their structural, electronic, elastic and optical properties are carefully calculated based on first-principle calculations, the plane wave pseudo potential approach (PW-PP) and LDA methods within the DFT framework were carried out with CASTEP code along the three main polarizations of the incident wave directions [100], [010] and [001].

The structural optimization of LiNaX (X = S_e, T_e) compounds reveals that their optimized crystal lattices calculations are quite accurate and agreed well with available theoretical and experimental measurements.

The electronic band-structures (GGA, LDA) calculations reveal that LiNaS_e compound exhibit direct wide bandgap semiconductor nature 2.58eV (2,65eV), while 2.27eV(2,50eV) for LiNaT_e, suitable with a great potential in a range of energy and optoelectronic applications and agreed well with experimental measurements.

Several optical properties are computed including the complex dielectric function, absorption coefficient, optical reflectivity, optical conductivity, refractive index and energy loss function. The findings calculations (GGA,LDA) results show that they exhibit high absorption coefficients in UV range up to (~$10^5 cm^{-1}$), peaks of optical conductivity (~$10^{15} sec^{-1}$) were found observed in UV range, lower reflectivity and loss function, make them the most promising candidate within UV ranges for optoelectronics devices.

Furthermore, this conducted research offers mechanical computational predictions based on various key parameters likes (elastic constants, bulk (B), shear (G) modulus and …). The calculated elastic constants using two methods (GGA, LDA) reveal almost identical results and perfectly satisfied the Born stability criteria indicating that are mechanically stable, have a character ionic and brittle, LiNaS_e compound is more resistant to compression and shear deformation than LiNaTe compounds and having an elastic anisotropy. The computed value of A^U shows a value greater than zero and reveals a decrease when replacing X-site of LiNaX from Te to Se as (0.65 and 0.13) exhibiting an elastic anisotropy. According to the A^U value

calculated, we can notice that both predicted compounds are anisotropic materials with less anisotropy for the compound LiNaSe. However, LiNaTe demonstrates the most elastic anisotropy.
Additionally, it was be observed that LiNaSe compound shows the higher T_D, which means its higher thermal conductivity. Another approach is used to study and confirm the anisotropic character of the mechanical properties for predicted compounds LiNaX by highlighting their bulk modulus B as well as the Young modulus E calculated using a three-dimensional plotting representation 3D.

Finally, we hope that all these findings results show a successful accurately prediction for inter-alkali metal chalcogenide compounds materials behavior including their wide band gaps, high optical absorption and stability, make them highly promising materials for optoelectronics applications (optical sensing, integrated photonics…).
Keywords: inter-alkali metal chalcogenide compounds, CASTEP, DFT, GGA-PBE and LDA methods, structural, elastic, optical-electronics properties

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Sol-Gel Autocombustion Process Synthesis and PhysicoChemical Characterizations of Copper substituted Cobalt Nickel Ferrite nanoparticles

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In this study, the five Cu-Ni substituted cobalt ferrite nanoparticles: $Co_{0.8}Ni_{0.2}Fe_2O_4$; $Cu_{0.2}Co_{0.6}Ni_{0.2}Fe_2O_4$; $Cu_{0.4}Co_{0.4}Ni_{0.2}Fe_2O_4$; $Cu_{0.6}Co_{0.2}Ni_{0.2}Fe_2O_4$ and $Cu_{0.8}Ni_{0.2}Fe_2O_4$, have been prepared using eco-friendly sol gel autocombustion process. The physicochemical characterization results derived from Fourier transform infrared (FTIR), X-ray powder diffraction (XRPD), field emission scanning electron microscopy (FESEM), differential thermal analysis (DTA) and thermogravimetric analysis (TGA), have confirmed that the ferrite synthesized powders are pure and are formed by homogeneous crystallites having a size varying from 19.96 nm to 24.94 nm. In addition, the nanosized ferrite cubic spinel basic framework has an excellent stability versus copper substitution and thermal treatment beyond the combustion temperature and without any detection of tetragonal-cubic phase transition. Furthermore, the zero-field-cooled (ZFC)-field-cooled (FC) and the magnetization versus magnetic field strength measurements using superconducting quantum interface device (M-H SQUID) magnetometry have proved the presence of super paramagnetic behavior at room temperature. Also, the super paramagnetic parameter theoretical calculations have been performed by using Langevin function fitting on M-H(300 K) data and the results indicate the irremarkable dependence on crystallite size and copper composition impact. Indeed, during the substitution process a decrease has been observed in remanence, saturation magnetization, coercivity, blocking temperature and magnetocrystalline values. The complex impedance spectroscopy (CIS) study has highlighted the best electrical conductivity value 18.07×10^{-3} $S.cm^{-1}$associated to the lowest E_a = 0.360 eV of $Ni_{0.2}Cu_{0.8}Fe_2O_4$ at 373 K. The excellent magnetic and electrical features of the synthesized nanosized Cu-Ni substituted cobalt ferrites enable them to be useful for various nanotechnological applications in the precious fields of modern life.

Enhanced Energy Conversion and Storage Using Fractal Nanostructures

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The integration of advanced nanostructures for both energy conversion and storage present a promising pathway for improving the performance of energy systems. This study describes a multifunctional approach for thermoelectric and supercapacitors that focuses on the design, synthesis, and characterization of dendritic and fractal nanostructures to enhance thermoelectric conversion and supercapacitor efficiency. The work combines efforts from multiple research projects to develop nanostructures that exhibit high surface area and unique morphological properties, making them ideal candidates for multi-functional energy applications.

The thermoelectric aspect explores the Seebeck effect on fractal nanostructured antennas made from preformed nanoparticles on carbon-coated silicon substrates. These nanostructures optimize the absorption of near-infrared (NIR) light, converting heat energy into electricity with increased efficiency. By adjusting the geometry and size of the nanostructures, a better thermoelectric response is achieved, demonstrating significant potential for waste heat recovery and complementing existing photovoltaic technologies.

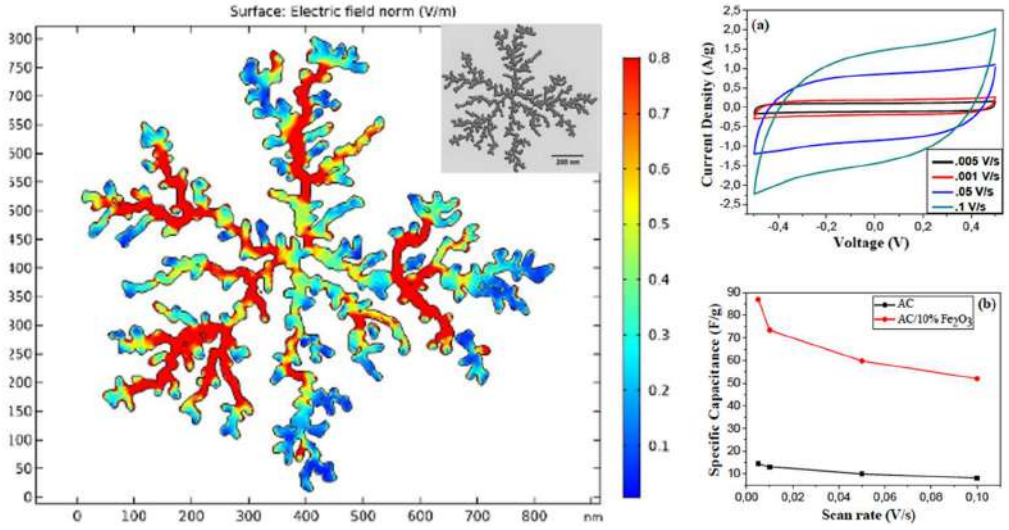

Figure. (Left) Simulation of the absorption distribution response on AgNF structures, under 1 V/m incident electric field. (Right) a) CVs of AC/Fe2O3 composite as a function of scan rates,
b) comparison of specific capacitance of pristine activated carbon and composite (AC/Fe2O3).

In parallel, the study addresses energy storage by synthesizing hybrid nanomaterials incorporating conductive nanoparticles (e.g., metal oxides) with carbon-based nanostructures, resulting in supercapacitors with enhanced energy and power density. These materials are characterized using advanced techniques, such as electrochemical impedance spectroscopy and cyclic voltammetry, to identify the key factors influencing charge storage and retention.
Preliminary results show a substantial increase in both energy conversion efficiency and supercapacitor performance, attributed to the unique properties of the fractal nanostructures. This research highlights the dual potential of these materials for combined energy harvesting and storage, opening new opportunities for their application in next-generation energy systems. Future work will focus on optimizing these properties and scaling up the fabrication process for industrial applications.

Biopolymer Ionogels: A Novel Gel Polymer Electrolyte for Asymmetric Supercapacitors

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Liquid electrolytes in supercapacitors have long posed considerable issues related to safety and packaging, especially for wearable and microdevices. To address these challenges, gel polymer electrolytes provide a valuable alternative with their benefits, including lower activity, minimal leakage, increased safety, flexibility, and robust manufacturing integrity[1].This study introduces a novel approach for systematically developing new electrolytes by embedding ionic liquids within a biopolymer matrix, leading to the formation of solid and flexible ionogels.The presence of polar groups in biopolymers helps to dissociate ion pairs in ionic liquids, leading to stronger interactions and more effective immobilization within the polymer matrix[2].Consequently, our method emphasizes the functionalization and cross linking of biopolymer sprior to incorporating various ionic liquids into them. The electrolytes we synthesized were initially employed in a symmetric supercapacitor utilizing activated carbon. Then, in order to further enhance the electrochemical stability window, these electrolytes were subsequently incorporated into an asymmetric supercapacitor, with MnO_2 as the positive electrode and activated carbon as the negative electrode. Alternatively, other exfoliated 2D electrode materials will be used. These developments mark a significant improvement in addressing the limitations associated with conventional liquid electrolytes and foster the development of safer, more efficient energy storage solutions.

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Improve efficiency of Perovskite-Based Solar Cell by photon recycling

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In recent years, significant advancements have been made in thin-film planar heterojunction solar cells, emerging as cost-effective photovoltaic devices with high power conversion efficiency. Among the materials utilized, organometal trihalide perovskite (CH3NH3PbI3) stands out as a promising absorber material. Its appeal lies in the affordability of organic-inorganic perovskite compounds, readily available in nature, ease of fabrication, and compatibility with large-scale processing at low temperatures [1-2].
In addition to its effective absorption in the ultraviolet range, this material exhibits captivating optoelectronic properties, including high crystallinity, elevated carrier mobility, and extensive carrier diffusion lengths. Despite these advantages, the highest reported power conversion efficiency for perovskite solar cells is currently at 26.1%, as of 2022 [3].
This study introduces a thin-film organometal trihalide perovskite solar cell featuring hybrid interfaces between carefully chosen materials. These selections are the result of an in-depth study aimed at minimizing recombination and optimizing performance. Furthermore, we enhance the absorption of the incident solar spectrum by incorporating a 1D photonic crystal at the cell's bottom, facilitating the photon recycling process.
The proposed solar cell parameters are numerically computed using the rigorous coupled wave algorithm through the SYNOPSYSRSOFT CAD tool. The thickness of each layer in the structure is optimized using the MOST scanning and optimization module of the RSOFT CAD tool, achieving the highest power conversion efficiency at a minimal device thickness (approximately 2.5 µm).
Remarkably, the power conversion efficiency achieved is 27.5%, with a fill factor of 87.4% at AM 1.5, showcasing great promise. This demonstrates the remarkable potential of the proposed design to achieve efficiencies exceeding 5%, positioning it as a competitive contender in the existing crystalline silicon photovoltaic market.

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THE RELEVANCE OF CATALYTIC SILICATE AND CARBON DUST SURFACE REACTIONS IN THE INNER SOLAR NEBULA

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We live in a dusty Universe! Dust is not only found in our solar system among the planets, but it is present in a wide variety of objects throughout the Universe, mainly in those regions between stars called interstellar clouds. The interstellar medium particles -generally composed of an intimate mixture of silicate and carbon grains- and the interstellar gas are perpetually interacting. The aim of our study is to understand the dynamics of this interaction between the matter in the gas phase and the nanoparticles in new physical conditions and see how this influences the chemical complexity of space, particularly on the formation of planets. A coherent and interdisciplinary approach is required to quantify the active and catalytic role of dust in space [1].

First of all, we will produce in the laboratory dust particles analogous to the silicate dust observed in the interstellar medium. Then, we will perform experiments to study the reactions on the surface of the dust grains under astrophysical conditions and characterize the obtained products using the techniques: X-Ray Photoelectron Spectroscopy (XPS). Finally, we will exploit the results of our study to define relevant astrophysical environments using a molecular dynamic simulation and develop additional modules for these simulations that describe the new dust functionality.

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The effect of unmodified fumed silica nanoparticles on recycled high-density polyethylene matrix properties using stearic acid as an interface modifier

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To prevent environment pollution, recycling and recovering plastics wastes has remained to be a major concern worldwide in the 21st century to sustain its circularity. Among the various plastic pollutants that threaten our planet, polyethylene (PE) based polymers especially high-density polyethylene (HDPE) which is considered as non-biodegradable polymer and accounted in the top three most used plastics in industry and has a wide variety of applications [1, 2]. By adding fillers to the recycled and neat HDPE, we can improve their physical and mechanical properties, tackle the quality degradation when necessary, and meet industrial requirements for various applications [3]. This research investigated the effect of untreated fumed silica (SiO_2) as nanofillers on recycled high density polyethylene (HDPE) properties in presence of unmodified and modified recycled PET fiber. PET materials were treated with aqueous solutions of sodium hydroxide in a different concentration. The stearic acid (SA) was used as an interface modifier in order to overcome the incompatibility problems with the HDPE Matrix. The nanocomposites were prepared by melt blending and compression molding with 3 and 5 wt% filler loading rates. Thermal, structural, and morphological tests were conducted to analyse the performance of the silica and the compatibilizing agent on the dispersion and properties of the studied composites. Results revealed that 3 wt% of unmodified silica filler reinforced the obtained nanocomposites. Untreated PET fiber has significantly improved the modulus and Izod impact strength of the composite. The treatment of the fiber as well as the interface modifier caused a slight increase in stress. Some formulations were found to be the ideal combinations which could provide novel mechanical applications to meet industrial requirements at a larger scale.

Keywords: recycled HDPE matrix, Silica, Stearic acid, PET fiber, polymer nanocomposites.

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One-pot synthesis of low-cost CuS/Vulcan carbon composites applied as electrode materials for supercapacitors

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CuS microflowers composites with Vulcan carbon black (CuS/Vulcan) were synthesized by a low-cost one-pot hydrothermal process and investigated as electrode materials for supercapacitor applications. The phase integrity of pristine CuS and CuS/ Vulcan composites was confirmed by XRD measurements. The immobilization of CuS nanoparticles on the Vulcan support prevented their agglomeration and improved the specific surface area, the electric conductivity and the electrochemical response time of CuS-based electrodes. The electrochemical performance of CuS/Vulcan composites was characterized in a three-electrode setup and a two-electrode cell configuration as a function of the CuS/Vulcan weight ratio. The CuS/Vulcan composite electrodes with a mass ratio of 70:30 demonstrated the highest specific capacitance of 285 F g−1 and a capacitance retention of 97% after 2000 galvanostatic charge–discharge cycles at 5 A g−1 in 3M KOH. The assembled CuS/Vulcan (70:30)//CuS/Vulcan (70:30) symmetric cell exhibited an improved specific energy of 12.6 Wh kg−1 at a specific power of 907 W kg−1 (at the discharge current density of 0.25 A g−1). Overall, this study presented a facile, convenient and scalable approach for designing cost-effective and high-performance composite electrodes based on copper sulfide.

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Carbonaceous Nanomaterials for Electrochemical Sensing of Pesticides

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In today's agriculture, pesticides play a part in meeting the demand for population growth. However, pesticides are utilized for more than just agriculture; they are extremely hazardous to the environment and human health due to their highly poisonous nature. Therefore, when they are used widely and without safety precautions, they have a detrimental effect on farmers and cause social unrest.

In this study, we report an electrochemical sensing method that can detect cymoxanil fungicide at low concentrations. It is less expensive, extremely sensitive, and non-selective. We have performed various electrochemical experiments using two types of carbonaceous nanomaterials on GC electrodes: quasi-amorphous carbon (activated Biochar micro nano-system) and nanostructured carbon (f-MWNTs and Graphene oxide). Because of the high capacities of these selected carbonaceous nanomaterials due to their specific surface area and functional groups, the modified electrodes have improved the pesticide sensor performance. Their enormous surface-to-volume ratio aspect, great mechanical strength, outstanding electrical conductivity, quick electron transfer kinetics, and environmental friendliness all contribute to their electrochemical sensing capabilities.

Furthermore, the electrochemical tests conducted on the targeted analyte under optimal conditions were carried out using appropriate cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS) techniques.

Keywords: Biosensor, Biochar, Carbon nanotube, Graphene oxide, Fungicide.

Development of Molecularly Impressed Polymer-Based Electrochemical Sensor for Ultra-Sensitive and Sensitive Determination of Lincomycin in Beverage Samples

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Lincomycin (LIN) is one of the lincosamide antibiotics which is used as a bacteriostatic agent and inhibits protein synthesis [1]. This study aims to develop a high-sensitivity MIP-based electrochemical sensor to detect LIN using the molecularly imprinted polymer (MIP) method. Using the electropolymerization method, the MIP sensor was designed after gold nanoparticles were dropped onto the glassy carbon electrode surface. LIN showed high sensitivity and selectivity towards the template molecule in the developed sensor. Surface and morphological characterizations of the MIP-based electrochemical sensor were performed. The electrochemical impedance spectroscopy (EIS) technique was successfully applied with high sensitivity and accuracy in the determination of LIN in standard solution, milk sample, and various fruit juices using 5 mM $[Fe(CN)_6]^{3-/4-}$ as a redox probe. Optimization experiments were conducted for the sensor developed for LIN. The calibration range under optimal conditions was found to be between 1 pM and 10 pM, and very low limit of detection (LOD) and limit of quantification (LOQ) were found. Recovery studies were conducted on beverage samples to prove the accuracy of the sensor. Finally, the sensor's selectivity was evaluated using common interfering agents and model drugs. The results showed that the MIP-based sensor can specifically recognize LIN compared to structurally related drugs and can be reliably applied to directly determining LIN from real samples.

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All solid-state Laser-Induced Graphene-Based Microsupercapacitor Modified with Poly(Methylene blue) for improved Energy Storage

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The development of new instruments for environmental monitoring, energy storage, and medicinal analysis is greatly facilitated by nanomaterials (1). Given their high potential for electron storage, using carbonaceous materials to elaborate electrodes is a highly recommended (2). To produce carbon-based electrodes, the laser-induced graphene (LIG) technique has been found to be a practical, economical, and high-throughput approach (3). Polyimide-based LIGs have the potential to function as good electrode materials for supercapacitors (4).
Our work aims to improve the capacitive performance of polyimide-based LIG electrodes for supercapacitor energy storage. By enhancing the electrical capacitance of the double layer and adding a pseudo-capacitive component, the introduction of conductive polymers with large specific areas can considerably increase the specific capacitance which improve the total energy storage capacity.With the use of a gel electrolyte, the elaborated microsupercapacitor, which was formed by modifying the surface of a PI-based LIG with electrochemically deposited poly(Methylene Blue), displays an exceptionally large and stable potential window up to 3.0 V. The microsupercapacitor provide enhanced surface capacitance, energy density, and power density. In fact, the specific capacitance increased by 250% after modification. Notably, over 5,000 cycles, this supercapacitor exhibits remarkable cycle stability. These outcomes demonstrate the potential of the microsupercapacitor as an energy storage device.

Key words: Laser-induced graphene, Energy storage, redox polymer, supercapacitor.

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Effect of PLD parameters on Mo (110) thin film properties Title

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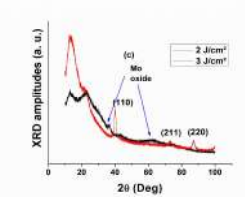
In this work, the structural and electrical properties of Mo thin films deposited by pulsed laser deposition at low substrate temperature were investigated. Films were deposited in argon (Ar) atmosphere onto corning 7059 glass substrate. We have focused our study on: (i) the optimal deposition conditions to produce bcc (110) molybdenum (Mo) thin films, (ii) the effect of the PLD parameters such as laser fluency, gas pressure and substrate temperature on structural and electrical properties of Mo films, and (iii) find out how the structural properties can affect the electrical properties of Mo films. In addition, the processes that influence the film microstructure are discussed. Results show that there is a trade-off between PLD parameters in order to define the optimal species mobility and deposition rate to grow well oriented (110) bcc Mo Figures (1-10). High deposition rate results in amorphous or poor crystalline films. Best texture was obtained at relatively low deposition rate. Mo resistivity increases with Ar pressure and deposition rate, whereas it decreases with substrate temperature. Highest values were obtained for films deposited at the highest Ar pressure and the lowest substrate temperature. Poor crystalline or amorphous Mo films are more resistive.



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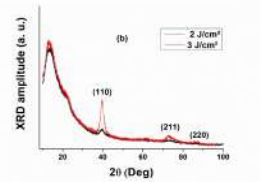

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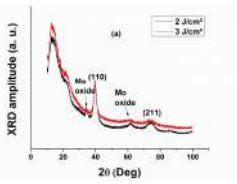

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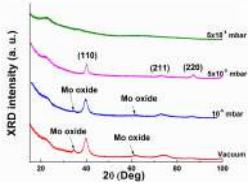

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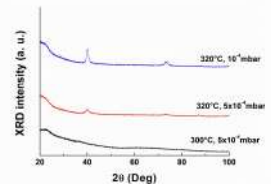

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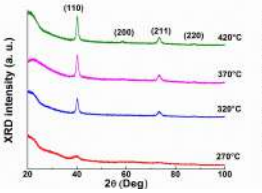

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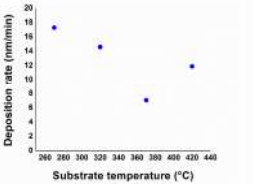

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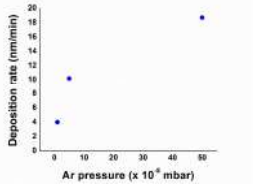

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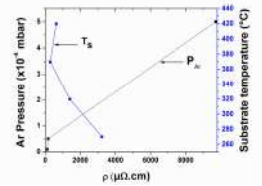

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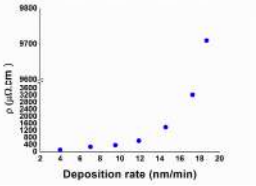

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Concentration TTIP Effect on Thickness of Titanium Oxide Nano Layers Synthetized by Spray Pyrolysis and on its Performance as Gas Sensors

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Layers of titanium oxide (TiO2) are synthesized by spray pyrolysis for titanium concentrations of 0.07M; 0.10M and 0.13 M. These layers are deposited on glass and FTO substrates. The structural, optical and electrical properties of the layers thus produced are studied as a function of the substrate and as a function of the concentration. The XRD spectra obtained show that the TiO2 is well crystallized for all concentrations in the tetragonal anatase phase and in the preferential direction (101). The thickness varies with the concentration but the grain size is optimal for a concentration of 0.1 M. The layers of titanium oxides are transparent in the visible range have a gap energy of 3.49 eV. The electrical properties of the layers deposited on FTO are studied by impedance measurement. A significant variation is observed for a concentration of 0.13 M. Gas detection tests are performed using NO_2 and Ozone as gases. These tests reveal that the TiO2/FTO layers are selective for ozone and that the detection is optimal for a concentration of 0.1 M.

Binuclear spin-crossover [Fe(bt)(NCS)2]2(bpm) complex: A study using first principles calculations

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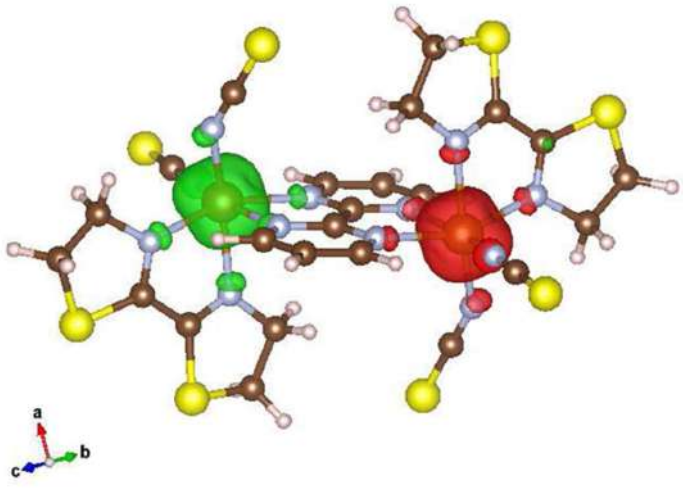
The spin-crossover [Fe(bt)(NCS)2]2(bpm) complex is studied using spin-polarized density functional theory within the generalized gradient approximation, the Hubbard U and the weak van der Waals interactions in conjunction with the projector augmented wave method in its molecular and periodic arrangements. It is shown that the considered complex has three magnetic configurations [high spin state (HS)–HS, HS–low spin state (LS), and LS–LS] corresponding to those observed experimentally after two transition temperatures Tc(1) of 163 K and Tc(2) of 197 K. For the HS–HS magnetic state, we found that the two Fe centers are antiferromagnetically coupled for both molecular and periodic structures in good agreement with the experimental observations. Our results show that the computed total energy difference between the magnetic state configurations of the considered Fe2 complex is significantly smaller compared to those reported in the literature for other mono- or binuclear compounds.



Design and conception of an IoT-Controlled UVc Sterilization System

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Due to the emergence of airborne infectious diseases in recent years, disinfection of high-risk contamination spaces, such as hospitals and large public areas, has become essential for ensuring better health safety against bacteria and viruses [1]. UV light is widely recognized for its effectiveness in eliminating pathogenic microorganisms and has proven effective in various applications, including healthcare facilities, laboratories, food processing industries, and public spaces. This project focuses on utilizing UV light, known for its germicidal properties, to sterilize and disinfect environments [2].
The project is based on an ESP32 microcontroller, a passive infrared (PIR) motion sensor (HC-SR501), a TFT display, a mobile application connected with Firebase cloud, and UV light sources such as UV-C lamps (wavelength 245 nm) that emit short-wavelength ultraviolet light.

We have successfully developed a prototype and tested our product in a biological laboratory. Our tests showed that at a distance of 150 cm and with an exposure time of 30 minutes, no bacterial colonies detected, demonstrating the lamp's efficiency. The results of the biological tests support the use of this technology for disinfection in various environments, such as ambulances and operating rooms.

Keywords: Sterilizer, ultraviolet; UV; motion sensor (PIR); esp32

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Temperature effect on some optical and electric properties of a solar cell

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The objective of the study is to understand the energy behavior of materials used in solar photovoltaic capture systems through the study and modeling of the influence of optical properties and on solar cell performance by simulation using the Python language on a wide range of solar cells, quantum well devices with multi-junction solar cells. The model used is a multi-scale simulation that takes into account nanoscale phenomena such as the quantum containment effects of semiconductor nanostructures and at the micro-level propagation of light. The study of the structural and electronic properties of the solar cell has allowed us to show that the variation in absorption as a function of wavelength causes a weak and constant transmission to react as well as the definition of voltages, the concentration factor of sunlight and the execution of the calculation in a loop. In addition, the main effect of temperature on solar cells results from the variation of three main parameters, which are short circuit current, open circuit voltage and form factor. The study of the optical properties of the solar cell allowed us to conclude that the spectral variation of Fresnel coefficients describing reflection, the transmission and absorption of the multilayer structure is measures a change in the polarization of the incident light and reflected to the sample surface. A number of mechanisms affect the refractive index for energies above the gap that have not been taken into account. These mechanisms are indirect optical transitions, absorption of free carriers, the vibration effect of the crystalline network and the effect of impurities present in the crystal, which leads us to define a mixing law allowing modeling the evolution of the refractive index according to the wavelength whatever the composition of the alloy.

Abstracts of Poster Communications

Session I

X-RAY Diffraction analysis of nanoparticles

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Powder X-ray diffraction (XRD) is a common characterization technique for nanoscale materials. Analysis of a sample by powder XRD provides important information that is complementary to various microscopic and spectroscopic methods, such as phase identification, sample purity, crystallite size and morphology. One application of powder XRD is phase identification, which is often accomplished by comparing an experimental XRD pattern with a reference pattern that is either simulated or obtained from a database (*International Community of Diffraction Data*). To accomplish this comparison, experimental XRD patterns must have sufficient signal-to-noise ratios. For some samples, especially nanoscale materials, powder identification can be particularly challenging because of nearly indistinguishable diffraction patterns. In these cases, additional characterization techniques, as TG-DSC and MET, are important for achieving phase identification.
X-ray Diffractometer parameters are also very important to achieve accurate phase identification. At the "*Unité de Services Communs pour la Recherche USCR- Diffraction des Rayons X*" of Faculty of Sciences of Tunis, diffraction data were collected with PANalytical X'Pert PRO diffractometer which equipped with automatic slit, X'celerator detector and Cu-Kα radiation at a scan speed of 0.01° 2θ/s. The acceleration power applied was 45 kV and 40 mA. The difference between experimental and theoretical peak positions of Si (1.1.1) was within 2θ=0.002°. The phase identification was realized with the High Score *Plus*software.
Powder XRD provides useful information about structure, phase, composition, shape, size, crystallinity and other important features of nanoscale materials, although unambiguous sample characterization almost always requires complementary experimental methods. Powder XRD data for nanoscale materials can often be straightforward to analyze for the key information that is needed, but other times, it can be quite complex.

Keys words: *X-ray diffraction, Phase identification, PANalytical X'Pert PRO.*

Efficient Prediction of Modal Indices in Silicon Waveguides Using Machine Learning Techniques

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This study presents a novel machine learning approach for predicting modal indices in silicon waveguides. Our methodology employs a deep neural network (DNN) architecture to establish a robust link between waveguide geometric characteristics and their corresponding effective refractive indices (neff) for both transverse electric (TE) and transverse magnetic (TM) modes.
The DNN is trained on a comprehensive data set generated by precise finite differenceeigen mode (FDE) simulations. The input features include waveguide width, height, and operating wavelength, while the outputs consist of the fundamental TE and TM mode indices. We employ a dual training methodology and a dynamic learning rate to improve model convergence and g
Our methodology demonstrates remarkable accuracy, achieving a mean absolute error of less than 10^{-4} for neff predictions a cross many geometries relevant to silicon photonics. Notably, post-training, our method can predict modal indices for arbitrary waveguide dimensions within milliseconds, achieving a speed improvement beyond 1000 times relative to conventional si
We evaluate our model's effectiveness using experimental data and demonstrate its application in accelerated design space exploration for silicon photonic devices. Furthermore, we illustrate the application of this strategy to complex waveguide designs, including multi-layer and slot waveguides, thereby enabling the efficient optimization of advanced photonic integrated circuits.

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Nanocristalline nickel synthesis by pulsed current

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The synthesis of nickel by pulse electrodeposition has attracted much attention during the last decades. Pulse electrodepotion has been reported to improve the deposition process and deposit properties such as porosity [1], ductility [2], hardness [2] and surface roughness (3).It has been reported that pulse plating strongly modifies the properties, the structure, the surface morphology and the macroscopic characteristics of nickel coatings. In the present research nickel deposits were produced by pulse current electrodeposition from watts bath. The optimization of the conditions of deposition was established and the influence of pulse parameters, on the grain size, surface morphology and crystal orientation was determined. The morphology of the coatings was characterized by observations in scanning electronic microscopy (SEM). X-ray diffraction in symmetric mode was also used to evaluate the structure and principal crystallographic orientations of the deposits. The results obtained, showed that the development in pulsed induced a marked improvement in the morphology and grain refinement.

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Investigating the impact of Interfacial Layer on the I-V Characteristics of Schottky Diodes based on SiC Polytypes

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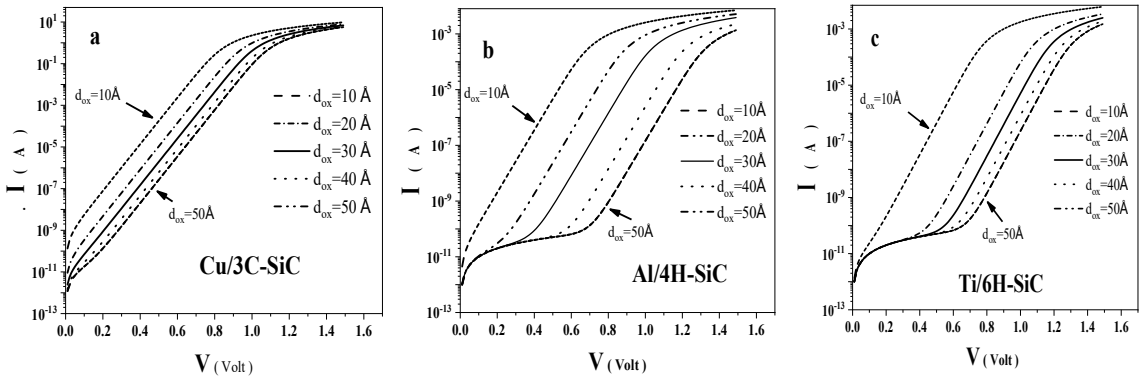
Silicon carbide (SiC) is an attractive semiconductor for sensing applications in harsh environments due to its exceptional material characteristics when compared to silicon and other semi conductors. Its wide band gap, excellent thermal conductivity, and high breakdown voltage enable SiC devices to operate effectively under extreme conditions [1]. As a result, numerous researchers have investigated the properties of SiC Schottky rectifiers, initially focusing on 3C–SiC, followed by 6H–SiC, and more recently on 4H–SiC. This paper presents an analytical simulation using MATLAB of the I(V) characteristic of Schottky diodes based on SiC polytypes, focusing on the impact of a key factor: the thickness of the interfacial layer (dox) on the formation of the reel Schottky barrier. The chosen doping type is moderate n-type doping with Nd = $5\times10^{15}cm^{-3}$.

In the ideal case the barrier height Φ_B Φ_B is calculated directly as the difference between the metal's work function Φ_M and the semiconductor's electronaffinity χ_{sc}:

$q\Phi_{Bideal}= q(\Phi_M - \chi_{sc})$, in the reel situation, the calculation of the Schottky barrier height takes into account the interface states (N_{SS}), the thickness of the native oxide layer formed at the interface [2]:

$$\Phi_{Bn} = C_2(\Phi_M - \chi) + (1 - C_2)\left(\frac{E_g}{q} - \Phi_0\right) - \Delta\Phi_{Bn}\,\gamma = \frac{\varepsilon_i}{\varepsilon_i + q.dox.Nss}\Phi_{Breal} = C_2(\Phi_M - \chi) + (1 - C_2)\left(\frac{E_g}{q} - \Phi_0\right) \text{and} C_2 = \frac{\varepsilon_i}{\varepsilon_i + q^2 D_{ox} N_{ss}}$$

The charge transport mechanism in the Schottky contact is described by the thermionic model [2]. $I_{STE}\left(e^{\frac{qV-R\times I}{nkT}} - 1\right) + \frac{V-Rs\times I}{R_p} I_{STE} = AA^*\,T^2\,\exp\left(\frac{-q\Phi_B}{kT}\right)$



Simulation of I-V characteristics as a function of dox:
a) Cu/3C-SiC, b) In/4H-SiC, c) Ti/6H-SiC.

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Analytical modeling of transport mechanisms in Ti/ 6H-SiC (n) Schottky diode as function of temperature

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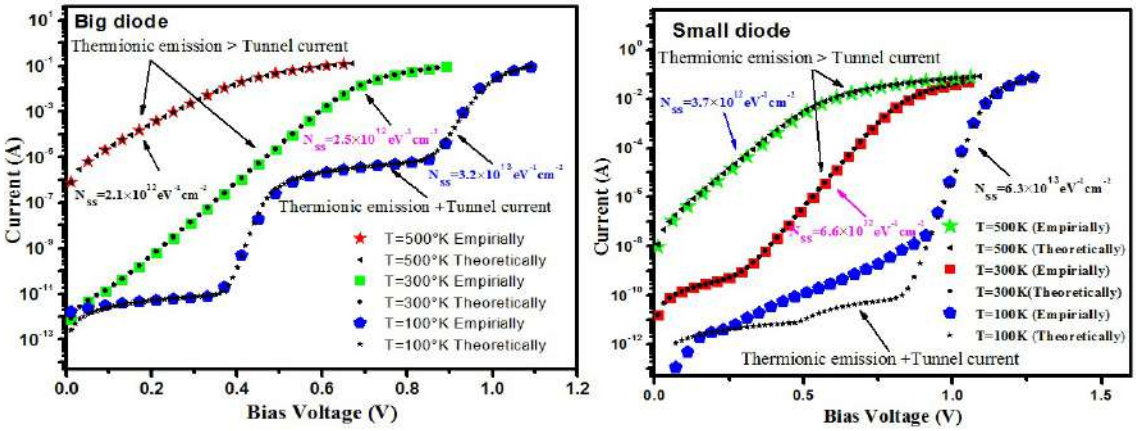
In this contribution, we used a computational model to calculate the I-V-T forward current in Ti/6H-SiC(n) Schottky diode elaborated in two different contact sizes (1.6 × 1.6 $mm^2$and 0.4 × 0.4 mm^2). This model takes in account all the electrical conduction mechanisms, such as, the thermionic emission, the tunneling and the leakage currents. The aim is to strive for maximum alignment between the experimental and the theoretical I-V-T curves.

For the selected temperatures of 100 K, 300 K, and 500 K, the adjustment steps were taken by introducing, on the one hand, the experimental parameters (doping concentration, contact area....), the parameters extracted from the experimental curves (ideality factor and Richardson constant), and on the other hand, the fitting parameters which particularly describe the barrier height Φ_{bn}, as well as the interface density N_{SS}. At each temperature, the physical, electrical, and technological parameters are recalculated, generating the respective simulated current curves.

Forward current-voltage fit revealed many interesting aspects: the diodes behaved very well exhibiting linear I-V characteristics as described by thermionic emission theory only at 300K and 500K. However, for low temperature, the diodes exhibited significant tunneling components that distorted the linear behavior by introducing a double barrier.

For the bigger diode, there is an excellent agreement between the experimental and modeled data for all temperatures. However, the fitting for small diodes proved notably inadequate at the low temperature of 100 K. An array of studies on polytypes-based SiC Schottky diodes with various metals has shown that N_{SS} increases with decreasing temperature [1][2]which aligns with our treatment results.



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Optimization of Eco-friendly synthesis of Zinc Oxide Nanoparticles via-Box-Behnken design: Removal of Paracetamol

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Through this research, zinc oxide nanoparticles (ZnO NPs) were successfully synthesized via easy route "co-precipitation" using Box-Behnken Design (BBD). The method was systematically optimized using response surface methodology (RSM) based BBD, considering the effect of various independent variables such as zinc acetate concentration, pH, and reaction time and temperature calcination on the responses like particle size. The accuracy of the model was confirmed by the coefficient of determination (R^2) value of 0.9968. The significance of the regression model was found to be high which is validated by the low probability value of $P < 0.0001$. The X-Ray Diffraction (XRD) results confirmed that the ZnO NPs had a hexagonal wurtzite structure. The average crystalline size of around 45 nm was observed by the Debye–Scherrer formula. The purpose of this research is to investigate the removal of Paracetamolvia adsorption processin the presence of the optimized ZnO. The results revealed that an amount of 0.15 g/L ZnO-NPs showed maximum removal efficiency at pH 3.5. The adsorption process of the paracetamol followed the Langmuir model with a correlating constant (R^2) higher than 0.99 and with a maximum capacity (qm) value of 44.5 mg/g. The pseudo-second-order ($R^2 > 0.9796$) model was most appropriate in the description of the adsorption process. These results revealed that the nanoparticles have the potential to be used in the removal of pharmaceutical wastes.

Keywords: Zinc oxide; Box-Behnken design; optimization; new adsorbent; pharmaceutical effluent; Paracetamol.

Photocatalytic Activity of Co-Zn ferrites nanoparticles in wastewater treatment

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Dyes and pigments present in wastewater discharged from textile, pharmaceutical, leather, food, cosmetics and plastic industries have adverse impacts on the aquatic life as well as on human health because of their toxicity [1]. In the past decade, semiconductor photocatalysis driven by solar light has emerged as one of the most promising and efficient methods for removing organic pollutants. On the other hand, magnetic nanoparticles have gained research interests as photocatalysts in view of ease of magnetic recyclability and their good catalytic response. Herein a study of simple, low-cost and reproducible strategy to synthesis Co-Zn ferrites nanoparticles was investigated. The Co-Zn photocatalysts was prepared via co-precipitation method. XRD data confirm the purity and the formation of the desired phase. The formation of two-dimensional (2D) nanosheets like morphology was observed by SEM images. The measurements of the hysteresis loop, performed at room temperature, indicate a ferromagnetic behavior of Co-Zn nanoparticles. The photocatalytic activity of the photocatalysts for degradation of pharmaceutical dye (Rhodamine B) under sunlight irradiation shows a good efficiency. It reaches to 86 % after 3 h for a concentration of 10 mg/L of dye.

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TiO_2 QUANTUM DOTS ON TiO_2 NANOTUBES: A NOVEL APPROACH TO PHOTOCATALYSIS

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Among its many applications in the environmental and energy fields, TiO_2 photocatalysis is used for self-cleaning surfaces, air and water purification systems, sterilization, hydrogen evolution, and photoelectrochemical conversion [1]. Recently, nanotechnology has demonstrated that nano-sized titanium dioxide photocatalysts, are highly effective in photodegrading organic and inorganic contaminants in water [2]. In fact, several approaches have been employed to formulate structures and electronic properties of TiO_2 at the nanocrystal level, including the control of the band structure, doping and heterojunction interaction [4-6]. In this work, we present an alternative approach to constructing TiO_2 homojunctions by assembling TiO_2 quantum dots (QDs) onto titanium nanotubes (TNT). These homojunctions were thoroughly characterized using X-ray diffraction (DRX), Nitrogen physisorption, photoluminescence spectroscopy (PL), and UV-Visible spectroscopy. From the outcomes, a strong interfacial interaction between the TNT and TiO_2 QDs significantly reduces the recombination of photogenerated electron-hole pairs and enhances charge transport efficiency [7]. In terms of catalytic application, TiO_2 catalysts showed high photocatalytic activity for the degradation of methylene blue present in water (up to 70% in 140 min). Currently, efforts are being made to optimize and characterize other TiO_2-based catalysts, which exhibit promising performance and highlight alternative proposals and assumptions about QDs/support coupling. As a result of this work, a new vision of homojunction based on quantum dots is being created, and new paths are being opened for practical applications of photocatalysis in the field of water treatment.

Keywords: Heterogeneous photocatalysis, TiO_2, quantum dots, homojunction, semiconductor, water treatment.

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Some recent advances in 2D materials using ab initio calculations

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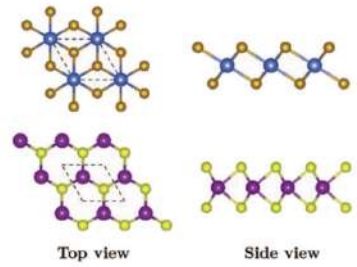
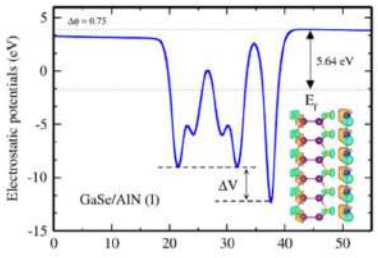
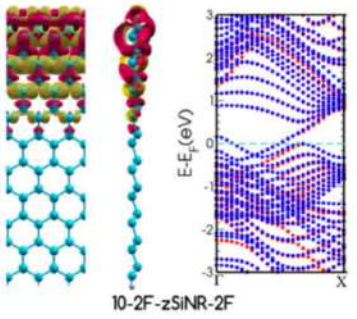
In the field of nanosciences, research on materials has made spectacular progress over the last twenty years. In this talk, I will present, through some examples from recent works, how ab initio calculations can provide a better understanding of the physical and chemical properties of different compounds. In particular, I will discuss our recent works on the properties of 2D systems interfaced with other bidimensional systems such as graphene, silicene, AlN, or ZnO [1, 2, 3]. Then I will present our recent results concerning the electronic structure of 2D silicene nanoribbons system [4]. Finally, I will discuss our calculations on the structural and electronic properties of 2D quaternary monolayers and their vdW heterostructures [5].



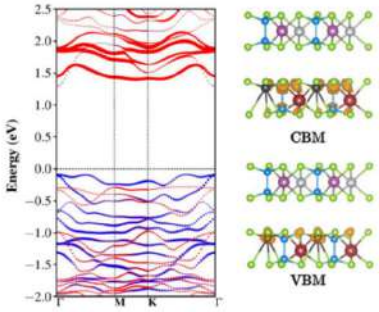
(a) Top and side views of TDMs monolayers



(b) Potential drop across the interface of the GaSe/AlN



(c) The spin-charge densities and band structure of zSiNR



(d) PBE+D2 calculated projected band structure and band-resolved charge density of the heterogeneous AgBiP2 Se6/AgScP2 Se6

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Synthesis, Characterization, and Evaluation of the Antimicrobial Activity of the Magnetic Nanocomposite Fe_3O_4/HAP Hydroxyapatite

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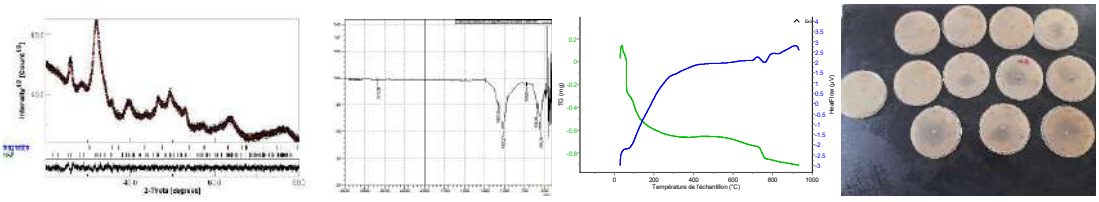
Magnetic nanocomposites are increasingly recognized for their diverse applications in the medical and pharmaceutical fields, particularly for their potential to counteract bacterial resistance. In this context, our work focused on the synthesis of a Fe_3O_4/HAP (hydroxyapatite) nanocomposite powder from a reaction medium containing precursors such as iron oxide, calcium nitrate, and ammonium dihydrogen phosphate, in the presence of a weak base, NH_3. The synthesis was carried out using a soft chemistry method, involving filtration, drying, and calcination steps, to ensure optimal physicochemical properties and evaluate the antimicrobial efficacy of the nanocomposite, whose size was determined to be at the nanoscale. The protocol was characterized by its simplicity, low cost, and feasibility for industrial or laboratory-scale production. Characterization analyses, based on infrared spectroscopy and thermal analysis, confirmed the high quality of the Fe_3O_4/HAP nanocomposite. Additionally, the assessment of its antimicrobial activity demonstrated notable efficacy, particularly against Bacillus, a bacterium commonly implicated in infections and contaminations, as well as against a yeast sample. These results demonstrate the antibacterial and antifungal effectiveness of our nanocomposite and underscore the significance of the advancements achieved through a simple synthesis technique, offering promising prospects for various applications.



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Nickel Copper Ratio Effect on Nanohybrid Products Electrochemical Performance for Energy Storage

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In terms of energy storage, supercapacitors are currently getting a lot of interest where outstanding performance benefits include their extended lifespan, high energy density, high level of safety, and low cost.
We report in this investigation samples rich in nickel and copper hydroxide with highest specific capacitance and moderate cycle stability. Therefore, high conductivity and rate capability, two distinctive electrochemical features, guarantee the material's practical application potential as an electrode for supercapacitors. So, we present in this work a simple, inexpensive, and environmentally friendly method for producing electroactive nanomaterials based on Ni and/or Cu hydroxides by varying the precursors' ratios from 0 to 2 under optimized growth condition (6 h/120 °C). Hence, XRD, FTIR, FESEM, and BET are most techniques used to characterize the obtained products.
Additionally, we performed their electrochemical tests via a three-electrode arrangement system in 6M KOH electrolyte. We clearly observed a synergistic relationship between the Ni/Cu precursor ratio and the electrochemical performance of the hydroxide-based products.

Keywords: Energy storage, Supercapacitors, Nanohybrids, electro-active materials, Electrochemical measurements.

The Study Of based FeCo Nano Powder Using Mössbauer Spectroscopy

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Understanding the behavior of crystal structure in Iron based Nanoparticles powder (NPs) is important for predicting its properties during its lifetime in a micro-sensors and subsequent long-term data storage. Mössbauer spectroscopy (MS) is a nuclear non- destructivetechnique that meet the requirements of characterizing the structure-property relationships in the nanometer range. In this work, the structure and properties at nanoscale physical and chemical hyperfine interactions and parameters such as isomer shifts I_S, quadruple splitting Q_S and hyperfine magnetic field B_{hf} are investicated using transmission ^{57}Fe Mössbauer spectra measured at room temperature using ^{57}Co γ-ray source to provide valuable insights into the local environment and understanding of the crystallographic structure and magnetic behavior of binary$Fe_{15}Co_{85}$ NPs synthesized by hydrothermal method. The analysis of Mössbauer spectra curves was by using Recoil with two subspectra observe two Zeeman sextet and one broad doublet which confirms the body-centered cubic structure BCC of disordered alloy. The structure and properties of powders are governed by nanoscale physical and chemicalinteractions. Therefore, it is necessary to investigate both structure and properties ofmaterials at the nanoscale so that nano structure-property relationships can be utilized to predict bulk properties of materials to highlight the importance of nanoscale materials analysis for future technologies.

Keywords: Mössbauer spectroscopy, Hyperfine interactions,magnetic properties, Nanopowders.

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Crystallography of Apatite from Tunisian phosphorite deposits

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The crystallography structure of Apatite from Tunisian phosphorite deposit was investigated to determine the crystallographic parameters, crystallite size and the degree of substitution which affect this mineral. The diffraction data were realized with X rays Diffractometer in the "*Unité de Services Communs pour la Recherche - Diffraction des Rayons X"* of Faculty of Sciences of Tunis;model PANalytical X'Pert PRO which equipped with automatic slit, X'celerator detector and Cu-Kα radiation at a scan speed of 0.01° 2θ/s. The acceleration power applied was 45 kV and 40 mA.
In the apatite structure, calcium and oxygen form columns that are attached with phosphorus and oxygen atoms. These Ca-O columns are parallel to the c-axis of the crystal and thus define the hexagonal prisms of apatite. Fluorine occupies a central position in the channel as well as other Ca ions [1] [2] [3] [4] [5]. Substitutions affecting sedimentary apatite are frequent and directly influence the symmetry of the crystal lattice which results in a modification of the "*a"* and "*c"* parameters. The decrease in the crystallographic parameter "*a*" of apatite can be hidden by the substitution of F by OH^-. Substitution of F^- by Cl^- and OH^- in the channels can transform the hexagonal crystal lattice of apatite to monoclinic or triclinic lattices [4] [6]. Substitution of PO_4^{3-} ions by CO_3^{2-} ions in apatite causes distortions in the crystal lattice. The parameter "*a*" from Tunisian apatite varies inversely proportional to the substitution rates of CO_3^{2-} ions (from 9.387Å to 9,325Å) and the parameter "*c*" remains relatively constant (6,900Å to 6.888Å). The determination of crystallite size of Tunisian apatite reveals a positive correlation with increasing of CO_3^{2-} content. The crystallite size of this apatite varies from 490$Å^3$ to 525$Å^3$ when CO_3^{2-} varies from 6.02% to 8.3%.These substitutions in apatite can cause crystallographic changes and therefore the exact determination of these parameters can provide useful information on the mineralogical and chemical characteristics of apatite.

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DFT simulation of structural and electronic properties of SiC/Graphene Interfaces

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The humanity is in front of energy crisis with the exhaustion of fossil energy so the development of smart systems with electrochemical energy storage sources has become a crucial solution. The Li-ion batteries and supercapacitors are the next generation of energy storage systems for powering miniaturized embedded electronic devices. Many heterostructures design have been developed for enhancing the electrochemical performance of energy storage devices [1]. In this work, we have systematically investigated the structural and electronic properties of hybrid systems composed of monolayer SiC and Graphene using first-principle calculations based on density functional theory (DFT). The theoretical results illustrated that the employment of SiC/Graphene material can greatly improve the electrochemical performance which improve a new perspective for the development of heterostructures based on SiC/Graphene material.

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Manganese oxide sprayed thin films as a second absorber layer in CIGS solar cell: Solution concentration effect

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Dimanganese trioxide (Mn_2O_3) thin films were, successfully, deposited on glass substrates using spray pyrolysis method. The study focused on examining the influence of varying solution concentration (C = 0.07, 0.1, 0.13, and 0.16 M) on the physical properties of Mn_2O_3thin films. Thus, DRX analysis proved that a concentration of about 0.13 M revealed an optimal Mn_2O_3 film growth, as shown in Fig.1. SEM images revealed a well-connected surface morphology (Fig.2). Optical properties, including transmission and reflection (Fig.3), were measured to determine the direct band gap energy, which was approximately 1.48 eV. Additionally, all layers exhibited low transmission in the visible spectrum ($0\% \leq T \leq 10\%$), making them suitable for use as an absorber layer in solar cell applications. Refractive index was calculated using Moss, Reddy, and Ravindra models. PL spectra indicated multiple emissions in visible region (Fig.4). One-dimensional Solar Cell Capacitance Simulator (SCAPS-1D), based on one-dimensional Poisson equation [1],has been employed to study the photovoltaic performance of both TiO_2/CdS/CIGS and TiO_2/CdS/Mn_2O_3/CIGS solar cells. It was found that the addition of Mn_2O_3, as a second absorber layer in CIGS solar cell, enhances, notably, the photovoltaic efficiency to achieve 21.43 % (Fig.5).

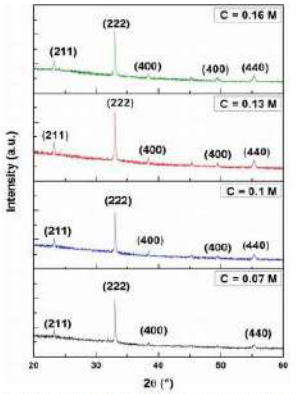

Fig.1. XRD spectra of Mn_2O_3 thin films deposited at various solution concentrations.

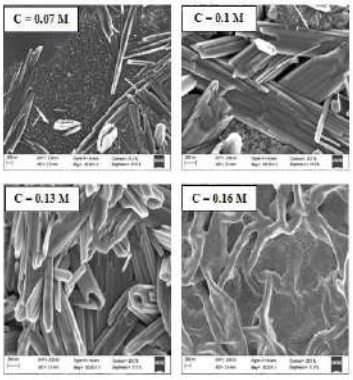

Fig.2. SEM topography of Mn_2O_3 thin films.

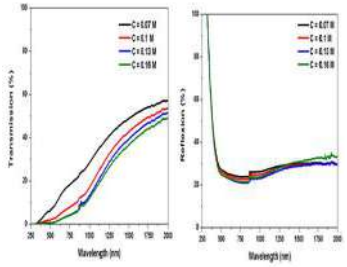

Fig.3. Reflection and transmission spectra of Mn_2O_3 thin films

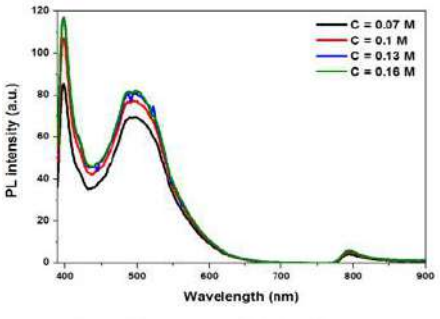

Fig.4. PL spectra of Mn_2O_3 thin films.

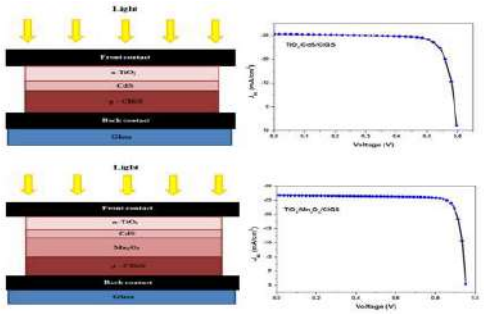

Fig.5. CIGS solar cell parameters with and without second absorber layer.

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Optical selective filters using quasi-periodic photonic crystal based on Si/SiO_2

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We elaborated a one-dimensional quasi-periodic photonic crystal [1,2] based on Si/SiO_2 materials [3]. We investigated its optical properties using the transfer matrix method, determining the reflectance spectra at normal incidence in the near-infrared wavelength range. The results demonstrate that this quasi-periodic photonic structure exhibits sharp localized light modes within the photonic band gaps, covering the optical telecommunication wavelengths of 0.85, 1.33, and 1.55 µm, with varying numbers and positions depending on the nature and characteristics of the build system. This phenomenon presents a promising alternative for the design of selective filters applicable in various fields, such as telecommunications and optoelectronics.

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Advancing LDPE Properties with Ni Nanoparticles: A Thorough Investigation of Structural, Magnetic, and Mechanical Enhancement

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In this study, we examine the influence of varying concentrations of Nickel (Ni) nanoparticles on the morphological, magnetic, and mechanical properties of a low-density polyethylene (LDPE) polymer matrix. Nickel nanoparticles (NPs) were synthesized using a solvothermal method. Subsequently, LDPE/Ni nanocomposite films were fabricated via a solution mixing technique, with Ni contents of 1%, 3%, 5%, and 10%. X-ray diffraction analysis revealed that the inclusion of Ni NPs enhances the crystallinity of the polymer nanocomposite. Nanoindentation tests demonstrated that the nanomechanical elastic properties, specifically hardness, of the LDPE/Ni composites increased with the addition of Ni NPs. Magnetic property measurements indicated that the nanocomposites exhibit soft ferromagnetic behavior at room temperature. These findings suggest that LDPE/Ni magnetic nanocomposites hold significant promise for the development of materials with unique, adjustable magnetic and mechanical properties. This enhanced functionality could be particularly beneficial in applications requiring precise control over material properties, such as in advanced electronics, magnetic storage devices, and mechanically resilient components.

Annealing temperature effect on charge recombination and dissociation in bulk hetero-junction polymer solar cells under open circuit conditions

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This study evaluates the current density-voltage (J-V) characteristics and magneto-conductance (MC) of ITO/PEDOT/AnE-PVstat:PCBM/LiF/Al solar cells subjected to thermal annealing at temperatures ranging from 25°C to 120°C, using an AM 1.5 G (100 mW/cm²) solar simulator. Our findings reveal a positive magneto-conductance effect (+MC) at 25°C, 100°C, 105°C, and 110°C, while a negative magneto-conductance effect (-MC) was observed at 120°C. To describe the MC effect, we applied the triplet-doublet quenching (TQD) model, which accounts for triplet-charge interactions affecting current flow, based on density matrix formalism and the Stochastic Liouville Equation. Notably, the rates of dissociation and recombination for triplet-doublet pairs increased at lower temperatures (25°C, 100°C, 105°C, and 110°C) but decreased at higher temperatures (115°C and 120°C).

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Spectral, crystal structure, DFT/HSA of novel Zwitterion Schiff derivative of DHA

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A novel Schiff base (SB) derivative, (E)-3-(1-((2,6-diisopropylphenyl)-imino)-ethyl)-4-hydroxy-6-methyl-2H-pyran-2-one, was synthesized in a high yield through the direct condensation of 2,6-diisopropylaniline with 3-acetyl-4-hydroxy-6-methyl-2H-pyran-2-one in ethanol under reflux conditions. The synthesized ligand was identified using different elemental analysis (CHN-EA) and spectroscopic techniques (2D-nuclear magnetic resonance (^{1}H- &^{13}C- NMR), Fourier transform infrared (FT-IR) and mass (MS) spectroscopies, and their structural analysis was performed by single crystal X-ray diffraction (XRD). The results showed that the ligand exhibits a zwitterionic form stabilized by an intramolecular single proton transfer process between the enol and imine tautomerism. The enol↔iminetautomerization was determined by XRD and computed by DFT/HSA calculations, which proved the stabilization of the [N^{+}–H···O^{-}] zwitterionic form via S6 intra-H-bond.

Keywords: Schiff base, Zwitterionic; enol↔iminetautomerism, XRD, DFT/HSA.

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Solvent effects on the electrical and optical properties of SnO_2 thin films

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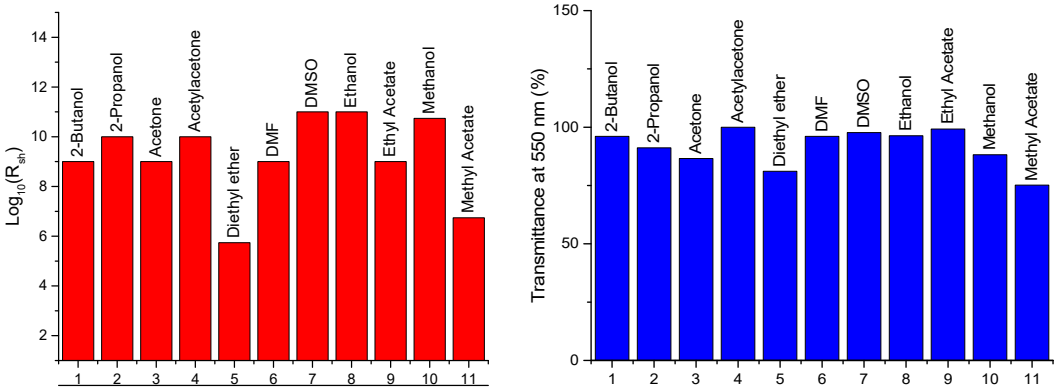
The study of the impact of solvents on the electrical and optical properties of thin-film tin dioxide (SnO_2) is crucial for optimizing its performance in various applications, such as photovoltaic devices, gas sensors, and field-effect transistors. SnO_2 is a transparent semiconductor material known for its excellent electrical and optical properties, including high conductivity and transparency in the visible range. The preparation of SnO_2 thin films can be influenced by several factors, including the choice of solvent used during deposition [1, 2].

The solvent plays a significant role in determining the microstructure of the thin film. Solvents with different polarities can affect the grain size, surface roughness, and crystal orientation of SnO_2. A well-defined microstructure is essential for improving the quality of thin films, as it directly influences the mobility of charge carriers and the scattering of light through the film.

In our experiments, we deposited thin films of SnO_2 using the sol-gel dip-coating method with 30 different solvents, such as ethanol, acetone, and toluene. The resulting films were then characterized using various techniques, including X-ray diffraction (XRD) to analyze crystal structure, UV-Visible spectroscopy for optical properties, and two-probe resistance measurements to assess sheet resistance.



Acknowledgments:
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Dielectric Relaxation Processes and Magnetic Field Effects in Organic Diode Using a Novel Co-Polymer

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We used a novel conjugated polymer, P18-8, which is a combination of poly(1,4-phenylene−ethynylene) and poly(1,4-phenylene-vinylene), to fabricate an organic diode with the ITO/PEDOT: PSS/P18-8/LiF/Al structure. Various electrical properties of the fabricated device were investigated over a wide frequency range (100 Hz–1 MHz) and at different applied voltages using impedance spectroscopy (IS). The current density-voltage (J-V) characteristic exhibited ohmic behaviour at low applied voltages, whereas at higher voltages, it conformed to the space charge limited current (SCLC) theory. The charge carrier mobility in P18-8 was measured from the J-V characteristic on a double logarithmic scale and from the frequency dependence of conductance using the so-called method. The impedance (Z*) of the device, as a function of frequency and bias voltage, was modeled using a single parallel resistor and capacitor network connected in series with resistance. The dielectric loss (ε") decreased with increasing frequency for all the applied voltages, mainly owing to the deformation and relaxation polarization effects. Peaks in the dielectric loss tangent (tan(δ)) at approximately 105 Hz indicate a dipolar polarization behaviours. The lower values of the real part of the complex electric modulus (M') observed in the low-frequency region were attributed to the long-range mobility of the charge carriers. Additionally, the imaginary part of the complex electric modulus (M") reaches its maximum value at all applied voltages, resulting in a peak at a specific frequency.

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Quantum-chemical calculations of structure, electronic properties, and spectra of neat PBDB-T:ITIC heterojunctions

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To improve the performance of polymer: fullerene heterojunctions in organic solar cells, it has been proposed to replace fullerene with alternative organic compounds, such as ITIC. Within this situation, we simulate the structural, electrical, and optical properties of PBDBT:ITIC interactions on a quantum chemical level. We constructed oligomers in various conformations to depict a segment of the donor polymer PBDB-T (Poly[(2,6-(4,8-bis(5-(2-hexyl)thiophen-2-yl)-benzo[1,2-b:4,5-b']dithiophene))-alt-(5,5-(1',3'-di-2-thienyl-5',7'-bis(2-ethylhexyl)benzo[1',2'-c:4',5'-c']dithiophene-4,8-dione)]) (Figure 1) and three ITIC (3,9-bis(2-methylene-(3-(1,1-dicyanomethylene)-indanone))-5,5,11,11-tetrakis(4-hexylphenyl)-dithieno[2,3-d:2,3-d]-s-indaceno[1,2-b:5,6-b]dithiophene) conformers (Figure 2). These were combined into donor-acceptor dimers in both parallel or T-shaped layouts and optimized using DFT computations with the B3LYP-GD3 functional, which accounts for Van der Waals interactions semi-empirically. By comparing the MO-energies of optimized PBDB-T oligomers, ITIC conformers, and dimers, we classified the resulting heterojunctions. Moreover, TD-DFT was employed to calculate the excited states of the dimers, allowing us to determine exciton binding energies and distinguish between charge transfer and excitonic states. Finally, we provide insights into the impact of the PBDB-T donor-acceptor interface design on solar cell performance.

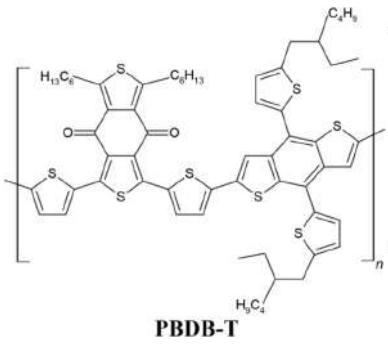

Figure 1

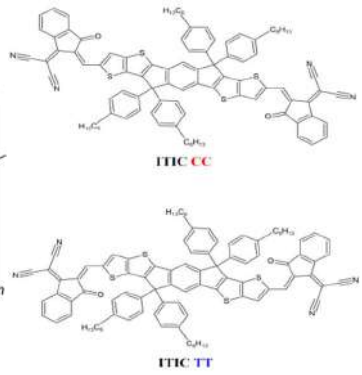

Figure 2

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Study of the complexation of the antiviral Ganciclovir by metal ions: Nickel (II), Cobalt (II) and Copper (II)

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Abstract

Enhancing the efficiency of antiviral drugs is crucial given the emergence of numerous viruses such as Ganciclovir [1]. Ganciclovir (L), an acyclic analogue of 2'-deoxyguanosine (2-Amino-1,9-dihydro-9-[[2-hydroxy-1-(hydroxymethyl)ethoxy]methyl]-6H-purin-6-one), exists in solution as two forms: keto and imine, identified via UV spectroscopy. A novel series of Cu(II), Ni(II), and Co(II) transition metal complexes were synthesized from ganciclovir (L). These complexes' structural characteristics were elucidated using UV-Vis, IR, XRD, and TGA/DTG thermal analysis. Results confirmed that the three metal ions coordinate with oxygen and nitrogen atoms. Job's method determined the complexes' stoichiometry as [1:1]. Finally, biological testing revealed that the toxicity of these complexes increased, while their activity decreased relative to ganciclovir.

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Ni/Fe Hydroxides based Nanohybrid for Energy Storage

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Abstract:

Transition metal oxide and hydroxide nanomaterials have attracted considerable attention especially due to their wide application in many fields.Among the numerous transition metals, Nickel-and Iron- based hydroxides with more complex metal compositions and binding have been extensively studied for their large scale applications as **energy storagedevice (super-capacitor)**, biosensing, catalysts, ….

In our investigation, we report the synthesis of a new kind of heterostructure and bi-phase nanocomposites based of $Ni_{0.75}Fe_{0.25}(CO_3)_{0.125}(OH)_2.0{,}38H_2O/NiFe_2O_4$using simple and low cost free template hydrothermal process at two different growth temperature120 °C and 180°C during 6 h. The obtained products have been characterized with different techniques such as: XRD, FT-IR, FESEM, Raman and BET analysis in order to investigate their physico-chemical properties. The obtained bi-phase nanocomposites have shown important effect of hydrothermal growth parameters that will be used as Ni-Fe based electroactive nanomaterials. They possess nano-heterostructure based of (Ni, Fe) with two kind of pores in 3D morphology, illustrating important specific surface area, pore volume and size around 98 m^2/g, 0,31 cm^3/g and 13 nm, respectively.

Keywords: Hydrotalcite materials, Ni-Fe oxide, LDH, hydrothermal synthesis, Supercapacitors. Energy storage.

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Metal Oxides in Catalytic Applications

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The use of metal oxides in catalytic applications has become increasingly important due to their wide range of tunable properties and their potential to improve reaction efficiency in various chemical processes. This study explores the catalytic behaviour of various metal oxides, focusing on their structural, surface, and electronic properties. The objective is to understand how the composition and morphological characteristics of metal oxides influence their performance, particularly in photocatalytic systems.

A comprehensive approach was employed, integrating advanced characterization techniques such as X-ray diffraction (XRD) for crystalline structure analysis, Raman spectroscopy to identify the vibrational modes of metal oxide bonds, and scanning electron microscopy (SEM) to study surface morphology and particle size distribution. Additionally, UV-Visible (UV-Vis) spectroscopy was used to evaluate photocatalytic properties, particularly concerning bandgap energy and light absorption efficiency. The results show that metal oxides with optimized structural properties, such as nanoscale particle size and controlled morphology, demonstrated enhanced catalytic activity, particularly in photocatalytic degradation reactions. Moreover, the study revealed that fine-tuning the surface properties of metal oxides, including their surface area, crystallinity, and defect density, can significantly improve catalytic efficiency by increasing the number of available active sites and enhancing light absorption.

Green synthesis and characterization of platinum nanoparticles loaded with paclitaxel and coated with chitosan: a promising approach for breast cancer treatment

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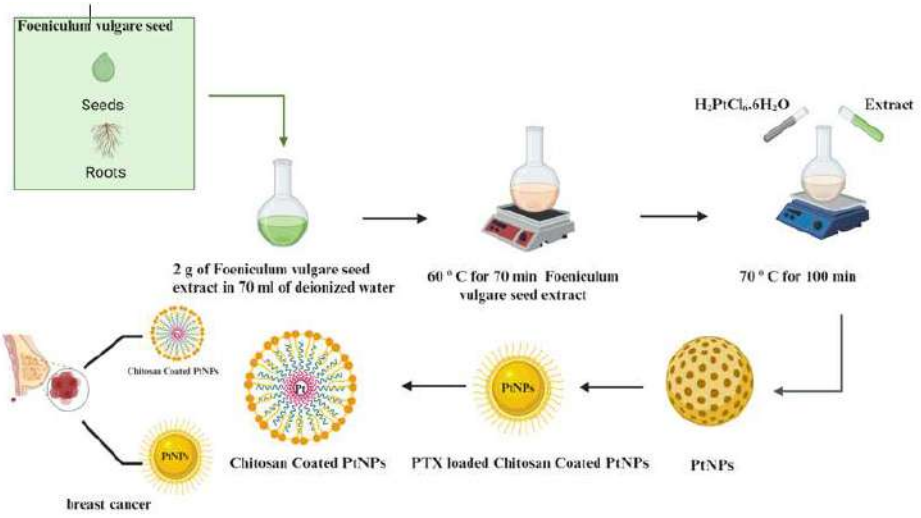
In the pursuit of more effective and safer cancer therapies, the development of novel drug delivery systems has gained significant attention. This study presents the green synthesis of platinum nanoparticles (Pt NPs) loaded with Paclitaxel (PTX) and subsequently coated with chitosan, offering a targeted and controlled release system for breast cancer treatment. The Pt NPs were synthesized using a biocompatible and environmentally friendly approach, ensuring minimal toxicity and enhanced biocompatibility. Characterization of the synthesized Pt NPs was performed using various techniques including UV-Vis spectroscopy, Fourier Transform Infrared Spectroscopy (FTIR), Transmission Electron Microscopy (TEM), and Field Emission Scanning Electron Microscopy (FESEM). The results confirmed the successful loading of PTX onto the Pt NPs and the effective coating with chitosan, which provides stability and facilitates targeted drug delivery. The in vitro cytotoxicity of the Pt NPs-PTX-chitosan complex was evaluated on breast cancer cell lines, showing enhanced anticancer activity compared to free PTX. The chitosan coating not only improved the stability and biocompatibility of the nanoparticles but also promoted cellular uptake and sustained release of PTX, resulting in a significant reduction in cancer cell viability. This green synthesis approach for developing Pt NPs loaded with PTX and coated with chitosan presents a promising strategy for targeted breast cancer therapy, offering potential improvements in therapeutic efficacy and safety. Further in vivo studies and clinical trials are necessary to validate these findings and explore the full potential of this innovative drug delivery system in cancer treatment.


Foeniculum vulgare seed
Seeds
Roots
2 g of Foeniculum vulgare seed extract in 70 ml of deionized water
60 ° C for 70 min Foeniculum vulgare seed extract
$H_2PtCl_6.6H_2O$
Extract
70 ° C for 100 min
PtNPs
PTX loaded Chitosan Coated PtNPs
Chitosan Coated PtNPs
breast cancer

Properties of mesoporous and microporous materials modified by iron nanoparticles as potential catalysts for water purification

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Abstract:
The aim of this work is to seek solutions to purify water from organic pollutants, in particular pharmaceutical residues such as Diclofenac, using the ozone degradation method catalyzed by synthetic porous materials and industrial waste such as zeolites. With this in mind, we have also deployed a new method for producing iron nanoparticles supported on these basic materials for the degradation of Diclofenac by ozone.
Firstly, we synthesized and characterized the two mesoporous materials (SBA-15 and SBA-16) with hexagonal and cubic structures respectively [1], where the results of the characterization techniques showed that these materials present very promising properties due to a higher degree of order, very large pore diameters and a very large specific surface areas.
Secondly, we used these materials as matrices in order to develop iron nanoparticles with more interesting properties than those of the parent materials using coffee and tea extract as a solvent [2] to replace the harmful reducing agent such as sodium borohydride.
Finally, these materials were tested in their purely silicic and iron nanoparticle forms for the degradation of Diclofenac using the ozonolysis method. The ozonation results showed that silicates and aluminosilicates such as SBA-15 and SBA-16 as well as type 4A zeolite are excellent catalysts for water purification with total mineralization at ambient temperature.

Keywords: Zeolite 4A, SBA-15, SBA-16, Nanoparticle, Ozonation, Diclofenac

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Investigating the Structural and Electronic Properties of AlN/GaN Superlattices Along (110), (110), and (111) Growth Axes Using First Principles

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In this study, we employ first-principles calculations to investigate the structural and electronic properties of AlN/GaN zinc-blende/zinc-blende superlattices. Our approach involves utilizing the full potential linear muffin-tin orbitals (FPLMTO) method within the plane wave approximation (PLW). This method offers accurate treatment of interstitial regions and avoids the reliance on adjustable parameters, ensuring a reliable and microscopic analysis. We explore the AlN/GaN superlattices in three different growth directions: (001), (110), and (111). By calculating the electronic structures of these superlattices, we compare and analyze their properties. Our investigation includes examining the partial density of states, which allows us to understand the changes in the nature of the band gaps observed in the (110) and (111) growth axis superlattices. We find that these modifications can be attributed to the strong hybridization of the Ga and N atoms' pd and sporbitals.

Kkeywords: AlNGaN110 and 111 growth axis Superlattices Electronic structure

Simulation and optimization of highly efficient n-i-p planar Perovskite Solar Cells using SCAPS-1D Software

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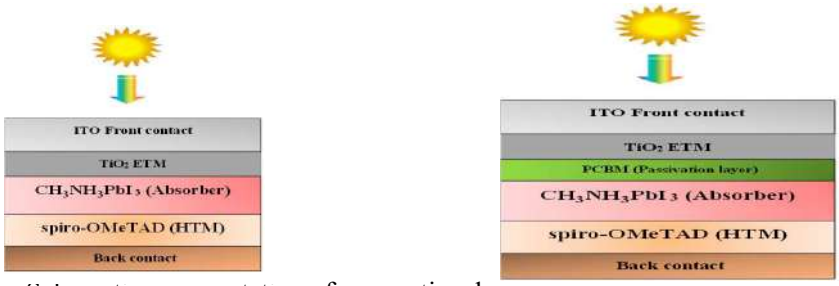
Recently, the conversion efficiency of Perovskite solar cells has reached 25.2%. However, further research is necessary to enhance their lifetime, reduce and control defects, and optimize their design structures and stability. In this study, we perform simulations using the Solar Cell Capacitance Simulator (SCAPS) to construct a more realistic model of a conventional n-i-p planar Perovskite solar cell (Fig 1), utilizing typical data values from the literature. After validating our model against experimental data, we investigate the main limiting factors responsible for the degradation of PSC performance. Subsequently, we propose a new structure based on an interface engineering strategy, aiming to improve performance by optimizing various physical and dimensional parameters, such as the thickness and doping level of each layer. The optimized structure achieves an impressive power conversion efficiency of 24.38% versus 21.5%, with a Voc of 1.12 V, a Jsc of 26.03 mA/cm², and an FF of 81.73%.



Schematic representation of conventional and proposed n-i-p planar PSC structure.

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Synthesis and Characterization of Mn_3O_4 Thin Films: Multifunctional Properties for Optoelectronic and Magnetic Applications

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The present investigation involved the synthesis of Mn3O4 thin films by the chemical spray deposition process, with a temperature of 350 °C being employed. The films were analyzed to determine their structural, optical, and magnetic characteristics. The X-ray diffraction study showed that the hausmannite structure was polycrystalline, with a tetragonal shape and most of its orientation along the (101) plane. The crystallite size was determined by employing both the Scherrer and Williamson-Hall techniques, yielding an average value of 36.56 nm. The optical experiments indicated a transmittance of 70% in the visible spectrum and 80% in the near-infrared spectrum, with an optical band gap of 2.61eV. Photoluminescence research revealed the presence of many emission peaks, indicating emissions that are associated with defects. The material's magnetic characteristics were examined using a vibrating sample magnetometer, which revealed that the material exhibited ferromagnetic behavior with a saturation magnetization of 3.17 x 10^{-4} emu. The findings illustrate the capacity of Mn3O4 thin films for use in optoelectronic devices, UV detectors, and magnetic sensors.

Impact of Miniaturization on Electrical Properties of High-k Interface Diodes

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This study explores the electrical and dielectric properties of the TiN/Al_2O_3/p-Si MIS structure within the temperature range of 380-450 K at 1 MHz. These properties were derived from experimental measurements. Results indicate that for wardbias plots show a distinct peak at higher temperatures, primarily due to series resistance and interface states between Al_2O_3 and p-Si. The dependence of the dielectric constant, dielectric loss, dielectric loss tangent, and AC electrical conductivity on temperature and bias voltage was examined. Findings reveal that these values vary with changes in bias voltage and temperature. The characteristics confirm that the series resistance and interface states significantly influence the electrical parameters in the MIS device. The interface state density, dependent on temperature, was determined using the Hill-Coleman Method. An Arrhenius plot of AC conductivity at 1 MHz shows the activation energy. Additionally, electric modulus form alisms were used to understand the relaxation mechanism of the structure.

Highly Sensitive RGB and HSV-Based Detection of Bromates Using Smartphone

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Bromate ions, used in the food industry and generated during water treatment using ozone, are recognized for their toxicity and alarming carcinogenicity. Faced with this public health risk, this work proposes a new, highly sensitive, rapid and cost-effective detection approach, based on smartphone photometry. By exploiting the oxidizing feature of bromate ions, the principle of this method is based on the oxidation of leuco methylene blue (LMB), a colorless compound, into methylene blue (MB - blue colored) in an acidic medium. The as-formed blue coloration, proportional to the bromate concentration, is captured after one minute using a level entry smartphone camera. The careful optimization of the reaction parameters such as HCl concentration, concentration of LMB, concentration of the thickening agent, reaction time, etc. allowed to link the coloration of the reaction solution to the intensities of the colors. The intensities of the RGB, HSV and HSL color systems are then analyzed with the RGB Color Detector app, offering a simple, reliable and sustainable alternative for bromate monitoring.

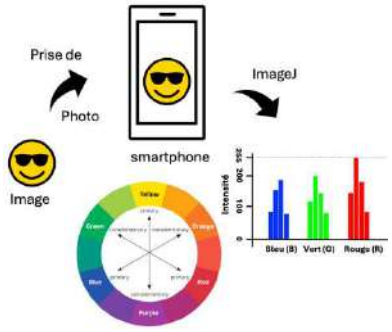

Figure: Principle of the smartphone photometry for color decomposition

Keywords: Bromate ions, Cancer, Smartphone, Color, Color systems, Sensing.

Abstracts of Poster Communications

Session II

Optimization of Graphene Electrodes Preparation for Biosensing Applications

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The use of graphene as an electrode material has known significant growth due to its extraordinary electrical properties [1]. The electron transfer rate and the analytical performance of graphene-based electrodes are considerably influenced by the preparation method and the quality of the graphene [2]. For such applications, producing high-quality graphene remains a challenge.
In this work, we focused on developing graphene electrodes prepared in the lab by combining wax printing with screen-printing technology. The electrodes are prepared following a multi-step protocol. The reference electrode and counter electrode are pre-printed on PET using a screen-printing machine. The working electrode was prepared first by filtering a graphene oxide solution through nitrocellulose membranes on which the electrode pattern was printed by wax machine, followed by the transfer and reduction of the film. The final step involves depositing an insulating film to prevent any undesirable contact during electrochemical measurements. The fabricated electrodes demonstrated good conductivity and were applied for the detection of BRCA1 as a breast cancer biomarker. The biosensor development is simple and cost-effective, relying on the modification of the graphene electrode surface with electroactive organic molecules, followed by the immobilization of DNA probe. The detection curves show ultra-sensitivity in a wide dynamic range of concentrations.

Keywords: Graphene electrode, screen printing, wax printing, Biosensor, cancer.

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Mineralization of Paraquat aqueous solutions by gamma irradiation

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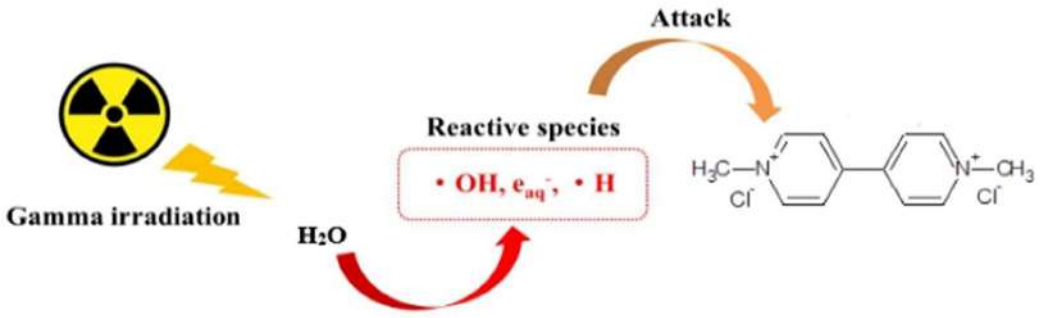
In the present work, gamma radiolytic degradation of paraquat (PQ), an extensively used yet highly toxic herbicide, from aqueous solutions was investigated. The effect of different gamma irradiation doses (from 1 to 8 kGy) was explored. After a 5-hour treatment period, 96% and 90% removal of Total Organic Carbon (TOC) and Chemical Oxygen Demand (COD), respectively, were observed. NMR1H and 13C analysis prove that 8 kGy dose is highly effective in completely eliminating the herbicide at 50 ppm. PQ removal kinetic was found to obey the pseudo-first order model. The obtained apparent rate constant was *k*app,PQ= (0.0059 ± 0.001) min−1.In order to determine the potential industrial application viability, the energy consuming was evaluated. Finally, a comparison was done between gamma degradation and other methods. It was found that gamma radiolytic degradation is an effective, fast and clean process that induce complete mineralization of PQ and its degradation by-products.



Keywords: Gamma irradiation, paraquat removal, Advanced oxidation process, energy consumption.

Synthesis of $CuO/WO_3/gC_3N_4$ nanocomposite used as a new efficient sensor for the sensitive and selective detection of H_2O_2

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In recent years, interests in designing and developing new, faster, and more reliable materials and methods for hydrogen peroxide sensing have increased significantly. In fact, they emerge from the use of this product in several industrial sectors like water treatment as well as in clinical research **[1-2].**

In this work, the design of a novel electrochemical hydrogen peroxide (H_2O_2) sensor, which is based on a new $CuO/WO_3/g\text{-}C_3N_4$ nanocomposite is presented for the first time.

The crystal structure, the morphology, the elemental composition, the phase purity, and the products' electrochemical properties were properly examined using numerous scientific tools including infrared spectroscopy (IR), X-ray diffraction (XRD), and transmission electron microscopy (TEM). In terms of its application, the electrochemical sensing ability of $CuO/WO_3/g\text{-}C_3N_4$ nanocomposite toward H_2O_2 analyte was examined through cyclic voltammetry (CV) and amperometry (*i-t*) evaluation. The obtained findings indicate that the dispersion of CuO and WO_3 nanoparticle oxides on the $g\text{-}C_3N_4$ nanosheet surfaces improves the electro-oxidation signal around 0.6 V and the overall performance of the hybrid sensor. A substantial linear correlation was shown between the peak current and the H_2O_2 concentration in the linear range of 0.5 to 1400 µM for the nano-composite electrode $CuO/WO_3/g\text{-}C_3N_4$. Based on the amperometric evaluation, the sensitivity of the modified hybrid electrode is 1720 $\mu A.mM^{-1}.cm^{-2}$ with a low detection limit of 0.5 µM. The constructed electrode has been successfully applied for testing H_2O_2 concentrations in real water samples. The novelty of this work revolves around the simple way of synthesizing for the first time, the ternary nanocomposite $CuO/WO_3/g\text{-}C_3N_4$, and its use as an H_2O_2 electrochemical sensor. These combined results pave the way for the design of new and more effective heterostructures with tailored activities for other environmental and health-related concerns.

Keywords: Nanocomposite, Non-enzymatic sensor, H_2O_2, Amperometric tests.

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Systemic scleroderma diagnosis using UV-visible fluorescence

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The ability of our body to protect itself against external chemicals is known as immunity. An immune system malfunction that results in the body attacking its own tissues is what defines an autoimmune illness [1],[2]. By identifying mineral and molecular markers, traditional medical analytical techniques offer a comprehensive understanding of illness states; nevertheless, the complexity and expense of these procedures are constrained [3],[4].The goal of our research is to develop a new method for screening for systemic scleroderma by analysing skin using UV-visible fluorescence. The skin fluorescence study sites, which took into consideration the sun exposure of patients who were grouped together as healthy patients and others suffering from scleroderma, allowed for the construction of an approach that produced significant results in terms of distinguishing between patients with scleroderma and those in good health. These data highlight an intriguing correlation between the fluorescence-measured molecular diversity of the skin and the presence of trophic problems in the context of Raynaud's disease, a severe clinical manifestation of sclerodermie [5]. This correlation strengthens the previously established link between trophic problems and sclerodermie, providing new insights into the understanding and treatment of this complex disease. The findings open up new possibilities for the medical dermatology by demonstrating the viability of this approach as a dependable and affordable tool for the early detection of an autoimmune illness.

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Fabrication and Characterization of a Porous Silicon-Based SERS Substrate for Acetamiprid Pesticide Detection

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This work presents the fabrication and detailed characterization of a Surface-Enhanced Raman Spectroscopy (SERS) substrate based on porous silicon (PSi) for the sensitive detection of acetamiprid pesticide. The substrate was developed via electrochemical anodization of highly doped p-type silicon wafers with <100> crystallographic orientation, followed by gold deposition to create a nanostructured surface. The porous silicon layer was formed using an electrolyte solution of hydrofluoric acid, ethanol, and water, followed by thermal oxidation to improve the stability and surface functionalization.
The nanostructured surface, achieved through gold sputtering, enables significant enhancement of the Raman signal of adsorbed molecules. Scanning Electron Microscopy (SEM) and Atomic Force Microscopy (AFM) analyses confirmed a uniform distribution of gold nanoparticles across the substrate surface. UV-Vis reflectivity measurements further validated the presence of localized surface plasmon resonance (LSPR), confirming the substrate's strong SERS activity.
Energy Dispersive X-ray Spectroscopy (EDX) was employed to confirm the elemental composition of the Au/PSi substrate, while Raman spectroscopy demonstrated the substrate's efficiency in detecting trace amounts of acetamiprid, highlighting its selectivity and sensitivity. These findings establish the potential of porous silicon-based SERS substrates in environmental monitoring, offering a reliable and reproducible platform for detecting pesticide residues.

Keywords: SERS, Porous Silicon, Acetamiprid Detection, Gold Nanoparticles, Electrochemical Anodization, Localized Surface Plasmon Resonance, Environmental Monitoring.

Cobalt(II)-functionalized graphitic carbon nitride improved laser-induced 3D graphene electrodes for the sensitive sensing of diclofenac

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Laser-induced graphene electrodes (LIGEs) were fabricated and characterized for the detection of diclofenac. The CO_2 laser was manipulated to develop LIG electrodes on a polyimide film by laser irradiation. This method of manufacturing allows for the engravement of conducting electrodes on a polymeric substrate in a single step. The LIG electrode surface was changed using Co (II)-functionalized graphitic carbon nitride (Co(II)@gC_3N_4) to improve detection sensitivity. The Co(II)@gC_3N_4-modified LIGEs were characterized by SEM/EDAX analysis, Raman spectroscopy and X-ray diffraction. Furthermore, electrochemical assessment of the physicochemical properties showed the improvement of the electrochemical features in terms of heterogeneous electron transfer rate, k_0, and electrochemically active surface area. In presence of increasing concentrations of DFC, the Co(II)@gC_3N_4-modified LIGEs can detect the target in the range from 1 – 200 µM, with limit detection of 0.36 µM (S/N = 3). Two ranges are distinguishable from 1–80 µM and from 80–200 µM with sensitivities of 0.99±0.03 and 0.28±0.02 $\mu A \cdot \mu M^{-1} \cdot cm^{-2}$. Furthermore, the electrode can discriminate between DFC, uric acid, ascorbic acid and salicylic acid. The applicability of the modified electrodes was also evaluated in real samples of DFC tablets and urine samples doped with DFC. These cost-effective electrodes had great potential for analyzing of drugs for various healthcare and environmental applications.

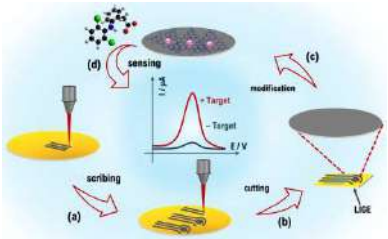

Figure: Schematic illustration of the LIG electrode preparation for DFC sensing

Keywords: Graphene; Sensing; LOD; Pharmaceuticals; Serum.

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Sjögren's syndrome diagnosis through in situ investigation of the oral cavity employing frontal optical fluorescence

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The mouth is an indispensable minor ecosystem of the human body. It consists of various divisions and areas that have diseases specific to their location. This study suggests an innovative strategy to in situ analysis employing spectroscopic techniques to identify causal relationships between specific chronic and systemic auto-immune disorders and oral health. This study aims to understand how these illnesses may exacerbate dental issues, such as caries and parodontitis, by potentially promoting bacterial growth [1], [2]. A cross-sectional study was conducted in a hospital to explore a specific sites and areas within the oral cavity of patients with chronic and/or systemic diseases as well as a health control group (HC). All the sites were excited by a light source, and participants were divided into groups. The disease's fluorescence profile has been determined. The oral cavity sites analysed by UV-visible fluorescence spectroscopy allowed for the separation of the groups of participants with diseases from the healthy control participants. The patients' buccal cavity analysis allowed for their grouping according to their stage of development. Fluorescence UV-visible spectroscopy is a promising, quick, and non-invasive tool for early diagnosis of buccal diseases, chronic affections and systemic autoimmune diseases, as well as for monitoring patients' health states [3], [4], [5].

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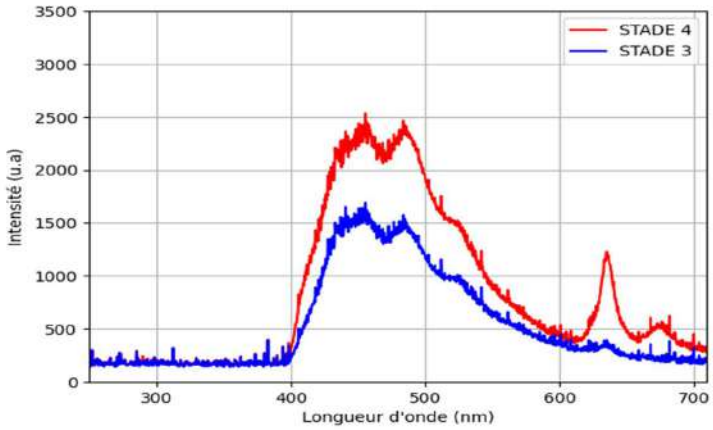

Fig1: Fluorescence spectra for patients with Sjögren's at different stages

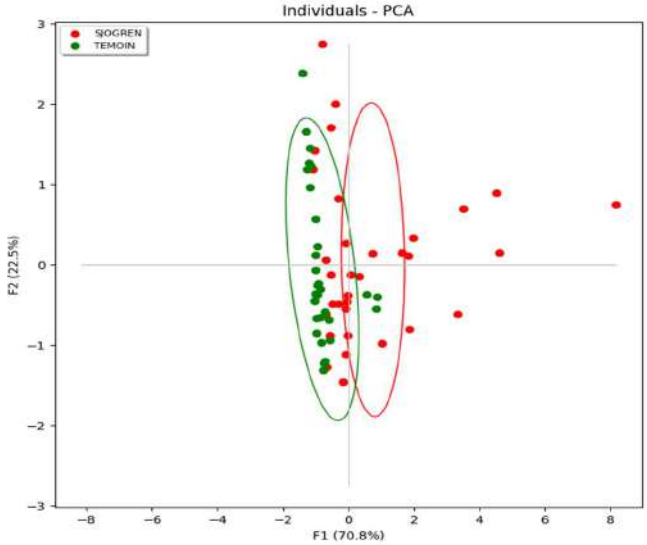

Fig2: Principal component analysis (PCA) of oral site.

Electrochemical Sensing of Levofloxacin and Warfarin Using Laser-Induced Graphene Electrodes Modified with Gold Nanoparticles.

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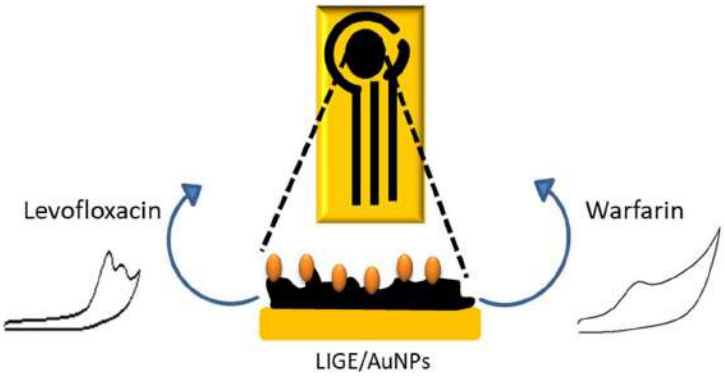
In this work, we report the design of a miniaturized electrochemical platform for the detection of pharmaceuticals (levofloxacin and warfarin) using laser-induced graphene electrodes (LIGEs) modified with gold nanoparticles (AuNPs). Firstly, a CO_2 laser with a fixed laser speed and power for the direct writing of graphene on a polyimide film by photochemical transformation of the polymer materials into graphene. This technique enabled us to efficiently produce the porous graphene three electrode under ambient conditions without solvent or further purification.[1] The electrochemical modification of the working electrode surface by gold nanoparticles lead to the final analytical device (LIGE/AuNPs) used for the detection of the electroactive biomolecules.[2] The LIGE/AuNPs demonstrated a Warfarin linear range of concentration between 10^{-4} and 5.10^{-4} M with a detection limit of $0{,}931.10^{-4}$M. However, the detection of Levofloxacin by the LIGE/AuNPs device exhibit excellent performances compared to conventional screen-printed carbon electrodes (SPCE). Indeed, the LIGE/AuNPs decreases the detection potential of Levofloxacin by 100 mV while improving the electrochemical behavior of the biomolecule.



Schematic depiction of the laser-produced graphene electrodes and the redox signals recorded for the studied drug molecules

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Development of new hybrid nanocomposites for effective photocatalytic degradation of toxic dye pollutants

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Photocatalysis has been considered as a potential technology to detoxify and clean-up water contaminated with toxic chemicals and harmful microorganisms. Herein, silver-doped hydroxyapatite copper nanocomposite Ag-HAp/CuO was synthesized via facile hydrothermal technique using low-cost precursors. The structure and functional groups of the prepared material were analyzed by XRD and FTIR spectroscopy, the optical property was examined by UV–Visible spectroscopy. The catalytic behavior is examined through the decomposition of methylene blue and rhodamine B, as a standard dyes, under visible light irradiation. The efficiency of the novel Ag-HAp/CuO composite in the remediation of these dyes was attributed to the combined synergistic actions of the bending functional groups of HAp surface and the high photocatalytic activity exhibited by CuO as a semiconductor. Thus, this study shows the great potential of Ag-HAp/CuO nanocomposite material as a catalyst under visible light radiation for the decomposition of industrial organic dyes.

Nanostructured "in-lab" aptasensor for electrochemical detection of vancomycin

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Electrochemical sensors based on aptamers are sensitive strategies capable of performing molecular measurements *in vivo*, regardless of the chemical properties (e.g., enzymatic, redox, spectroscopic) of the target analyte. In this study, an innovative, sensitive and robust aptasensor was designed for the detection of vancomycin (VAN) antibiotic. The electrochemical sensor is based on an in-lab printed carbon electrode (C-PE) functionalized by gold nanostructures (AuNSs) on which a blocking layer and aptamer strands specific to VAN are immobilized. The AuNSs, characterized by scanning electron microscopy (SEM) and atomic force microscopy (AFM), enhanced the electrochemical properties of the platform and the aptamer immobilization active sites. The developed disposable aptasensor allowed label-free detection of VAN via electrochemical impedance spectroscopy (EIS) across a wide range of concentrations (50 -1000 nM), with a limit of detection (LOD) of 1.721 nM. The developed aptasensor presented good selectivity against some commonly found interferences in human serum and milk and was successfully applied for the analysis of these samples.

Enzymatic biosensor for the detection of pesticides by fluorescence inhibition

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Pesticides, such as organophosphates and neonicotinoids, are recognized for their toxicity, present significant risks to both human health and the environment, highlighting the need for stringent control and regulation. Faced with this public health risk, this work proposes a new, highly sensitive, rapid and cost-effective detection approach based on fluorescence inhibition, for the detection of triazophos and acetamiprid which have an inhibitory effect on tyrosinase activity. The principle of this biosensor is based on the inhibition of the production of dopaquinone, our probe, produced during the oxidation of tyrosine. This reaction is catalyzed by the tyrosinase immobilized on magnetic beads. An optimization of reaction parameters such as tyrosinase concentration, incubation temperature, pH of the buffer solution, and substrate concentration, should be studied to determine the optimal catalytic activity of the enzyme. The rate of fluorescence inhibition is then determined in the presence of each pesticide at different concentrations. The platform implemented in this work has allowed to obtain a biosensor particularly efficient, reliable and sustainable alternative for triazophos and acetamiprid monitoring.

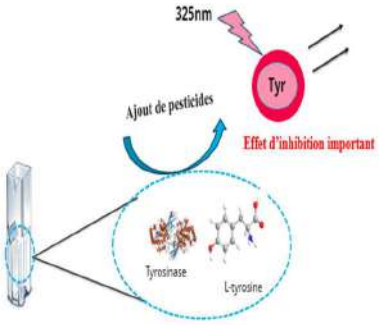

Figure: Principle of the enzymatic biosensor based on fluorescence inhibition

Keywords: Triazophos, Acetamiprid, Tyrosinase, Fluorescence inhibition, Probe, Substrate, Sensing.

First Electrochemical Bioplatform for Personalized 5-Fluorouracil Chemotherapy Assistance

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This work reports a simple biotool for the determination of 5-fluorouracil(5-FU), a drug often used in chemotherapy for the treatment of certain cancers. The methodology involves an indirect competitive immunoassay performed on the surface of magnetic microbeads (MBs) and amperometric transduction at screen-printed carbon electrodes (SPCEs). In brief, free 5-FU competes with 5-FU-BSA covalently immobilized on HOOC-MBs for the limited recognition sites of a FU-selective detection antibody (DAb) labeled with a secondary antibody conjugated to the peroxidase enzyme (HRP-antimIgG). Amperometric transduction was made using the H_2O_2/hydroquinone (HQ) system. The method provides analytical characteristics in terms of sensitivity (LOD of 1.0 ng mL^{-1}) and selectivity suitable with clinical useful nessand is competitive with other reported electrochemical non-biosensing detection strategies in terms of simplicity and assay time. Most interestingly, the method exhibits high accuracy in the analysis of a pharmaceutical formulation and of serum samples even from a patient with colorectal cancer (CRC) undergoing treatment with 5-FU thus showing potential for chemotherapy monitoring and personalized chemotherapy.

Keywords: 5-fluorouracil; competition immunoassay; screen-printed electrode; amperometry; magnetic beads; personalized chemotherapy.

Solar photoreactor photocatalytic/adsorbents based on doped and functionalized zinc oxide nanocomposites for the solar degradation of phenols in water samples

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Innovation in advanced oxidation process (AOP) technologies is increasingly focused on the direct utilization of solar radiation for photochemical conversion, with particular attention to the treatment of micropollutants in water. This approach involves the generation of radical species capable of degrading organic matter and trace micropollutants that persist in water due to the limitations of conventional wastewater treatment processes, which are often insufficient for complete removal. Solar photo-oxidation offers the potential for an autonomous and ecologically sustainable process by harnessing solar energy as the primary power source, resulting in more sustainable, cost-effective, and energy-efficient solutions [1]. In this study, a photocatalytic nanocomposite consisting of doped and functionalized zinc oxide (ZnO) nanoparticles, incorporating metal elements and conductive polymers, was employed to address the challenges associated with solar energy utilization. To explore the synergistic adsorption effect, the ZnO nanocomposite was combined with activated carbon (AC), forming a composite adsorbent/photo-catalyst material capable of storing pollutants during periods of low sunlight and concentrating micropollutants on the catalyst surface, thereby enhancing contact with photo-generated charges. The composites were characterized using various physico-chemical techniques to investigate their crystallographic, morphological, and structural properties.

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Efficient electrochemical nanoplatform based on gold nanofoam modified polypyrrol decorated with tungsten disulfide for the quantification of heavy metals in water

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Heavy metal contamination in water has become a critical global concern, with significant implications for both human health and environmental sustainability. Recent statistics suggest that nearly 40% of the world's lakes and rivers are affected by heavy metals [1]. These contaminants are prone to bioaccumulation in living organisms and food chains, which can lead to severe organ damage and contribute to the onset of neurodegenerative disorders such as Alzheimer's and Parkinson's diseases [2]. Therefore, the need for accurate and sensitive detection methods for heavy metals, even at trace levels, has become increasingly urgent. In this study, an efficient electrochemical platform was developed using a modified screen-printed carbon electrode (SPC) for the detection of heavy metals in various water samples. Specifically, the SPC electrode was functionalized with polypyrrole-coated gold nanofoam and tungsten disulfide nanosheets. Electrochemical analysis demonstrated that this sensor could simultaneously detect multiple heavy metals across a wide linear range of 0.01–10 µM, achieving a remarkably low detection limit of 2.3 nM. Additionally, the sensor's performance was evaluated in tap, river, and seawater samples, confirming its broad applicability in environmental monitoring.

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Highly Efficient Catalytic Performances for Nitro Aromatic Compounds Removal via Environmentally Friendly Polyvinyl Alcohol/ Silver Nanocomposites Synthesized through Gamma Irradiation

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Hazardous chemicals like toxic nitroaromatic compounds are very harmful to the environment and their removal is quite challenging. Therefore, there is a necessity to develop techniques, which are environment friendly, cost-effective and easily available in nature for water purification and remediation. However, the conventional preparation methods are limited by conditions such as cumbersome operation, high energy consumption, and high pollution. The present research work is focused on the development of a simple method to remediate wastewater contaminated by nitroaromatic compounds through the synthesis of nanocomposites materials (Ag/ PVA) using gamma radiation able to act as a catalyst for the reduction of nitroaromatic compounds. Silver nanoparticles were prepared in the environmentally friendly polyvinyl alcohol polymer as a support polymer after exposer to gamma radiation from 25 kGy to 100 kGy. The catalytic reduction of nitroartomaic compounds to their equivalent amine was particularly efficient using the Ag/PVA nanocomposites. Fourier Transform Infrared Spectroscopy (FTIR), UV-Visible, and Transmission Electron Microscopy (TEM) examinations were used to investigate the induced in structural changes of Ag/PVA nanocomposites. The reduction reaction of three nitroaromatic compounds (Trinitrophenol, 2-Nitophenol and 4-Nitrophenol) follow a pseudo-first-order. Therefore, the research of Ag/PVA nanocomposites has important potential value for environmental management and sustainable development of human health, and provides new clues for the future research of PVA new catalyst materials.

Keywords: Silver nanoparticles, nitroaromatic compounds, kinetic study, Ag/PVA catalyst.

Enhanced Efficiency of Free Convection in Al_2O_3-Ag-CuO Ternary Hybrid Nanofluid inside closed Differential-Heated Domain

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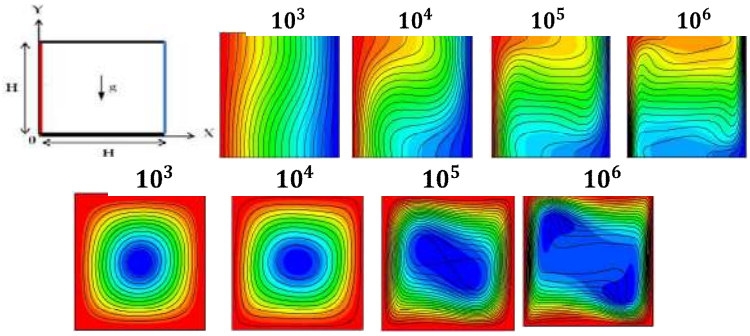
The aim of this paper is to scrutinize a free convection of Al_2O_3-Ag-CuO/water ternary hybrid nanofluid of equal volumetric nanoparticle (NPs) composition (30:40:30) respectively, in a differentially vertical heated square enclosure. The governing energy and Navier-Stokes equations are solved using finite volume approach, under several pertinent parameters namely, Rayleigh number ($10^3 \leq Ra \leq 10^6$) and NPs overall volumetric concentration($0\% \leq \varphi \leq 10\%$). Examination of flow and thermal fields through isotherms, streamlines, velocity, temperature profiles and Nusselt number is carried out lucidly. Results show that when Ra increases, the convection is intensified and a clockwise vortex develops inside the cavity as a consequences of high-energy transport through the flow associated with the irregular motion of nanoparticles. The ternary hybrid nanofluid appears to be the most efficient nanofluid in comparison with the other hybrid nanofluids, particularly at higher total volume fraction, thus it can be used for heat transfer intensification in closed chambers, e.g., for cooling of heat-generating elements or in solar panels applications.



Figures of physical domain of differentially heated cavity with isotherms and streamlines at several Ra numbers (φ=0.1)

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Zinc stannate $ZnSnO_3$sprayed thin film synthesis for photocatalytic degradation of methylene blue (MB) dye

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Zinc stannate or zinc tin oxide with chemical formula $ZnSnO_3$is a class of ternary oxide that is known for its stable properties under extreme conditions, higher electron mobility compared to its binary counterparts and other interesting optical properties [1]. The multifunctional material is thus ideal for use in different fields; such as solar cells, gas sensor, photo-electrochemical, optoelectronic device and phtocatalyst [2]. Photocatalysis is a highly appealing process for the degradation of harmful organic contaminants in water into harmless byproducts, mostly carbon dioxide and water [3]. Release of dye like methylene blue from textile industries is always one of the most problems of pollution environment. Research on photocatalytic materials and process has been a field in continuous expansion in the recent decades. The deposition of thin films have been attempted using a multitude of deposit methods. The deposition methods varies in terms of precursor forms, quality of thin films and cost of equipment. On the other hand, relies on simpler method of chemical synthesis such as ultrasonic or pneumatic spray pyrolysis (USP) or sol gel. USP is beneficial towards its low cost, a better stoichiometry control and homogeneity, covering large area films [4].
In this contribution, we have reported the fabrication of zinc stannate film by simple USP procedure. XRD, FTIR, Raman, UV-Vis spectroscopy techniques have been used to obtain the microstructure and phase of the sample as to characterize the physicochemical and optical properties. Photo-catalytic property of the oxide have been investigated and found that the MB degradation efficiency is of 95%. The Langmuir–Hinshelwood model has been used to evaluate the kinetics of dye degradation, estimated at 0.00785 min^{-1}. $ZnSnO_3$ is a suitable candidate for absorption and degradation for MB organic dye.

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Performance of PVK:ZnSe nanomaterial: solar cell application

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Considerable effort has been directed at hybrid thin film materials composed of polymer and inorganic nanoparticles [1,2]. In order to investigate their performance, the effect of oleic acid-capped ZnSe nanoparticles inclusion into poly(vinylcarbazole) (PVK) pristine on optical and electrical properties was investigated. The results showed that the incorporation of oleic acid-capped ZnSe strongly influenced the optoelectronic proprieties. This trend was described within the Förster formalism, which involves a non-radiative energy transfer from the donor PVK to the acceptor ZnSe NPs. A modified Stern–Volmer model was used to interpret the fluorescence quenching in this system.

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Investigation of the Optical and Structural Properties of Er^{3+}Doped Oxyfluoride Glass for Laser Applications

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This work focuses on the creation and investigation of the spectroscopic characteristics of an oxyfluoride glass enriched with Er^{3+} ions, based on the GeO_2-PbF_2-PbO system. The spectroscopic behavior of this sample was examined using a semi-empirical Judd-Ofelt (J-O) method. We identified the Judd-Ofelt parameters (Ω_t = 2, 4, 6), which turned out to be lower than those found in similar glasses, indicating that the material has less rigidity, a more ionic Er-O bond, and reduced asymmetry around the Er^{3+} ion sites.
These parameters allowed us to compute the probabilities of radiative transitions between different energy levels of the ^4f_N electron shell, along with the branching ratios for these transitions, and the radiative lifetimes of the main emission levels, particularly for the transition from the metastable $^4I_{13/2}$ level to the ground $^4I_{15/2}$ level of the Er^{3+} ion, in comparison with other Er^{3+}-doped glasses. Furthermore, we explored emissions in the visible region using a Stokes-type excitation, enabling us to examine the excitation spectrum and determine chromaticity coordinates. These findings suggest that this glass holds significant potential for use in laser applications and optical amplifiers, especially at wavelengths of 543 nm and 1512 nm.

Effect of Annealing Temperature on Structural, Optical and Morphological properties of $ZnTiO_3$provskitedeposited on porous silicon and its photocatalytic Application

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Nowadays, the world suffers from water scarcity caused by environmental pollution. Major pollutants are organic compound generated from industrial manufactory. The crystalline ceramics mainly perovskite-type oxides of $ATiO_3$ types, such as $ZnTiO_3$,$SrTiO_3$,$MgTiO_3$,$NiTO_3$,..,have attracted wide-spread attention in different frontier areas of research. Perovskite $ZnTiO_3$is a promoted material and has excellent results for various applications such as photocatalysis as we present in this work, a systematic study on $ZnTiO_3$ coated porous for photocatalysis application. The PS was elaborated by electrochemical anodization from the single- crystal p-type silicon wafer. In this work, we investigate the physical and photocatalytic properties of $ZnTiO_3$ Perovskite thin films deposited on porous silicon substrates. $ZnTiO_3$ layers were prepared by consecutive sol-gel method and further deposited on PS substrates by spin-coating.
In this paper, we investigate the effect of annealing temperature on structural, optical, and photocatalytic properties of $ZnTiO_3$ thin films deposited on PS substrates.
$ZnTiO_3$ coatings were prepared by consecutive sol-gel method and further deposited on Si substrates by spin-coating.
The obtained films were annealed at three various temperatures namely 700°C, 800°C, and 900°C. X-ray diffraction analysis shows that the crystallite size of the films grows from 180 to 216 nm as the annealing temperature increases from 700 to 900°C. At the same time, the roughness increases from 193 to 215 nm and the band gap dwindles from 3.64 to 2.57 eV.
$ZnTiO_3$ coatings annealed at 700°C exhibits the highest photodegradation rate about 94% to catalyze the degradation of the Methylene Blue aqueous solutionunder sunlight irradiation. We demonstrate that this high photocatalytic activity is attributed to the structural, optical andmorphological properties of prepared samples.

Keywords: $ZnTiO_3$, perovskite, porous silicon, Methylene Blue, photocatalytic activity.

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Biomaterials Synthesis for environmental application

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Heavy metals and organic pollutants constitute an environmental and agricultural pollution problem that threatens: humans, animals and plants. Among the solutions to reduce this problem is the recycling of organic and inorganic waste in the form of nanomaterial (Biochar) to treat the soil and improve the quality and quantity of crops.

In the present study, we report the production of activated Biochar (activated carbon) from organic waste by thermic activation (pyrolysis).

Nanostructured Biochar product has been characterized in order to determine its attractive physicochemical properties using various protocols (electrical conductivity, carbon content, ash, volatile matter, humidity, apparent density, and Iodine Number), in addition we have study also the morphological, structural and thermal properties with SEM, FTIR and Raman.

The test has shown very interesting properties on the physicochemical proprieties soil where nutrients increased with Biochar application: increase soil moisture and thus increase soil pH and EC values Significantly, as well as the development of soil fertility in terms of organic matter, including an increase in carbon levels, which have opened up a wide field of application especially environmental treatment and agricultural.

Keywords: Biomass; Activated Biochar; Pyrolysis; Environmental treatment; Soil treatment.

Novel electrocatalyst based on silver nanowires modified reduced graphene oxide functionalized with PEDOT/PSS for the efficient quantification of carbofuran pesticide in various samples

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The rapid expansion of the global population, along with intensified urbanization and industrialization, has led to the increased presence of emerging contaminants, particularly pesticides. These compounds are among the most pervasive organic pollutants worldwide due to their persistence, high stability, and water solubility, which contribute to their accumulation in diverse ecosystems [1]. To date, various analytical methods have been applied to detect pesticide residues. Of these, electrochemical techniques have proven to be the most sensitive, reliable, and portable, with the added advantage of being easily miniaturized and integrated, offering greater versatility than other analytical approaches [2]. In this context, a novel electrocatalytic platform based on PEDOT: PSS-functionalized reduced graphene oxide, decorated in-situ with silver nanowires, was developed for the quantification of the pesticide carbofuran in various samples, including water and food. The modification of the screen-printed electrode surface was confirmed using microscopic, spectroscopic, and electrochemical techniques. Pesticide detection was achieved through the electrocatalytic oxidation of the phenolic derivative of carbofuran, generated after its base hydrolysis. The electrochemical findings revealed that the detection platform exhibited a highly sensitive response to the target pesticide, with a detection limit of 4.27 nM. In terms of analytical performance, the sensing platform demonstrated high selectivity, excellent storage stability, and strong repeatability and reproducibility, with a relative standard deviation (RSD) of 3.9%. Moreover, the sensor's applicability was successfully tested in real samples achieving recovery rates of up to 96.8%.

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Investigation of methylene blue Adsorption by Fe_3O_4 Nanoparticles: An Optimization Study Using Response Surface Methodology

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Water coloring has the properties of resistance to mutagenic, toxic, aggressive, destructive, strong light and unstable oxidation and air pollution and has serious effects on environmental systems and human health. Because of its severe toxicity, methylene blue (MB) can cause cancer, mutagenesis, and teratogenic consequences in people as well as enter the food chain [1]. Diverse techniques, specifically membrane filtration, oxidation, ozonation, adsorption, and coagulation, were utilized to remove MB dye from wastewater [2,3]. Adsorption has garnered the greatest study to date on the effective removal of pollutants, mostly by virtue of ist simplicity, afford ability, and superior efficacy. The main objective of this investigation is to study the modelling and the optimization parameters of MB adsorption using a low-cost and Magnetic adsorbent Fe_3O_4. The parameters evaluated for adsorption are the adsorbent dosage, pH, contact time, and temperature using the response surface methodology. The principal variables affecting MB removal were pH (3–11), catalyst dosage (0.01–0.3 g), contact duration (10–180 min), and temperature (25–55 °C). To select an experimental domain, a preliminary study was performed first. The results showed that at pH 10, 1.4 g L^{-1} Fe_3O_4 -nanoparticles (NPs) had the highest removal efficiency of cationic dye MB (20 ppm) from aqueous solutions by batch adsorption technique. The pseudo-second-order (PSO) kinetic models and the Langmuir isotherm provided the best fit for the adoption of MB. To determine the effect of the investigated variables and their interaction on the adsorption process, a Box–Behnken design was used. A second-order polynomial equation was used to model the experimental results. The experimental findings were consistent with the suggested model as demonstrated by the high value of the determination coefficient. The performance of the model equation verified the experimental observation with just a slight divergence, and the values acquired from the experiment and model predictions were found to be in suitable agreement. Ac-cording to the numerical optimization, 98.61 % is the optimal elimination efficiency for MB adsorption. These results suggest that an adsorption process utilizing Fe_3O_4 NPs is efficient in environmental remediation.

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Electrocatalytic oxygen reduction over polypyrrole/iron electrode modified by gold nanoparticle susing electrochemical cementation process

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The slow of the oxygen reduction reaction kinetics in fuel cells has so far limited their commercialization. Moreover, a lot of work has gone into designing a robust catalyst to quicken the reduction reaction kinetics [1, 2]. The application of metal nanoparticle-modified polypyrrole film electrodes for electrocatalysis has generated a lot of interest [1, 3-5]. In the current work, electrochemical cementation process of gold nanoparticles was achieved onto polypyrrole film which had previously been electrodeposited on iron from aqueous solutions of oxalic acid and pyrrole.

Scanning electron microscope (SEM), energy dispersive X-rays (EDX) and X-ray diffraction (XRD) methodswere used for Fe@PPy@Au composite characterization. Better dispersion and smaller particle size are characteristics of the Au nanoparticles supported on the Fe@PPy surface.

Electrochemical cyclic voltammetry tests were used to assess the electroactivity of the Fe@PPy@Au composite toward the oxygen reduction reaction.High electrocatalytic activity was demonstrated by the Fe@PPy@Au in the oxygen reduction reaction. The performance of the Fe@PPy@Au composite electrode is significantly influenced by the thickness of the polypyrrolefilm and the duration time of the electrochemical cementation process.

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ACTIVATED BIOCHAR FOR ANIONIC DYE REMOVAL

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In recent years, numerous studies have investigated the use of biochar to remove organic and inorganic pollutants. Biochar is a carbonaceous material produced primarily from waste biomass through a thermochemical conversion process. This material has been used as a biosorbent in various pollutants removal processes including dyes.
Biochar, as adsorbent, offer a more cost-effective adsorption solution compared to most conventional adsorbents. Adsorption processes provide a cost-effective, easy-to-control and high-quality treatment processes.
The present work investigates the preparation of promising activated Biochar derived from biomass via a pyrolysis process. Our adsorbent was characterized and then used to remove the Azorubine (E112) from wastewater using adsorption technique. The effects of impregnation ratio, amount of adsorbent, pH and contact time on the adsorption activity of biochar on AZ were evaluated.
The obtained products were characterized using different techniques, such as: XRD, FTIR, RAMAN and FESEM in order to determine more precisely their surface chemistry basing on the functional group.

The maximum MB removal efficiency of our biosorbent reached 80 % at 20 ˚C at acide pH and this is due to the activation process efficiency, which has allowed to have a nanoporous structure.

Keywords: Biochar; Pyrolysis; AZ adsorption; Depollution; Wastewater treatment.

Synthesis, characterization and application of ZnO/zeolite X nanocomposite from Tunisian Clay

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Abstract

Nano NaXZeolite was successfully synthesized at low temperature (60 °C)via alkali fusionfollowed by hydrothermal treatmentfrom low-cost natural Tunisia.At optimized synthesis conditions, nano NaX has surfacearea of 358m^2 $g^{-1}$with external surface area of 88.36m^2 $g^{-1}$and average crystal size range between <40– 150nm.Wet impregnation and succeeding thermal treatment at 550◦Cfor ZnO/NaXresulted in a synergistic effect with the zeolite environment forming ZnO/NaX with a bandgap of 2.8 eV, which is lowerthan that of bulk ZnO(3.36 eV).The zeolite played an important rolein the formation of photocatalysts activated by visible energy photons.The antimicrobial activity of NanoZnO/zeoliteX and synthesized Ag supported NaXmatrixwas investigated.Hydrogen sensing behavior of ZnO/zeolite nanocrystals will be studied.

References

Gas detection on polar ZnO surfaces and Graphene/ZnO heterostructure: A DFT Approach

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Our study investigates the gas sensing capabilities of polar surfaces of ZnO and graphene/ZnO heterostructures using Density Functional Theory (DFT). The focus is on the adsorption of graphene on polar surfaces of ZnO and its impact on gas detection performance. Since we found that the O-polar surface of ZnO is more stable than the Zn-polar surface, we examined the adsorption behavior of NH_3 and NO_2 gas molecules, both on the O-polar surface of ZnO and on the Gr/ZnO heterostructure. We analyze the structural and electronic properties of each structure for different adsorption sites.
ZnO's polar surfaces are known for their high sensitivity in gas detection, and the adsorption of graphene improves the electronic properties, leading to improved detection performance.

Enhancing the performance of proton exchange membranes: Incorporating layered double hydroxides into low sulfonated polyether sulfone octyl sulfonamide composite membranes

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An interesting approach was employed to fabricate ion exchange membranes tailored for proton exchange membrane applications. This involved blending low sulfonated polyether sulfone octyl sulfonamide (LSPSO) with Layered Double Hydroxides (LDHs) clay at varying weight ratios (1 wt %, 3 wt %, and 6 wt %). Comprehensive characterization of the resulting composite membranes was conducted using diverse techniques, including Fourier-transform infrared spectroscopy, X-Ray diffraction, scanning electronmicroscopy, and thermogravimetric analysis, to evaluate surface morphology and thermal stability. Notably, the thermal performance of the composite membrane exhibited significant enhancements compared to the pristine LSPSO membrane. The inclusion of 6 wt % LDHs in the composite membrane led to a substantial increase in proton conductivity, rising from 35.04 mS/cm to 143.75 mS/cm at 100 °C. This discovery underscores the potential of the LDHs/LSPSO composite membrane as an electrolyte membrane for high-temperature fuel cell applications.

Keywords: SPESOS, Ion conductivity, Layered Double Hydroxides, Composite membrane, Fuel cells

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Optimization of batch and electrosorption of Cr (VI) from wastewater using Al_2O_3 nanoparticles

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The objective of this study was to apply the technique of electrosorption in order to assess the capacity of heterogeneous adsorption under electricfield. This was to enhance the adsorption capacity of the nanoparticles, to shorten the adsorption time and to reduce the cost of the purification of contaminated waters. A final objective of this study was to compare the free adsorption (FA) and the electrosorption (ES) to understand the interface adsorbent/adsorbate at different contact conditions. For these purposes, a potentially efficient, environment-friendly absorbent was synthesized for dechromation purposes. The experimental design method generated optimum conditions as t_c = 123 min, T = 318 °K and C_0 = 100 mg/L. Freundlich well fitted modeling proved that the adsorption of chromate (VI) on nano-Al_2O_3 occurred on a homogenous surface. In addition, the adsorption coefficient intensity n did not only confirm monolayer adsorption but also indicated a favorable adsorption process. Thermodynamic studies confirmed the reaction spontaneity and the physisorption of the process. The electrosorption process was also tested using 20mA/cm² as applied current density. Free-adsorption (FA) and electrosorption (ES) processes were compared. The maximum recordedyield was 99% for (EA) against 87% for (FA). EDS analysis recorded 11.3% of chromate adsorbate with free adsorption. The amount of Cr (VI) on nano-Al_2O_3 was 42.5 %. Nevertheless, the Al_2O_3nanoparticles lost their crystallinity and exploded after ES process. Mechanisms of both (FA) and (ES) were proposed.

Keywords: Adsorption, Electrosorption, Nano-Al_2O_3, Cr (VI), Isotherms

Cost-Effective Ceratonia Siliqua for Paracetamol Removal: Equilibrium, Regeneration Studies, and Modeling via Box-Behnken Design

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This study examined the use of Ceratonia Siliqua activated (CS-AC) to remove paracetamol (PAR) from aqueous solutions. To investigate the adsorption capacity, isotherm, and kinetic parameters of the adsorption process, batch adsorption experiments were conducted to test the effects of adsorbent dosage, time, pH, initial concentration of paracetamol, and contact time. The morphology and structure of this local adsorbent were performed using different analysis techniques and physicochemical measures, including Fourier transform spectroscopy (FTIR), scanning electron microscopy (SEM), surface area (BET) and point of zero charge (pH_{pzc}). The experimental results may be more accurately described by the Langmuir and pseudo-second order. Additionally, response surface methodology (RSM), which is based on Box–Behnken design (BBD) surface statistical design, was used to investigate the impact of variables on the adsorption of paracetamol. Higher coefficients of correlation and p-value values, by BBD, were in excellent adaption with the ideal combination of process variables, indicating the suitability of the selected model for assessing the experimental data.

Keywords: Ceratonia siliqua L., new adsorbent, Paracetamol, kinetics, isotherms, Modeling, Box-Behnken Design.

Elimination des micropolluants dans les effluents liquides pharmaceutiques par un bio adsorbant

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La quantité de substances pharmacologiquement actives utilisées pour traiter et prévenir les maladies et pour atténuer le stress associé à la vie moderne peut se mesurer en milliers de tonnes par an. Ces produits pharmaceutiques se retrouvent partiellement dans les effluents des stations d'épuration et par suite dans les eaux de surface. De nombreuses recherches sont actuellement menées afin de mettre en œuvre des méthodes appropriées pour l'élimination des produits pharmaceutiques des eaux usées.

Dans l'objectif de l'élimination des polluants pharmaceutiques, un substrat à base de plante (Caroube [1-3]) a été élaboré et caractérisé par : EDX, MEB, BET et FTIR. Le fruit séché est purifié et transformé en poudre selon un protocole bien déterminé. La rétention des micropolluants pharmaceutique sont été réalisée par adsorption sur la poudre de caroube sous deux formes : brute et activée. Une optimisation des paramètres opératoires contrôlant le procédé d'élimination des polluants (pHzéro, pH, temps de contact, vitesse d'agitation, masse d'adsorbant …) a été conduite, l'étude expérimentale d'élimination des micropolluants avec les substrats élaborés a permis de déterminer une efficacité d'élimination de 80 % pour la caroube brute, cette efficacité est améliorée jusqu'à 86% pour la caroube activée. Une étude cinétique a été menée, a révélé que la réaction d'élimination suit la loi du pseudo second ordre et l'étude d'adsorption a montré et que le modèle décrivant le processus d'adsorption est celui de Langmuir.

Les résultats obtenus montrent que la caroube est un bon adsorbant pour l'élimination du paracétamol cette efficacité est meilleure dans son état activé.

Keywords : micropolluants pharmaceutiques, adsorption, caroube.

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Growth and Characterization of Cadmium Carbonate Nanowires

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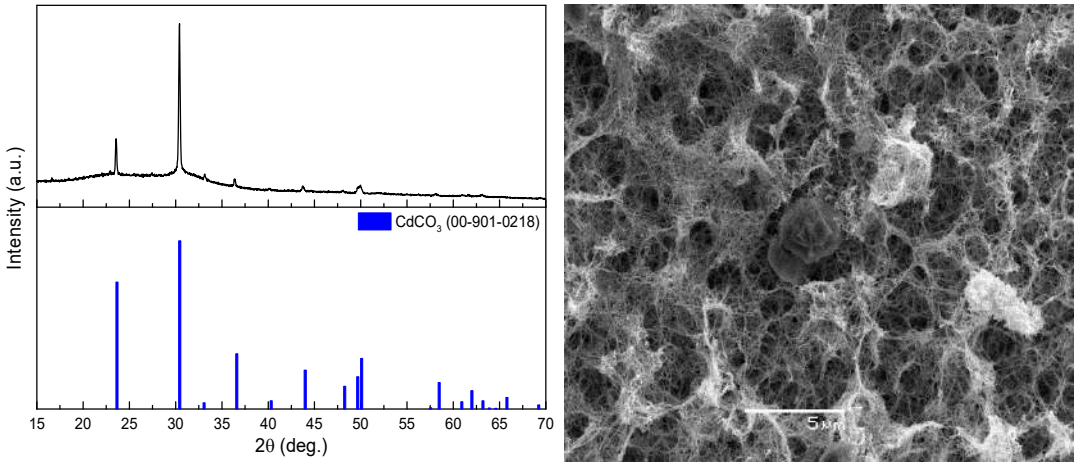
Nanostructured $CdCO_3$ thin films were synthesized via a low-temperature chemical bath deposition process. X-ray diffraction (XRD) confirmed the formation of hexagonal $CdCO_3$, while Scanning Electron Microscopy (SEM) revealed ultralong nanowires with lengths spanning several micrometers and widths of tens of nanometers. Optical characterization showed a band gap energy exceeding 4 eV. The material's synthesis is significant due to its wide range of applications, including the fabrication of cadmium-based films (CdX, X = O, Se, Te) [1-3], photocatalysis [4-5], and hybrid supercapacitors [6]. This highlights the potential of $CdCO_3$ for advanced technological uses.



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Synthesis of a new cement from waste glass powder and hydrated cement

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Abstract:
The cement industry is one of the major sources of pollution in the world. Its enormous activity causes remarkable releases of dust and greenhouse gases having a direct and indirect impact on the environment in all its aspects; the atmosphere, the soil and the human being. In this context, the recovery of waste, including waste glass and hydrated cement, makes it possible to minimize pollution caused by the cement industry.
In this framework, a study was established on the effect of incorporation of fine particle size additions such as glass powder and hydrated cement on the mechanical properties of the mortar produced according to different compositions based on these additions. Cements manufactured with additions make it possible to preserve the non-renewable natural resources necessary for the production of the semi-finished product (clinker) and thus reduce the impact of pollution [1-2].
We have developed new ternary and binary cements by partially replacing the clinker with powders resulting from the grinding of these two wastes (hydrated cement and glass). The substitution rate was from 5% to 40% of the binder mass.
The products obtained as well as the waste underwent several chemical analyzes such as: chemical analysis by XRF,as well as mechanical ones such as: mechanical resistance to compression at 2, 7 and 28 days according to Algerian and European standards [3] in order to test the influence of this waste on the cement paste and its binary and ternary mortar.
The results obtained indicate that it is entirely possible to evaluate these materials and produce a new cement whose mechanical properties are almost similar or superior to those of ordinary cement. Compressive strength at advanced ages is high in the case of ternary cement based on glass powder at a rate of 25% and hydrated cement at a rate of 10%.

Keywords: Glass powder, Hydrated cement, Cement additions, Ternary cement, Carbon footprint, Resistance.

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Structural, morphological, optical and dielectric properties of ZnAl2O4 nanoparticles prepared by sol gel auto-combustion technique

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Abstract

The structural, optical, and dielectric properties of the $ZnAl_2O_4$ nanoparticles synthesized by the sol-gel auto-combustion method have been studied. The X-ray diffraction, FTIR, and Raman analysis confirmed that this compound crystallizes in the cubic structure with a space group $Fd\bar{3}m$. Moreover, the optical properties were characterized by UV-Vis diffuse reflectance. The band gap value, in the range of 3.9 eV, indicates a semiconductor character of our compound, making it useful for photoelectronic devices. Later, the dielectric permittivity and dielectric loss are measured. We found that the $ZnAl_2O_4$ nanoparticle have a high permittivity at room temperature and a very low dielectric loss. These results offer the possibility of a nanoelectronic application using this high performance.

Keywords: nanoparticles, sol-gel auto-combustion, Raman spectroscopy, X-ray diffraction, dielectric permittivity.

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