The 2025 2nd International Conference on Materials Sciences and Mechatronics for Sustainable Energy and the Environment

المؤتمر الدولي الثاني لعلوم المواد والميكاترونيات من أجل الطاقة المستدامة والبيئة 2025

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Conference Chairman's: Younes Ziat and Yassine Lakhal **رؤساء المؤتمر:** يونس زيات وياسين لكحل

Guest editors

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Higher School of Technology, Sultan Moulay Slimane University
October 1-2, 2025 at Béni-Mellal, Morocco

المدرسة العليا للتكنولوجيا، جامعة السلطان مولاي سليمان
أكتوبر 2025 في بني ملال، المغرب 1-2

Preface

We are pleased to announce the outstanding success of the **2nd International Conference on Materials Sciences and Mechatronics for Sustainable Energy and the Environment (MSMS2E 2025)**, held from **October 1 to 2, 2025**, at the **Higher School of Technology, Beni Mellal, Morocco**. The event was organized by the **Engineering and Applied Physics Team (EAPT)** and the **Moroccan Association of Science and Technology for Sustainable Development (MASTSD)**, in collaboration with **Sultan Moulay Slimane University, the Journal of "*Solar Energy and Sustainable Development*", "*E3S Web of Conferences*", and the Libyan Center for Research and Studies in Solar Energy**.

This prestigious scientific gathering brought together leading researchers and international experts to discuss the latest advancements in **materials sciences and mechatronics**, focusing on **innovative solutions for sustainable energy and environmental challenges**. The conference featured enriching scientific sessions, including **keynote lectures, research presentations, and specialized workshops**, providing valuable opportunities for collaboration and knowledge exchange.

We extend our heartfelt gratitude to all the researchers for their valuable contributions, as well as to the **reviewers, session chairs, and committee members** for their dedicated efforts. A special thanks to our **sponsors and partners** for their support, which played a crucial role in the success of this significant scientific event.

We are also pleased to announce that the **proceedings of MSMS2E 2025 have been officially published in *E3S Web of Conferences* and "*Solar Energy and Sustainable Development*"**, ensuring broad visibility and accessibility to the high-quality research presented during the event.

We also express our deep appreciation to **the conference chairs, Professor Younes Ziat and Professor Yassine Lakhal**, for their outstanding leadership and invaluable contributions, which were instrumental in the organization and success of this international conference.

MSMS2E 2025 has been a remarkable opportunity to foster **scientific collaboration and expand research horizons** in the fields of sustainable energy and mechatronics. We hope that such initiatives will continue to promote knowledge exchange and contribute to the development of sustainable solutions for a brighter future.

We look forward to seeing you at the next editions of the conference

مقدمة

يسرنا أن نعلن عن النجاح الباهر للمؤتمر الدولي **الثاني لعلوم المواد والميكاترونيكس للطاقة المستدامة والبيئة(MSMS2E 2025)** ، الذي نُظم من 1 إلى 2 أكتوبر 2025 في المدرسة العليا للتكنولوجيا، بني ملال، المغرب، تحت إشراف **فريق الهندسة والفيزياء التطبيقية (EAPT) والجمعية المغربية للعلوم والتقنيات من أجل التنمية المستدامة(MASTSD)** ، وبالتعاون مع **جامعة مولاي سليمان، مجلة *الطاقة الشمسية والتنمية المستدامة*، E3S Web of Conferences, والمركز الليبي للبحوث والدراسات في الطاقة الشمسية**.

لقد جمع هذا الحدث العلمي المتميز نخبة من الباحثين والخبراء الدوليين لمناقشة أحدث التطورات في علوم المواد والميكاترونيكس، مع التركيز على الحلول المبتكرة للطاقة المستدامة والتحديات البيئية. شهد المؤتمر جلسات علمية ثرية تضمنت محاضرات رئيسية، عروض بحثية، وورش عمل متخصصة، مما أتاح فرصًا مثمرة للتعاون وتبادل الأفكار بين المشاركين.

كما يسعدنا الإعلان عن أن **أعمال المؤتمر (MSMS2E 2025) قد تم نشرها رسميًا في *E3S Web of Conferences* ومجلة الطاقة الشمسية والتنمية المستدامة(*Solar Energy and Sustainable Development*)** ، مما يضمن انتشارًا واسعًا وإتاحة البحوث عالية الجودة التي تم تقديمها خلال الحدث.

نود أن نعرب عن خالص شكرنا وتقديرنا لجميع الباحثين الذين قدموا مساهماتهم القيمة، وللمراجعين ورؤساء الجلسات وأعضاء اللجان على جهودهم المبذولة. كما نشكر الرعاة والشركاء على دعمهم الذي ساهم في نجاح هذا الحدث العلمي الهام.

كما نعبر عن امتناننا العميق **لرؤساء المؤتمر: البروفيسور يونس زيات والبروفيسور ياسين لكحل** على قيادتهم الحكيمة وإسهاماتهم القيمة التي كانت أساسية في تنظيم وإنجاح هذا المؤتمر الدولي.

لقد كان **MSMS2E 2025** فرصة مميزة لتعزيز التعاون العلمي وتوسيع آفاق البحث في مجالات الطاقة المستدامة والميكاترونيكس. نأمل أن تستمر هذه المبادرات في تعزيز التبادل المعرفي والمساهمة في إيجاد حلول مستدامة لمستقبل أكثر إشراقًا.

نتطلع إلى لقائكم في النسخ القادمة من المؤتمر

The 2025 2nd International Conference on Materials Sciences and Mechatronics for Sustainable Energy and the Environment

MSMS2E 2025

BENI MELLAL, MOROCCO

1-2 OCTOBER 2025

OBJECTIVES OF MSMS2E 2025:

The 2025 2nd International Conference on Materials Sciences and Mechatronics for Sustainable Energy and the Environment (MSMS2E 2025) will be held on October 1-2 in Beni-Mellal, Morocco. MSMS2E 2025 is to bring together innovative academics and industrial experts in the fields of energy, mechatronics, embedded systems, environment, and materials science in a common forum

TOPICS:

- **Photovoltaic and grid**
- **Solar collector and exchangers**
- **Semiconductors and thin films for photovoltaic**
- **DFT for Semiconductor Energy Applications**
- **DFT for Photocatalysts, Catalysts, and optic**
- **Wind Energy Engineering**
- **Electric and Hybrid Vehicles**
- **Smart Grid**
- **Batteries**
- **Biomass Energy Engineering**
- **Hydrogen storage technology**
- **Enegy Conversion and Power Systems Control**
- **Energy and smart cities**
- **Solar Energy Engineering**
- **Energy and sustainable development**
- **Energy and environment**
- **Energy storage Technology**

IMPORTANT DATES:

- **March 26, 2025:** Registration and Abstract Submission / Paper Submission
- **June 06, 2025:** Deadline for Registration / Deadline of Paper Submission
- **June 08, 2025:** Notification of Abstract Acceptance
- **June 17, 2025:** Payment Deadline for Registration
- **available soon :** Final Program
- **October 01, 2025**: Conference Start

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Theoretical and Measured PV System Output Using High-Resolution Data: Analysis and Comparative Performance

Nabeel I. Tawalbeh[1], and Sadeq A. Hamed[1]

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Abstract. This paper presents a high-resolution comparative performance analysis of a dual-layout photovoltaic (PV) system installed at the University of Jordan – Aqaba Branch. The system comprises a Car Park array and a Ground-Mounted array. AC power monitoring is conducted through five-minute interval basis across multiple seasons in 2023. A cosine-squared model was employed to simulate ideal clear-sky output based on actual sunrise and sunset times. Inverter data were filtered using a 12-point moving average to reveal daily trends and mitigate transient irradiance noise. Results demonstrate that the Ground-Mounted system consistently outperformed the Car Park configuration, particularly under low-sun-angle or diffuse-light conditions, with efficiency differences reaching up to 30%. Additionally, the analysis quantified the overestimation of energy in raw data, showing that daily energy can be inflated by nearly 9% if smoothing is not applied. These findings highlight the importance of combining theoretical modeling with high-resolution measurements to better interpret system performance, inform design decisions, and optimize operation under varying environmental conditions.

Keywords: Photovoltiac systems; High-resolution monitoring; Inverter performance; Specific yield; System efficiency; Cosine model; Shading.

Evaluating the Effects of Marine Oil Pollution on Oysters: A Laboratory Study on Ecosystem and Aquaculture Implications

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Abstract: The contamination of oysters by marine oils is a major environmental and food safety concern. As part of a laboratory-scale experiment conducted at the Institute of Fisheries and Marine Sciences (ISPM), the aim is to analyze the impact of hydrocarbons, particularly marine oils, on oysters and understand their accumulation in the tissues of these filter-feeding mollusks. Marine oils, often originating from spills linked to petroleum and maritime activities, end up in coastal waters where oysters absorb pollutants while filtering the water. In this context, laboratory experiments are conducted by exposing oysters to specific concentrations of marine oils. The monitored parameters include the concentration of hydrocarbons in the oyster tissues, their growth rate, filtration efficiency, and reproductive impact. The results show that exposure to hydrocarbons impairs the biological functions of oysters, reducing their filtration efficiency and their ability to feed properly. Hydrocarbons, particularly polycyclic aromatic compounds (PACs), accumulate in internal organs, affecting the health of the mollusks and increasing the risks of bioaccumulation along the marine food chain. Furthermore, the tests highlight the indirect environmental impact of contamination. The accumulation of marine oils in the water disrupts marine ecosystems by reducing water oxygenation and affecting biodiversity, including phytoplankton species essential to the food chain. These results emphasize the need to strengthen risk management measures related to marine oil spills and explore sustainable energy solutions to reduce marine ecosystem pollution, protect oysters, and ensure the safety of aquaculture products.

Keywords: Oyster contamination; Marine oils; Hydrocarbons;Aquaculture;Marine pollution.

Effect of Barrier Thickness and Temperature on Binding energy, Spin Polaronic Shift and Diamagnetic Susceptibility of Magnetic Impurity Confined in Semimagnetic Double Quantum Well

Hamza Azmi[1], Abdelghani Fakkahi[1], Amine Mazouz[1], Kamal El-Bakkari[1], Mohammed Jaouane[1], Reda Arraoui[1], Ayoub Ed-Dahmouny[2] Ahmed Sali[1]

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Abstract. The development of spintronic technologies has spurred considerable interest in understanding the thermal behavior of magnetic nanostructures, where the interplay between charge and spin degrees of freedom plays a critical role. This study aims to investigate the influence of temperature on key physical parameters namely the binding energy, spin polaronic shift, and diamagnetic susceptibility in a semimagnetic double quantum well (DQW) nanostructure. Utilizing a variational approach within the effective mass approximation, the analysis focuses on the thermal response of an electron bound to a hydrogenic impurity in a magnetically doped quantum system. The results reveal that as temperature increases, both the binding energy and diamagnetic susceptibility exhibit a noticeable reduction, attributed to the increase of the distance between the electron and the magnetic impurity induced by the decrement of quantum confinement effect. Furthermore, elevated temperatures lead to a disruption of spin alignment, reflected in the diminishing spin polaronic shift, indicating increased spin disorder. Additionally, it is found that increasing the barrier thickness of the DQW enhances the quantum confinement effect, resulting in a rise in binding energy, spin polaronic shift, and diamagnetic susceptibility. These findings provide insight into the thermally induced modifications of spin-dependent interactions and suggest a temperature-tunable control of magnetic and electronic properties. The conclusions underscore the relevance of this study to emerging spintronic devices, particularly in the optimization of components such as spin field-effect transistors, spin light-emitting diodes, and magnetic random-access memory (MRAM), where precise control over spin and charge dynamics is essential.

Keywords: Binding energy; Diamagnetic susceptibility; Semimagnetic double quantum well, Spin polaronic shift; Temperature

High-performance optimization and analysis of $Cs_2CuSbCl_6$-Based lead-free double perovskite solar cells with theoretical efficiency exceeding 27 %

Hicham Elassib[1]

[1]*UM5R, Rabat, MOROCCO*

Abstract. The primary challenges in photovoltaic solar energy include toxicity, stability, and the cost of solar cells. To address these issues, we propose the use of noble metal halide double perovskites, which are lead-free. CUS2CuSbCl6 stands out as a popular absorber due to its huge bandgap, high absorption coefficient, and affordable price. Our research analyzes and simulates solar cells with $Cs_2CuSbCl_6$ as the absorber material, utilizing SCAPS-1D software. Along with AZnO for the electron transport layer (ETL), we assess the material's stability and suggest less expensive substitutes for hole transport materials (HTLs) such MoO_3, Spiro-OMeTAD, MoO_3, NiO, Cu_2O, and CuSCN. Our goal is to find the ideal values for important photovoltaic parameters to increase the efficiency of the suggested solar cells. This entails examining how the thickness, temperature, and doping level affect the properties of the solar cell. Furthermore, numerous feasible back electrodes are investigated and their impact on performance is assessed to replace the pricey gold (Au) electrode. We discovered that the optimal configuration for $Cs_2CuSbCl_6$ is C (metal back contact)/MoO_3 (HTM)/$Cs_2CuSbCl_6$ (Absorber)/AZnO (ETM)/FTO, resulting in 300 K performance. PCE: 27.56%, Voc: 1.47 V, Jsc: 20.66 mA/cm2, and FF 89.83%.

MSMS2E 2025, October 1-2
Higher School of Technology, Sultan Moulay Slimane University, Beni Mellal, Morocco
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المدرسة العليا للتكنولوجيا، جامعة السلطان مولاي سليمان

Investigation of the chromium crystal field effect on the magnetic properties of the Sr_2CrWO_6 double perovskite: A Monte Carlo simulation

Mariam El Hamri[1], Omar El Rhazouani[2], El Bouazzaoui Choubabi[1], Fatima Majid[3], Abderrahmane Elmelouky[1]

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Abstract. The chromium-based double perovskite Sr_2CrWO_6 has attracted considerable attention from researchers because of its high critical temperature, half metallic behavior, high degree of spin polarization and low resistivity. These interesting properties make from it an interesting candidate for spintronic applications and room-temperature magnetoelectronic devices. Furthermore, the compound crystallizes in a cubic cell and has two magnetic sublattices, one occupied by chromium and the other occupied by tungsten. In this paper, the chromium crystal field influence on the magnetic and thermodynamic properties of the Sr_2CrWO_6 double perovskite has been studied by using Monte Carlo simulation within the framework of the Ising model. Interesting results have been found, such as the appearance of one compensation temperature below the transition one. Moreover, the chromium crystal field influences the compensation temperature, while the critical temperature shows less sensitivity to the chromium crystal field variation.

Keywords: The magnetic and thermodynamic properties; the Sr_2CrWO_6 double perovskite; Monte Carlo simulation; The chromium crystal field

Optimization of quaternary compound kesterite Cu2ZnSnS4 (CZTS) optical band gap using dip-coating for photovoltaic absorbers

Marius Armand Amou [1,2] ,Bouchaib Hartiti [1],Ahmed Ziti [1],Fransisco Kouadio Konan [1,2,3] ,Abdelkrim Batan [1,4], Youssef Doubi[1] Hicham Labrim[1,5] ,Boko Aka [2],Philippe thevenin[6]

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Abstract. This study focuses on the synthesis of Cu_2ZnSnS_4 (CZTS) thin films, a promising material for photovoltaic absorbers, using the sol-gel method combined with dip-coating technique, and optimized through a Taguchi design of experiments. Six factors were investigated (annealing temperature and time, dip-coating speed, solvent type, copper concentration, sulfur-to-metal ratio), each at three levels, according to a L27 orthogonal array. Analysis of the results, based on the signal-to-noise (S/N) ratio and analysis of variance (ANOVA), highlighted the predominant influence of annealing time, followed by annealing temperature and dip-coating speed, on the optical band gap energy (Eg). The optimal configuration (A3B3C1D1E3F1) yielded a band gap of 1.5 eV, which is ideal for thin-film solar cell applications. Structural (XRD, Raman), morphological (SEM), optical (UV-Vis, Tauc), electrical (four-point probe), and chemical (EDS) characterizations confirmed the formation of a pure CZTS phase, free from secondary phases, with good crystallinity, high absorption ($\alpha > 10^4$ cm^{-1}), and suitable conductivity ($\sigma \approx 13.61$ S/cm). These results demonstrate the relevance of the adopted approach for the fabrication of high-performance CZTS thin films, compatible with the requirements of photovoltaic devices. By this method, the optical band gap was adjusted to the optimal 1.5 eV, ensuring better light absorption.

Keywords: CZTS, sol-gel, dip-coating, Taguchi, thin films, photovoltaics.

Non-linear modeling and comparative analysis of damage mechanisms in Acrylonitrile Butadiene Styrene (ABS): approaches by stresses and residual ultimate energies

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Abstract. This study presents an in-depth comparative analysis of damage assessment methodologies in Acrylonitrile Butadiene Styrene (ABS) subjected to mechanical stresses. The research compares three distinct approaches: evaluation by residual ultimate stresses, by residual ultimate energies, and by applying the unified damage theory. Specimens with a combined defect (hole with notches of varying lengths) were subjected to standardized static tests to characterize the progressive evolution of damage. Analysis of damage-reliability curves identified three characteristic phases in the degradation process: initiation (up to $\beta \approx 0.20$), progressive propagation (up to $\beta \approx 0.70$), and rapid acceleration leading to failure. The results show a remarkable agreement between the methods based on stresses and residual energies, with deviations not exceeding 5% in identifying critical life fractions. This convergence validates the robustness of the proposed models to describe the non-linearity of damage in thermoplastic polymers, thus overcoming the limitations of Miner's linear rule. This research significantly contributes to the understanding of the physical mechanisms governing damage in polymer materials and offers an enhanced analytical framework for predicting the residual life of structural components with defects.

Keywords: Non-linear modeling, Damage mechanisms, Acrylonitrile Butadiene Styrene (ABS), Mechanical stresses

The Impact of Marine Oil Contamination on Oysters

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Abstract. The contamination of oysters by marine oils is a major environmental and food safety concern. As part of a laboratory-scale experiment conducted at the Institute of Fisheries and Marine Sciences (ISPM), the aim is to analyze the impact of hydrocarbons, particularly marine oils, on oysters and understand their accumulation in the tissues of these filter-feeding mollusks. Marine oils, often originating from spills linked to petroleum and maritime activities, end up in coastal waters where oysters absorb pollutants while filtering the water. In this context, laboratory experiments are conducted by exposing oysters to specific concentrations of marine oils. The monitored parameters include the concentration of hydrocarbons in the oyster tissues, their growth rate, filtration efficiency, and reproductive impact. The results show that exposure to hydrocarbons impairs the biological functions of oysters, reducing their filtration efficiency and their ability to feed properly. Hydrocarbons, particularly polycyclic aromatic compounds (PACs), accumulate in internal organs, affecting the health of the mollusks and increasing the risks of bioaccumulation along the marine food chain. Furthermore, the tests highlight the indirect environmental impact of contamination. The accumulation of marine oils in the water disrupts marine ecosystems by reducing water oxygenation and affecting biodiversity, including phytoplankton species essential to the food chain. These results emphasize the need to strengthen risk management measures related to marine oil spills and explore sustainable energy solutions to reduce marine ecosystem pollution, protect oysters, and ensure the safety of aquaculture products.

Keywords: Oyster contamination; Marine oils; Hydrocarbons;Aquaculture;Marine pollution.

Exploring the Optoelectronic and Photocatalytic Properties of $SrMg_2FeH_8$ for Advanced Energy Applications

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Abstract. $SrMg_2FeH_8$ is a novel hydride material with promising optoelectronic and photocatalytic properties, making it a potential candidate for advanced energy and environmental applications. In this study, the electronic structure was analyzed using the density of states (DOS) and projected density of states (PDOS), revealing a semiconducting nature with a moderate energy gap of 2.251 eV. This bandgap enables effective absorption of visible light, which is crucial for photocatalysis. Optical investigations, including refractive index, extinction coefficient, and absorption behavior, demonstrate the material's strong interaction with light in the visible and ultraviolet ranges, further supporting its potential in optoelectronic devices. The photocatalytic performance of $SrMg_2FeH_8$ was examined, emphasizing its ability to drive oxidation and reduction reactions. The valence band edge, positioned at 2.61 eV versus the normal hydrogen electrode (NHE), is well-suited for water oxidation. Although the conduction band edge at 0.36 eV facilitates hydrogen evolution, kinetic limitations suggest the need for co-catalysts to enhance efficiency. The material's robust optical absorption, coupled with its electronic and photocatalytic characteristics, underscores its versatility for hydrogen production, pollutant degradation, and energy conversion technologies.

Keywords: optoelectronic properties; photocatalytic properties; hydrogen production; semiconducting nature; hydride material.

Analysis of the influence of misalignment defects on the vibrational characteristics of drive systems equipped with different types of couplings (elastic and rigid)

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Abstract. This study looks at how misalignment defects affect the vibration behavior of drive systems using different types of couplings. It focuses on Rotex GS elastic couplings and rigid flange couplings. The results show a clear difference between vertical and horizontal vibration responses. For elastic couplings, each stiffness level has its own unique vibration pattern, while with rigid couplings, misalignment causes distinct spectral signatures. These insights help us make better recommendations for predictive maintenance and emphasize the need to monitor vibrations in both directions.

Keywords: Vibrational behavior, Rotex GS elastic couplings, Rigid flange couplings, Anisotropy vibration, Vibrational behavior, Mechanical faults

Effects of *Dactylogyrus* spp. Co-infection on Mortality in Two *Oreochromis niloticus* Strains and Evaluation of Potassium Permanganate Treatment Efficacy for Sustainable Aquaculture Development

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Abstract. This study investigates the impact of *Dactylogyrus* spp. co-infection on mortality rates in two strains of Nile tilapia (*Oreochromis niloticus*), the gray and red strains, under controlled aquaculture conditions. Over a seven-month period, 65 juveniles of each strain were monitored for growth performance, survival rate, and parasitic infection levels. Results show that the red strain significantly outperforms the gray strain in both growth (83.8 g vs. 51.3 g final weight) and survival (97% vs. 70%), primarily due to its higher resistance to *Dactylogyrus* spp. infections and environmental stressors. Treatment efficacy of potassium permanganate ($KMnO_4$) was evaluated and demonstrated rapid reduction in parasite load, improving fish health. This research highlights the importance of strain selection and effective parasite management to enhance productivity and sustainability in tilapia aquaculture, contributing to Sustainable Energy and the Environment.

Keywords: Sustainable aquaculture; Sustainable energy and environment; Co-infection; Mortality rates; Nile tilapia.

Effect of incidence angle and annealing on the structural properties of TiNi thin films: A molecular dynamics simulation study

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Abstract. TiNi thin film is now the most commonly used shape memory alloy (SMA) in various industrial and medical fields. To produce high-quality films, a thorough understanding of its growth mechanism is essential. However, experimental characterization techniques cannot analyse this process with sufficient precision. The use of advanced simulation methods, such as molecular dynamics (MD), is an effective approach for overcoming this limitation. In this study, we explored the growth of TiNi films at the atomic scale by applying the molecular dynamics method. The simulation results indicate that for low incidence energies (0.1 and 1 eV), the surface morphology of thin films becomes rougher with increasing incidence angle. In contrast, for higher incidence energies (10 and 15 eV), the surface roughness remains largely unaffected by the incidence angle up to 45°. The average stress increases significantly between 15 and 45°, this is associated with the increase in size of the voids and vacancies formed on the film surface.

Keywords: TiNi thin film; Molecular dynamics; Surface roughness; Interface mixing; atomic stress; Incident energy

A Biodegradable Allantoin-Cobalt Catalyst for Environmentally Friendly Quinazolinone Synthesis

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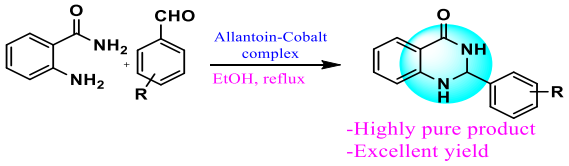
Abstract. Allantoin, widely recognized for its regenerative and soothing effects in dermatology, is emerging as a promising component in sustainable catalytic design. In this work, we introduce a novel allantoin-cobalt complex that serves as a highly effective and environmentally benign catalyst for green synthetic applications. This complex promotes the formation of nitrogen-containing bioactive heterocycles under mild, eco-friendly conditions, fully aligned with green chemistry principles. With increasing interest in biodegradable materials and sustainable cosmetic actives, this catalyst opens new possibilities for integrating allantoin's dermatological benefits into catalytic systems. By merging the fields of catalysis and cosmetic science, this approach offers an innovative path toward the synthesis of eco-conscious ingredients with dual functionality.



Scheme 1. *Cyclocondensation Pathway for the Synthesis of 2,3-Dihydroquinazolin-4(1H)-one*

The catalytic efficiency of the synthesized allantoin–cobalt complex was thoroughly investigated through its application in cyclocondensation reactions under a range of conditions. The results reveal that the catalyst delivers exceptional performance in terms of both activity and selectivity, positioning it as a promising green alternative for the synthesis of quinazolinone derivatives. This study highlights the value of incorporating allantoin into cobalt-based catalytic frameworks, contributing to environmentally responsible chemistry and the development of biodegradable systems. Overall, these findings open new directions for the creation of innovative, nature-inspired catalytic platforms that align with sustainable synthesis principles.

Keywords: Allantoin-based catalyst, cobalt complex, quinazolinone derivatives, green chemistry, biodegradable materials, sustainable synthesis

Heat Transfer Fluids for Concentrated Solar Power: A Comprehensive Bibliometric Analysis

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Abstract. Solar energy has emerged as a sustainable alternative to fossil fuels, addressing the growing global demand for clean and renewable energy sources. Among the various solar technologies, Concentrated Solar Power (CSP) systems play a pivotal role in large-scale electricity generation by utilizing mirrors to concentrate sunlight onto a receiver. One of the critical components of CSP systems is the Heat Transfer Fluid (HTF), which is responsible for efficiently transporting and storing thermal energy. The performance of HTFs significantly impacts the efficiency and feasibility of CSP plants, making research in this area crucial. Various HTF types, including synthetic oils, molten salts, nanofluids, and phase change materials (PCMs), have been investigated to enhance heat transfer efficiency, thermal stability, and energy storage capacity. Understanding the research landscape in this field is crucial for identifying emerging trends and directing future advancements. This study presents a comprehensive bibliometric analysis of HTF research in CSP applications. Using an automated search on the Scopus digital library, we compiled a dataset of 4055 scientific publications from 2000 to 2024. The analysis focuses on five key bibliometric indicators: descriptive statistics, author productivity, source productivity, scientific collaboration, and keyword analysis. The findings highlight major research trends, influential publications, and emerging topics, including advancements in nanofluids, molten salts, and phase change materials (PCMs).

An Overview of Silicone-Based Heat Transfer Fluids in Concentrated Solar Power Systems

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Abstract. This paper investigates the potential of silicone-based heat transfer fluids (HTFs) for use in Concentrated Solar Power (CSP) systems. These fluids, primarily composed of polymethylsiloxanes, offer significant advantages over traditional organic oils and molten salts, including superior thermal stability (up to 425–450 °C), low viscosity, chemical inertness, and reduced environmental impact. Commercial products such as HELISOL® 5A and SYLTHERM™ 800 demonstrate excellent performance in long-term stability tests and real-world CSP applications, with reduced degradation and maintenance requirements. Case studies and simulation models confirm improved efficiency and lower levelized cost of electricity (LCOE) when silicone fluid replace conventional HTF. Although initial costs remain higher, their operational reliability and safety make them attractive for next-generation solar thermal systems. This study concludes that silicone-based HTF is an excellent substitute for CSP applications and suggests more investigation into long-term deploymentt, recycling strategies, and performance optimization across various climatic and industrial contexts.

Current Flow Mechanisms and Photoelectric Properties of Solar Cells Based on p-CdTe-n-CdS and p-CdTe-n-CdSe Heterostructures with Deep Impurity Levels

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Abstract. In this paper, we consider the mechanisms of the flow current and photoelectric properties of solar cells manufactured on the basis of strongly mismatched semiconductor p-CdTe-n-CdS and p-CdTe-n-CdSe heterojunctions with a low density of surface states $N=3\cdot10^{11}sm^{-2}$. It was found that the forward current in heterojunctions is due to tunneling of thermally excited electrons, and at large forward biased currents, thermionic nature. The reverse current of such structures has a tunneling nature. It is shown that the structures have a photoconversion efficiency of 0.7÷0.8 el/sq in the spectral region of 0.4÷3.0 eV in the near-infrared region of the spectrum.

Keywords: heterojunction, heterostructure, photovoltaic, coefficient, Volt-pharadic

Elaboration and Characterization of Pure and Zn-Doped V_2O_5 Thin Films by Spray Pyrolysis for Photovoltaic and Optoelectronic Applications

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Abstract. In this study, pure and Zn-doped (2% and 4%) vanadium pentoxide (V_2O_5) thin films were successfully fabricated using the spray pyrolysis technique. The objective is to optimize their physical properties for potential applications in photovoltaic and optoelectronic devices. The structural properties were investigated using X-ray diffraction (XRD), confirming the formation of a well-crystallized orthorhombic phase. Surface morphology was examined by scanning electron microscopy (SEM), revealing homogeneous and compact film structures. Optical properties were studied using diffuse reflectance spectroscopy (DRS), showing a tunable optical bandgap depending on the Zn doping level. Electrical properties were evaluated using the four-point probe method and Mott-Schottky analysis, allowing assessment of the films' conductivity and semiconducting behavior. The results demonstrate that Zn doping significantly influences the structural, optical, and electrical characteristics of V_2O_5 thin films, highlighting their potential for integration into solar energy conversion and optoelectronic systems.

Keywords: V_2O_5 thin films, Zn doping, spray pyrolysis, structural properties, optical properties, electrical characterization, XRD, SEM, DRS, Mott-Schottky, photovoltaic applications, optoelectronics.

First-Principles Investigation of the Dual Thermoelectric and Hydrogen Storage Potential of Perovskite Hydrides

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Abstract. This work explores, via first-principles calculations based on density functional theory (DFT), the multifunctional properties of perovskite hydrides as promising candidates for next-generation energy applications. In particular, we investigate the interplay between electronic structure, lattice dynamics, and thermodynamic stability to evaluate their potential for both thermoelectric energy conversion and hydrogen storage. The electronic band structure and density of states reveal tunable semiconducting behavior, which is crucial for optimizing the Seebeck coefficient and electrical conductivity. Phonon dispersion calculations confirm the dynamical stability of the studied compounds, while also indicating low lattice thermal conductivity, a key requirement for efficient thermoelectric performance. In parallel, hydrogen adsorption and storage properties are assessed through binding energy calculations and structural analysis, showing favorable interaction strengths that ensure both reversibility and stability. The coupling between hydrogen incorporation and electronic transport properties is also discussed. Overall, this study highlights perovskite hydrides as dual-functional materials, combining efficient thermoelectric response with viable hydrogen storage capability, making them strong candidates for sustainable energy technologies.

***Keywords*:** Perovskite hydrides; Density functional theory; Thermoelectric materials; Hydrogen storage; Electronic structure

Optoelectronic Properties of Zr/Te Co-Doped $MgTiO_3$: A DFT Study for Photovoltaic Applications

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Abstract. This study employs DFT with GGA and mBJ potential to investigate the structural, electronic, and optical properties of Zr/Te codoped $MgTiO_3$ perovskites. Structural optimization indicates that both pure and codoped $MgTiO_3$ exhibit negative formation energies, confirming their stability. According to optoelectronic analyses, codoped materials with a direct band gap absorb more visible light and have higher optical conductivity, making them appropriate for visible light-driven photocatalysis, in contrast to undoped $MgTiO_3$, which has an indirect band gap and absorbs only UV light. The enhanced visible-light absorption of these co-doped materials suggests their suitability for renewable energy applications, particularly in photovoltaic and optoelectronic devices.

Keywords: Zr/Te codoped MgTiO3; DFT; Band structure; electronic structure and optical properties

Power Management in a PV-Battery Microgrid Grid Connected Using Hybrid ANFIS-Fuzzy Logic MPPT Control and an Adaptive Charge-Discharge Algorithm

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Abstract. This work presents an energy management strategy (EMS) for a microgrid that integrates photovoltaic (PV) panels, a battery energy storage system (BESS), and a grid connection. The primary objective is to maintain a dynamic and reliable power balance between PV generation, local load, BESS, and the grid, while maximizing the self-consumption of solar energy. The system architecture comprises a PV generator whose power is optimized by a hybrid Maximum Power Point Tracking (MPPT) algorithm based on the integration of an Adaptive Neuro-Fuzzy Inference System (ANFIS) and a fuzzy controller, acting as a PI regulator, which is used to optimize the operating point of the panels, even under variable sunlight conditions (uniform or partial shading). The BESS made up of Lithium-ion batteries, is managed by a bi-directional DC-DC converter and a fuzzy PI controller, which ensures fine, adaptive regulation of power flows. The core of the innovation lies in the battery management algorithm, which relies on a set of explicit rules to direct power flows. These rules include a strict 10 kW constraint on battery charging and discharging power, crucial for preserving battery life and system safety. The system was simulated considering various cases of irradiance profiles and charging demands of 35 kW and 55 kW, including normal and critical battery state-of-charge (SOC) situations. The simulation results demonstrate the success of the ANFIS-Fuzzy Logic (FL) MPPT control in maximizing energy capture and the effectiveness of the battery management algorithm in precisely controlling charging and discharging power while ensuring a robust and reliable energy balance between PV, battery, load, and grid. These results confirm the algorithm's ability to handle critical high and low SOC situations, intelligently redirecting power flows to maintain microgrid stability and power continuity.

Keywords: ANFIS; Battery; Fuzzy logic; Microgrid; PV

Comparative study of the physical properties of $InGeF_3$ and $InGeCl_3$ materials for efficient photovoltaic

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Abstract. The characteristics of ABX_3 perovskites were investigated and evaluated in this work. To do this, two halogenated perovskites, were compared. Although both $KGeF_3$ and $InGeCl_3$ have a cubic structure, their lattice parameters are different ; $InGeF_3$ (4.48 Å) is more compact than InGeCl (5.32 Å), which may have an impact on the mobility of charge carriers. With regard to the band gap, for example, InGeF favors superior light absorption due to its indirect band gap (1.51 eV) and InGeCl direct band gap (1.03 eV). Because of this distinction, InGeCl exhibits greater optoelectronic performance, rendering it more appropriate for use in photovoltaic applications. In conclusion, although being members of the same family, InGeCl performs better because of its straight band gap and higher absorption.

Keywords *— Absorption, Optoelectronics, Perovskites , Photovoltaic applications.*

Kinetic and Thermodynamic Insights into Dye Adsorption from Water Using Mechanically Modified Biochar

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Abstract. The growing need for eco-friendly and effective methods to eliminate organic pollutants, particularly synthetic dyes, has intensified interest in biochar-based adsorbents. In this work, we developed a high-performance adsorbent by modifying sugarcane bagasse-derived biochar through hydrogen peroxide (H_2O_2) treatment followed by mechanical activation. The adsorption efficiency of this engineered biochar was evaluated using methylene blue (MB) as a model dye. Key operational parameters: such as pH, adsorbent dosage, contact time, initial dye concentration, and temperature, were systematically studied. The adsorption behavior was further analyzed using kinetic and isotherm models to better understand the mechanisms involved. Our results demonstrated that mechanical treatment significantly enhanced the adsorption properties of the biochar, achieving a maximum capacity of 390 mg/g and a removal efficiency of 99.93% at 100 ppm MB. These improvements were mainly attributed to increased surface area, porosity, and functional group availability after treatment. In addition, the material showed excellent reusability, maintaining 87% of its initial capacity after five adsorption–desorption cycles, confirming its potential for practical application in wastewater treatment.

Keywords: Adsorption; Biochar; Isotherms; Kinetics; Mechanical Treatment; Thermodynamics.

Modeling of an energy management system for AC-DC microgrid using simple management logic

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Abstract. Microgrid (MG) is a concept that refers to any electrical installation that contains a set of renewable energy sources connected to the main grid with an energy storage system, electric vehicles and AC and DC loads. System stability and power quality are among the main problems encountered by microgrids due to the existing diversity in terms of loads and renewable energy sources. To solve this problem, we generally use the battery energy storage systems (BESS). To ensure a reliable and efficient energy supply, it is essential to optimize power flow by using an energy management system (EMS) and taking into account the availability of renewable energy sources and energy demand. This work proposes an energy management system (EMS) for a hybrid microgrid containing three renewable energy sources: photovoltaic (PV) system, wind system, fuel cell system, an energy storage system (ESS) and a diesel power source. The main and most important role of the EMS is to ensure an efficient balance between the energy produced and the energy consumed by controlling in real time and continuously the different energy sources, including photovoltaic, wind, fuel cell, energy storage, and grid systems. The proposed Energy Management System (EMS) attempts to control the flow of energy via the two AC and DC buses, taking into consideration the use of supplementary renewable production (PV, Wind and FC), and injecting into the grid the excess energy produced by the distributed sources (DG). This system uses control and conversion techniques to extract maximum power from the PV unit and wind system using a maximum power point tracking (MPPT) algorithm. PV, wind system and FC are sized to meet load demand, while ensuring battery charging in the event of excess energy. MATLAB/Simulink is the numeric computing platform used to test the energy management system proposed in this work.

Keywords: Battery energy storage system (BESS); Demanding power; Energy Management System (EMS); Micro-Grid (MG); Remaining power

Implementation of a robust droop control for the primary control of a low inertia AC microgrid

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Abstract. In isolated microgrids, precision and stability are important criteria for ensuring the production-consumption balance between different equipment, and are also essential for optimising the integration of renewable energies. These criteria not only extend the operating range of systems, but also guarantee optimal operation of microgrid equipment. Against this background, this research proposes advanced approaches to decentralized control, including robust droop control (RDC). The objective of this method is to guarantee precise, balanced power distribution between two grid-forming inverters (GFIs) operating in parallel. These devices feed linear resistive and inductive loads connected to the point of common coupling (PCC) of an isolated AC microgrid, operating at base voltage. To compare and confirm the effectiveness of the suggested method, conventional droop control (CDC) is also implemented for reference purposes. A Matlab/Simulink simulation validates our proposal. The RDC controller improve robustness, power sharing accuracy and stability compared with the conventional CDC. In both transient and steady-state conditions, both methods demonstrate their effectiveness, particularly during load variations. The RDC optimizes power sharing accuracy, reduces frequency oscillations and fluctuations, enhances the dynamics, robustness, accuracy of power distribution, and stabilizes voltage with less oscillation.

Keywords: Droop Control; Robust Droop Control; Microgrids; GFI; Renewable Energy

Investigation, using DFT, of adsorption of biomarker volatiles by fullerene and hetero-fullerene and possibility of biosensing of liver cirrhosis

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Abstract. In this investigation, density Functional Theory (DFT) calculations were used to explore the interactions of 2-pentanone, limonene, and methanol molecules, considering as a biomarker volatile for liver cirrhosis, with virgin C60 and hetero-fullerene M - C59 (M = B, Si, Al). The Geometric and electronic parameters such as adsorption configuration, adsorption energy, border molecular orbitals, and charge density difference are performed to explore the nature of these intermolecular interactions. The results show that after doping, the absorption spectrum of undoped material (C60) were affected and the interactions at the HOMO–LUMO energy gap were altered depending on the introduced atom, B, Si and Al. Examination of the response and the recovery time of the hetero-fullerene M-C59 where M = B, Si and Al, materials suggest that, these materials can be exploited as biosensor for liver cirrhosis.

Keywords: Fullerene ; Hetero-fullerene ; Liver cirrhosis ; methanol; 2-pentanone

Fe-Induced Electronic Modulation In α-MnO_2: A DFT+U Study For Advanced Cathode Materials

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Abstract. Manganese dioxide (MnO_2) is a widely studied transition metal oxide, particularly in its α-phase, due to its tunnel-type hollandite structure that supports efficient ion intercalation and robust structural stability. The electrochemical performance of α-MnO_2 is intimately linked to its electronic structure, including band gap characteristics and the nature of frontier orbitals. Here, we investigate the effect of Fe substitution on the electronic and structural properties of α-MnO_2 using DFT+U calculations performed with the Quantum ESPRESSO package, applying the PBE functional and Hubbard correction to account for electron correlation in Mn 3d orbitals. The pristine α-MnO_2 is confirmed to be an indirect band gap semiconductor (Eg = 1.08 eV), with a valence band maximum (VBM) composed of O 2p states and a conduction band minimum (CBM) derived from Mn 3d orbitals, both exhibiting notable hybridization. Upon Fe doping, the electronic structure is markedly altered. The system exhibits band gap narrowing and ultimately transitions toward metallic-like behavior under partial oxidation, with PDOS analysis revealing dopant-induced states at the Fermi level. Isosurface visualizations of the HOMO and LUMO using VESTA highlight localized charge redistribution and Mn–O orbital hybridization, critical for redox activity and electron delocalization. Structural analysis confirms that the tunnel architecture of α-MnO_2 is preserved post-doping, with only minor lattice distortions and no secondary phase formation. These findings demonstrate that Fe incorporation enables tunable electronic conductivity without compromising structural integrity, thereby enhancing the suitability of $FeMnO_2$ for lithium- and sodium-ion battery cathodes. The study underscores the role of targeted cation substitution in engineering advanced electrode materials with optimized charge transport, redox behavior, and electrochemical functionality.

Keywords: Band structure; Cathode materials; Electronic conductivity; Fe doping; MnO_2

Numerical Study of the Performance of a Solar Cell Based on the Tandem Perovskite/Silicon

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Abstract. The silicon/perovskite tandem cell technology allows to exceed the limits of theoretical efficiency of single junction photovoltaic cells. In this article, we studied the design and optimization of tandem two-pin (2T) cells using the SCAPS-1D software. The architecture in question combines a superior cell based on perovskite and a lower cell made of silicon. The results show promising photovoltaic performance.

Keywords: Cell; Silicon/Perovskite; SCAPS-1D Software; Photovoltaic Performance.

Exploring The Impact of Halogen (F, Cl; Br, I) Doping on $CaTiO_3$: A First Principles Study

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Abstract. The behavior of perovskite-based materials is greatly influenced by both their atomic composition and crystal structure, which contributes to their remarkable potential in various cutting-edge technological fields. In this theoretical work, the optoelectronic characteristics of the perovskite-analogue compound $CaTiO_3$ are studied through the formalism of density functional theory (DFT). The findings indicate a clear transition from p-type semiconducting behavior to a zero-bandgap metallic conductor as a result of doping. This transition suggests promising potential for use in electronic and optoelectronic technologies, particularly in applications that demand high electrical conductivity and controlled optical absorption. These results offer meaningful guidance for the targeted development and fine-tuning of materials for specialized functional purposes.

Keywords: $CaTiO_3$ Perovskite; Optoelectronics; Doping Effect; DFT Analysis; Halides

Enhanced Fuzzy MPPT Controller with Rules Compression for 10 kW Grid-Connected PV System

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Abstract. This paper proposes an enhanced fuzzy logic controller (FLC) for PV systems, featuring a novel reduced-order design. This work introduces a significantly simplified FLC for MPPT in a 10-kW grid-connected PV system. The proposed controller minimizes both the number of input variables and membership functions (MFs). Specifically, it utilizes only a single input, the sum of conductance and its increment, and employs just five rules, a substantial reduction compared to the 25-49 rules typical in standard FLCs. Integrated within a system architecture featuring a DC-to-DC converter and a 3-level voltage source converter (VSC) for grid power transfer via duty cycle control, this highly reduced FLC maintains robust MPPT performance through adaptive responses to varying weather conditions. Consequently, it achieves considerable simplification in implementation complexity without sacrificing operational efficiency. To our knowledge, this FLC represents one of the few controllers capable of such significant rule reduction while maintaining performance. Key results show: At 1 kW/m², IC achieves 99% efficiency vs. FLC's 96%. under medium irradiance (0.5 kW/m²), FLC outperforms IC by 5% (93% vs. 88%). For low irradiance (0.2 kW/m²), both reach 95.2%. Under large irradiance steps (0.4 to 1 kW/m²), the FLC achieves 22× faster convergence than IC (0.015 s vs. 0.33 s), demonstrating superior dynamic response to abrupt solar variations. This highlights the proposed algorithm's robustness for dynamic weather scenarios while maintaining competitiveness in steady operation.

Keywords: Power Grid; Fuzzy Logic Controller; MPPT; FLC.

Valorization of sugarcane bagasse for the sustainable biosorption of crystal violet dye: Kinetic, Isothermal, Thermodynamic Studies and Mechanisms Analysis

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Abstract. The contamination of aquatic environments by synthetic dyes poses a major environmental issue due to their toxicity, persistence, and harmful effects on ecosystems. This study investigates the use of sugarcane bagasse (SCB) as a low-cost biosorbent for the removal of crystal violet (CV) dye from aqueous solutions. SCB was characterized by X-ray diffraction (XRD) and Fourier-transform infrared spectroscopy (FT-IR). The effects of operational parameters such as contact time, biosorbent dosage, pH, and temperature were examined. Under optimal conditions 40 minutes of contact, 2 g/L SCB dosage, room temperature, and pH 10 a maximum removal efficiency of 95% was achieved. Isotherm and kinetic studies indicated a multilayer adsorption process dominated by physisorption, with the pseudo-second-order kinetic model providing the best fit to the experimental data. Thermodynamic analysis confirmed that the adsorption process is spontaneous and endothermic. Post-adsorption FT-IR spectra revealed the involvement of hydrogen bonding, electrostatic interactions, and ion exchange in the adsorption mechanism. These findings demonstrate the potential of sugarcane bagasse as an efficient, sustainable, and environmentally friendly biosorbent for the removal of synthetic dyes from contaminated water, offering a promising solution for wastewater treatment in a cost-effective manner.

Keywords: Crystal violet dye, Biomass, wastewater, Biosorption, Isotherm.

Doping-Induced Modulation of the Electronic, Optical, and Catalytic Properties for Next-Generation Photovoltaic and Photoelectrochemical Devices

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Abstract. In this study, we systematically investigate the effect of chemical doping on the structural, electronic, optical, and catalytic properties of functional semiconductor materials using first-principles calculations. The primary objective is to tailor material properties for enhanced performance in photovoltaic and photoelectrochemical (PEC) applications. Our results show that appropriate dopant incorporation leads to significant modulation of the band gap, enabling better alignment with the solar spectrum. The density of states analysis reveals the emergence of impurity states that contribute to improved light absorption in the visible range. Optical properties, including dielectric function and absorption coefficient, demonstrate enhanced photon harvesting efficiency upon doping. Furthermore, catalytic activity toward hydrogen evolution and oxygen evolution reactions is evaluated through adsorption energy descriptors and surface reactivity indicators. The doped systems exhibit improved catalytic performance due to optimized charge transfer and reduced reaction barriers. These findings demonstrate that doping engineering is an effective strategy to design multifunctional materials for high-efficiency solar energy conversion and sustainable hydrogen production technologies.

***Keywords*:** Doping engineering; Density functional theory; Photovoltaic materials; Photoelectrochemical devices; Optical properties

Energy Management of a Grid-Connected Microgrid Based on Linear Programming: A Case Study of Beni Mellal Province

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Abstract. This article examines the potential benefits for a user or an industrial company in Morocco operating a self-production microgrid, when the injection and sale of surplus local production become possible, notably thanks to the presence of an EMS. The objective is to highlight the importance and impact of surplus injection compensation on the overall costs and benefits for self-producers, especially in the industrial sector, and to support the acceleration of legal procedures related to electricity injection into the national grid, as well as the official publication of feed-in tariffs. To optimize producers' gains, an energy management strategy based on a linear programming optimization method is developed and analyzed. This strategy is evaluated under two scenarios: free injection of surplus energy and injection with sale at a reference tariff inspired by neighboring countries. Simulations are used to assess the impact of this approach on the company's energy costs and highlight the economic viability of establishing a legal framework for compensated electricity injection into the national grid.

Keywords: Microgrid, Linear Programming, Energy Management System, Energy Storage System, optimization algorith

Application of the Box–Behnken Design for Optimizing the Parameters of Crystal Violet Removal from Aqueous Solutions Using Quercus ilex of Acorn Waste: Kinetic and Equilibrium Study

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Abstract. This study explores the optimization of Crystal Violet (CV) dye removal from aqueous solutions using *Quercus ilex* acorn waste (AW), a natural and low-cost adsorbent. The Box–Behnken Design (BBD), a response surface methodology (RSM) approach, was employed to evaluate the influence of three key operational parameters: adsorbent mass, initial CV concentration, and temperature. The main objective was to maximize removal efficiency while minimizing operational costs. Seventeen experiments were conducted, and the results were modeled using a second-order polynomial equation. Analysis of variance (ANOVA) confirmed the statistical significance of the model ($\mathbf{p} < 0.0001$), with a high coefficient of determination ($\mathbf{R^2} = 0.96$), demonstrating strong predictive capability. Adsorbent mass and initial CV concentration had positive effects on adsorption efficiency, whereas temperature had a negative influence. The optimal conditions for maximum removal were an initial CV concentration of 100 mg/L, an adsorbent dosage of 0.5 g/L, and a pH of 10. This study highlights the potential of AW as an effective and sustainable adsorbent for textile dye remediation and demonstrates the value of BBD in optimizing adsorption processes for environmental applications.

Keywords: Box–Behnken design; crystal violet (CV); adsorption; *Quercus ilex* acorn waste (AW); dye removal.

Sustainable Synthesis of Activated Carbon for Efficient Removal of Methylene Blue from Wastewater

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Abstract. The removal of organic contaminants such as methylene blue from aqueous media remains a pressing environmental challenge. In this study, a sustainable and efficient adsorbent was synthesized via hydrothermal carbonization of biomass, followed by chemical activation to produce high-performance activated carbon. The impact of each processing step on the physicochemical properties of the material was systematically evaluated through a suite of characterization techniques, including scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDX), Fourier-transform infrared spectroscopy (FTIR), thermogravimetric analysis (TGA), and X-ray diffraction (XRD). The adsorption performance of the resulting activated carbon was assessed through batch experiments, revealing a high affinity for methylene blue with a maximum adsorption capacity of 382 mg/g. These findings underscore the potential of biomass-derived activated carbon as a green and effective adsorbent for wastewater treatment applications.

Keywords: Activated carbon; Biomass valorization; Methylene blue; Wastewater treatment

Linear and nonlinear optical behavior of Mg-doped $BaTiO_3$

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Abstract. This study examines the structural as well as the linear and nonlinear optical properties of Mg-doped $Ba_{1-x}Mg_xTiO_3$ powders synthesized using the sol-gel method, with doping levels ranging from x = 0.00 to 0.06. X-ray diffraction (XRD) analysis confirmed the formation of a pure perovskite structure in all samples, indicating the successful incorporation of Mg^{2+} ions into the $BaTiO_3$ lattice. Increasing Mg content leads to a shift toward a pseudo-cubic phase, evidenced by reduced tetragonality, as further supported by Rietveld refinement. Crystallite sizes were calculated using the Debye-Scherrer formula. UV-visible spectroscopy showed that with rising Mg concentration, the Urbach energy increased from 0.115 to 0.153 eV, while the optical band gap decreased from 3.228 to 3.080 eV. In addition, various optical properties including the linear refractive index (n), optical conductivity (σ_{opt}), and static refractive index (n_0) were determined and correlated with variations in Mg concentration (x). Analysis of the linear (LO) and nonlinear optical (NLO) properties of $Ba_{1-x}Mg_xTiO_3$ revealed that both the nonlinear refractive index (n_2) and third-order nonlinear susceptibility ($^{(3)}$) increase with increasing Mg content. These findings highlight the potential of $Ba_{1-x}Mg_xTiO_3$ nanoparticles (for x ranging from 0 to 0.06) for use in a wide range of optical device applications.

Keywords: Band gap; Magnesium; Optical properties; UV-visible; XRD

Preparation of Magnetite-Organic Matter as an adsorbent for cationic and anionic dyes removal from aqueous solution

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Abstract. Recent trends in material science emphasize the growing significance of utilizing industrial and agricultural residues as raw materials for production. A prime example is sugarcane bagasse. Additionally, the use of magnetic nanoparticles as adsorbents for pollutant removal is an emerging field in wastewater treatment. In this study, we propose a novel approach by combining iron oxide (Fe_3O_4) magnetic nanoparticles with sugarcane bagasse to develop a low-cost adsorbent. This composite material exhibits strong reactivity and effective interactions with dyes, offering a promising solution for pollutant removal. The synthesized materials were characterized using X-ray diffraction (XRD), Thermogravimetric/ differential thermal analysis (TG/DTA), Fourier transform infrared spectroscopy (FTIR) and Vibrating Sample Magnetometry (VSM). According to adsorption experiment results, our adsorbents show a promising adsorption capacity for congo red and methylene blue removing.

Keywords: Adsorption; Cellulose; Congo red (CR); Magnetite (Fe_3O_4); Methylene blue (MB);

Study of the doping effect on mechanical proprieties and thermal stability of $Ni_3Al - Cr$ alloy by molecular dynamic simulation

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Abstract. Atomic-scale structural analysis has clearly demonstrated the important role of nickel-based materials in providing cohesion. Nickel has the potential to significantly enhance the high-temperature stability of heat-resistant alloys. In this paper, we present a theoretical study of pure Ni_3Al doped with various percentages of chrome (Cr), and we conducted deformation by traction studies using molecular dynamics simulation. We subsequently performed a simulation of Ni_3Al doped with 10% Cr at various temperatures. For each temperature, we performed relaxation followed by dynamics (NPT) to determine the volume over a temperature range of 300–1000 K. The simulation was carried out using the LAMMPS program with a Modified Embedded Atom Method (MEAM) potential for the Cr-Ni-Al system. The use of molecular dynamics to model the Ni_3Al alloy with an FCC structure doped with various levels of chromium (Cr) makes it possible to anticipate deformation processes and evaluate mechanical characteristics. This method highlights the impact of chromium on the ductility of the material at a fixed temperature (300K). Furthermore, analysis of volumetric behavior as a function of temperature demonstrates a nearly linear increase in volume, typical of standard thermal expansion. The results suggest that adding 10% chromium (Cr) improves the ductility of the Ni_3Al alloy at high temperatures.

Keywords: MD simulation, MEAM potentials, Mechanical properties, Ni_3Al-Cr, Tensile properties

Electronic Structure Tuning of $NiFePO_4$: A DFT+U Investigation Toward High-Rate Li/Na-Ion Battery Cathodes

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Abstract. $NiFePO_4$, a partially Ni-substituted variant of the well-known olivine-type $FePO_4$, is emerging as a promising cathode material for lithium- and sodium-ion batteries. Building on the structural robustness and thermal stability of the $FePO_4$ framework, the incorporation of Ni offers the opportunity to enhance electronic conductivity and redox kinetics by tuning the electronic structure. Previous studies have demonstrated that transition metal substitution, particularly with Ni^{2+}/Ni^{3+}, can effectively modulate the electronic states near the Fermi level and facilitate electron delocalization. In this work, we employ Density Functional Theory (DFT) calculations with on-site Hubbard corrections (DFT+U) to investigate the electronic properties of $NiFePO_4$. Simulations were performed using the Quantum ESPRESSO package with the PBE functional within the GGA framework. To accurately describe the localized 3d states of transition metals, we applied $U^{fe} = 4.3$ eV and $U^{ni} = 6.0$ eV. We computed the electronic density of states (DOS), band structures, charge density maps, and Fermi surfaces for both pristine and partially oxidized forms of the material.Our results show that fully lithiated $NiFePO_4$ is a semiconductor with a band gap of approximately 1.02 eV. The valence band is dominated by hybridized Fe 3d and O 2p orbitals, while the conduction band includes contributions from Ni 3d states. Upon partial oxidation, the band gap narrows, and partially filled bands cross the Fermi level. These bands, derived from hybridized Ni 3d and Fe 3d orbitals, yield an anisotropic Fermi surface, indicating a transition toward semi-metallic behavior.This evolution enhances electronic conductivity and supports faster redox kinetics. The coexistence of mixed-valence Fe and Ni centers suggests polaron hopping mechanisms. In summary, Ni substitution modulates the electronic landscape of $FePO_4$, promoting conductivity and semi-metallicity under partial oxidation.

Keywords: DFT+U; Electronic structure; Lithium-ion batteries; $NiFePO_4$; Redox kinetics.

Study of the inhibition of corrosion of carbon steel in a 1M HCl solution by a natural extract

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Abstract. The study of carbon steel corrosion is a subject of both academic and industrial importance because of the increased industrial applications of acid solutions. Natural products and other environmentally-friendly materials, have gained much attention as a possible replacement to inorganic corrosion inhibitors because they are cheap, biodegradable, and in high abundance. The purpose of this investigation is to study the inhibition efficiency of natural extract on the degradation of carbon steel in hydrochloric acid (HCl 1M) by potentiodynamic polarization (PDP) and electrochemical impedance spectroscopy (EIS), and the effect of concentration, temperature and immersion time parameters on corrosion. The results of this study showed that the inhibition efficiency of the extract raised from 85 to 97%, with concentrations from 0.5 to 2 g/L. However, as temperature increased from 293K to 323 K, inhibition efficiency decreased from 97 to 91%. EIS method confirmed that the inhibition efficiency of extract remained virtually constant with rising immersion time. The polarization method (PDP) indicates that the extract acts as a mixed-type inhibitor with an anodic influence.

Keywords: CORROSION; EIS; Extract; INHIBITION EFFICIENCY; PDP

Valorization of natural support for the degradation of a cationic dye by photocatalysis

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Abstract. the removal of synthetic dyes from wastewater remains a critical challenge in environmental protection, especially in textile industries. Cationic dyes such as methylene blue are frequently found in industrial wastewater and represent a serious environmental concern due to their toxicity, persistence, and resistance to conventional treatments. Photocatalysis is a promising advanced oxidation process for the removal of such pollutants. In this study, a natural support material was prepared and used as a substrate for titanium dioxide (TiO_2) to enhance photocatalytic degradation of methylene blue. Snail shells, a biowaste rich in calcium carbonate, were calcined to obtain a porous and thermally stable support. TiO_2 was deposited onto the surface of the calcined material via a simple dopping method. The resulting material was characterized using UV-Visible and Fourier-transform infrared spectroscopy (FTIR). Photodegradation tests were carried out under UV light to evaluate the efficiency of the catalyst under varying conditions, including dye concentration, catalyst dosage, and pH of the solution. The optimized system achieved over 90% dye removal and followed pseudo-first-order kinetics. This work demonstrates the effectiveness of using natural biomaterials as photocatalyst supports, contributing to sustainable wastewater treatment technologies through the valorization of biowaste.

Keywords: Photocatalysis; Cationic dye; Natural support; Titanium dioxide; Wastewater treatment

Drying Kinetics and Characteristic Curve Development for Ziziphus Leaves in a Hybrid Forced Convection Solar Dryer

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Abstract. This study explores the convective drying kinetics of Ziziphus lotus (jujube) leaves using an innovative hybrid solar dryer that integrates indirect heating and forced convection. Drying experiments were conducted at temperatures ranging from 40 °C to 70 °C with a constant air velocity of 1.55 m/s. The drying process exhibited a typical falling rate period with no constant rate phase, highlighting the moisture diffusion-controlled nature of the process. Moisture content and drying rate curves demonstrated that higher temperatures significantly accelerated water removal. A characteristic drying curve (CDC) was developed using Van Meel's method and modeled with a second-degree polynomial (R^2 = 0.9567), providing a generalized representation of the drying behavior. Comparative model fitting showed that the Modified Henderson & Pabis model yielded the best prediction accuracy (R^2 = 0.9576; RMSE = 0.0651). These results confirm the strong temperature dependency of drying kinetics and support the use of the proposed CDC for predictive modeling and optimization in hybrid solar drying applications.

Keywords: Drying kinetics ; Hybrid solar dryer ; Characteristic drying curve (CDC) ; Convective drying ; Polynomial modeling

Molecular Dynamics Simulation of Phase Change Behavior in a Mg-Al-Zn Alloy for Thermal Energy Storage Applications

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Abstract. The necessity of creating sophisticated phase change materials (PCMs) with specific thermal and diffusion properties has been brought to light by the growing need for effective thermal energy storage devices. This study uses conventional molecular dynamics (MD) simulations to examine the phase transition behavior of a ternary Mg-Al-Zn alloy. In order to assess the alloy's potential as a PCM for thermal energy storage applications, the main goals are to describe the diffusion mechanisms and determine the alloy's phase transition temperatures. With the ability to precisely depict interatomic interactions inside the system, the simulations were carried out utilizing the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) with the Modified Embedded Atom Method (MEAM). Under constant pressure and recurring boundary conditions, the Mg-Al-Zn alloy model was continuously heated from 300 K to 1200 K. Atomic mobility and phase transition events were recorded by monitoring important thermophysical parameters, such as the mean squared displacement (MSD) and system energy. Phase transitions inside the alloy were indicated by the data, which showed clear increases in atomic diffusion rates and system energy fluctuations around particular temperature ranges. Temperature-dependent trends were seen in the diffusion behavior of Mg, Al, and Zn atoms, which shed light on the atomic-scale processes controlling heat storage efficiency. In order to support the design and optimization of Mg-Al-Zn alloys for energy storage technologies, this study advances our understanding of their temperature response and phase change properties.

Keywords: Thermal energy storage, phase change material, Mg-Al-Zn alloy, molecular dynamics, LAMMPS.

Using AI-Based Method for Fault Detection and Localization in Smart Grids model

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Abstract. Many services depend on the existence of electricity. To ensure the continuity of service, the distribution networks depend heavily on the time needed to detect and accurately localize faults. A fault results in the destruction of equipment, interruption of service, instability of the network, and poor system reliability. These consequences wool become financial losses for both distribution companies and, most importantly, users. Traditional fault location techniques, particularly for distribution networks that are geographically large and spread out, can be time-consuming and expensive to perform on a large scale. This paper made an application of an AI method for fault detection and localization in smart grid. The method developed has been programmed and is integrated in MATLAB Simulink model, this model contains a wind farm, a solar farm, a diesel generator and some loads, for the proper simulation of the system. the creation of the location Faults is randomized, using short-circuit, cable break, and high impedance faults types. An artificial neural network (ANN) is used for detection and localization, confirming the ability of the system to operate reliably in complex and realistic scenarios. This method aims to enhance both the accuracy and efficiency of fault diagnosis in modern smart grids.

Keywords: Smart grids; Detecting and locating faults; Artificial neural network; Renewable Energy

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Comparative Study Between Two BMS architecture in a PV-battery off-grid: Centralized and Modular topologies

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Abstract. The aim of this study is to provide a comparison of two Battery Management System (BMS) topologies, modular and centralized in a photovoltaic generator whose power is optimized by a hybrid MPPT algorithm based on the integration of an Adaptive Neuro-Fuzzy Inference System (ANFIS) and a fuzzy controller, functioning as a PI regulator. The battery pack, which is composed of lithium-ion batteries, is controlled by a fuzzy PI controller and a DC-DC buck/boost converter, which guarantees precise, flexible management of power flows. This paper stresses the compromise between the two architectures in multiple uniform irradiations through simulations 1000 W/m^2, 800 W/m^2 and 600 W/m^2. The result shows that generalized systems are well suited for cost-sensitive, space-limited applications. However, modular BMSs have better scalability, and increased fault isolation and are thus well suited for electric vehicles, renewable energy storage, and mission-critical applications.

Keywords: BMS Topology, MPPT, ANFIS, PV, Uniform irradiation

Title: Recycling Plastic and Construction Waste for the Development of Sustainable Building Materials

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Abstract. In the context of growing environmental pressure, the construction sector offers both a challenge and a strategic opportunity for solid waste recovery. This study explores several approaches for integrating recycled materials—specifically used plastics (PET, HDPE, LDPE), construction and demolition waste (CDW), and agro-industrial residues—into the production of bricks and masonry units. Drawing from recent experimental studies, we assess the mechanical, physical, and environmental properties of these composite materials. Results show that incorporating plastics can enhance lightness, moisture resistance, and thermal insulation, though mechanical strength tends to decrease, making them suitable for non-structural components. Similarly, crushed brick or recycled concrete aggregates show promising bearing capacity (CBR) and durability, particularly for road base layers or low-carbon mortars. This research contributes to circular economy initiatives and ecological transition, using locally available resources in Morocco. It lays the groundwork for standardizing sustainable construction materials and reducing both waste volumes and CO_2 emissions in the building industry.

Harmonic Mitigation in a Hybrid PV-Wind Smart Grid Using UPQC method

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Abstract. The rising integration of photovoltaic (PV) and wind power sources within SMART GRIDS introduces significant challenges related to power quality (PQ), especially due to harmonic distortions that can address grid. Stability, high power quality, and optimal efficiency of all connected devices. This research focuses on compromising harmonic problems in the smart grid by proposing the use of a Unified Power Quality Conditioner (UPQC) as an effective solution for comprehensive harmonic elimination. By combining series and shunt active power filters, the UPQC allows for the lowering of voltage and current harmonics. The control method using the synchronous reference frame approach (SFR) to detect and compensate for undesirable harmonic elements in real time. To validate the performance of the proposed approach under various loading and generation scenarios, simulation studies were performed. The findings demonstrate that the UPQC significantly reduces total harmonic distortion THD in voltage and current signals, therefore improving overall power quality and enhancing smart grid operation. Moreover, The UPQC surpasses traditional separate filtering methods, emphasizing its capability to enable reliable integration of renewable energy sources. This research contributes to the development of advanced power quality solutions for modern hybrid renewable energy systems, ultimately enhancing grid resilience and efficiency.

Keywords: Harmonic mitigation; Power quality; Smart grid; Unified power quality conditioner UPQC; Wind energy; Photovoltaic.

Development of a coupled ANN- BEM Framework for Smart Blade Aerodynamic Modeling

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Abstract. Accurate prediction of aerodynamic coefficients is essential for the design and control of smart blades featuring morphing airfoils. This study presents a data-driven metamodel based on Artificial Neural Networks (ANNs) developed to predict the aerodynamic behavior of airfoils within the NACA series. The model accepts geometric descriptors of airfoils along with the angle of attack (AoA) as input and outputs corresponding lift (Cl) and drag (Cd) coefficients. A high-fidelity aerodynamic database was generated through systematic simulations across a wide range of AoAs and NACA profiles to train and validate the ANN. The model is trained on NACA 4-digit series profiles covering a wide range of AoA and geometric parameters. The ANN model achieved a mean squared error of 2.10805 e-3 and an R^2 above 0.997 on test data. The trained metamodel demonstrates excellent generalization accuracy while drastically reducing computational requirements compared to conventional CFD or BEM-based methods. The model is particularly suited for integration into larger simulation frameworks, such as Blade Element Momentum (BEM) codes or adaptive control systems, enabling real-time performance estimation for morphing smart blades. This work contributes a scalable and efficient surrogate modeling approach for aerodynamic prediction across diverse airfoil geometries.

Keywords: NACA, airfoil, wind turbine metamodeling, ANN, BIM, morphing blade, CFD, Smart blades

Pressure-Induced Tuning of Structural, Electronic, and Optical Properties in $XZnF_3$ (X = Na, K, Rb) and $InGeF_3$ Perovskites: Toward Adaptive Optoelectronic Materials

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Abstract. This work presents a theoretical investigation of the effect of hydrostatic pressure on the structural, electronic, and optical properties of fluorinated perovskite compounds $XZnF_3$ (X = Na, K, Rb) and $InGeF_3$ using density functional theory calculations. The goal is to understand how external pressure can be used as an efficient tuning parameter for adaptive optoelectronic applications. Structural analysis under pressure reveals systematic lattice compression accompanied by changes in bond angles and interatomic distances, which strongly influence electronic behavior. A pressure-driven band gap evolution is observed, indicating possible semiconductor-to-semiconductor transitions and tunable optical response. Optical properties such as absorption coefficient, refractive index, and dielectric function show significant pressure dependence, with enhanced light–matter interaction in specific pressure regimes. These changes suggest strong potential for pressure-controlled photonic and optoelectronic devices. The comparative study between alkali-metal-based and indium-based perovskites highlights distinct sensitivities to external pressure, providing insight into structure–property relationships. Overall, this study demonstrates that hydrostatic pressure is an effective route to engineer the performance of fluorinated perovskites for next-generation adaptive optoelectronic technologies.

Keywords: Hydrostatic pressure; Perovskites; Density functional theory; Electronic properties; Optical properties

First-Principles DFT and BoltzTraP Investigation of Multifunctional Properties of XNiH3 (X = Li, Na, K) Perovskite Hydrides: Thermoelectric and Hydrogen Storage Potential

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Abstract. In this study, we explore the structural, electronic, thermoelectric, and hydrogen storage properties of perovskite compounds XNiH3 (X = Li, Na, K) using density functional theory (DFT) in the GGA approximation, with the Wien2k code coupled to the BoltzTrap code. The main objective is to evaluate the potential of these materials for applications in energy conversion and reversible hydrogen storage. Structural calculations reveal crystallization in a perovskite-type cubic structure with lattice parameters of 3.57 Å (LiNiH3), 3.72 Å (NaNiH3), and 3.87 Å (KNiH3). Electronic analysis indicates metallic behavior for all three compounds, which is favorable for electrical conduction and hydrogen desorption kinetics. Thermoelectric performance evaluated in the temperature range 300–900 K shows that these compounds are n-type, with negative Seebeck coefficients and maximum ZT factor values reaching 0.09 for LiNiH3 at 800 K. At the same time, the estimated gravimetric capacities are 4.37% (LiNiH3), 3.54% (NaNiH3), and 2.98% (KNiH3), confirming their suitability for hydrogen storage. These results suggest that XNiH3 compounds, particularly LiNiH3, are promising candidates for integrated energy applications, combining waste heat recovery and energy storage.

Keywords: Electrical; DFT; Merit factor; XNiH3.

Experimental investigation of the impact of misalignment defects on the vibration behavior of drive systems using various coupling types (elastic and rigid) in rotating machinery and power generation equipment.

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Abstract. This study explores how misalignment affects vibration patterns in drive systems using two common types of couplings: elastic (Rotex GS) and rigid flange couplings. By measuring vibrations in both vertical and horizontal directions under controlled conditions, the research reveals that vertical vibrations are consistently more intense than horizontal ones. In systems with elastic couplings, the stiffness of the material strongly influences how vibrations are transmitted and in some cases, increases the risk of failure. Rigid couplings, on the other hand, produce unique vibration signatures when misaligned, making it easier to detect mechanical issues. The type of misalignment matters too: axial misalignment causes strong, low-frequency vertical vibrations, while radial misalignment results in more complex patterns. These findings highlight the need to monitor vibrations in both directions and suggest that the ratio of vertical to horizontal vibration could serve as an early warning signal, helping teams catch problems sooner and plan maintenance more effectively.

Harmonic Mitigation in a Smart Grid Using a PV-Powered Series Active Power Filter

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Abstract. The rising integration of photovoltaic PV sources within SMART GRIDS introduces significant challenges related to power quality PQ, especially due to harmonic distortions that can address grid. Stability, high power quality, and optimal efficiency of all connected devices. This research focuses on compromising harmonic problems in the smart grid by proposing the use of a Series Active Power Filter SAPF as an effective solution for comprehensive harmonic elimination. The SAPF allows for the lowering of voltage harmonics. The control method using the synchronous reference frame approach SFR to detect and compensate for undesirable harmonic elements in real time. To validate the performance of the proposed approach under various loading and generation scenarios, simulation studies were performed. The findings demonstrate that the SAPF significantly reduces total harmonic distortion THD in voltage signals, therefore improving overall power quality and enhancing smart grid operation. Moreover, The SAPF surpasses traditional separate filtering methods, emphasizing its capability to enable reliable integration of renewable energy sources. This research contributes to the development of advanced power quality solutions for modern hybrid renewable energy systems, ultimately enhancing grid resilience and efficiency.

Keywords: Harmonic mitigation; Power quality; Smart grid; SAPF; Photovoltaic

Numerical Simulation of Enhanced Clay-Phase Change Material (PCM) Composites for Thermal Regulation in Traditional Earthen Buildings

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Abstract. The confrontation aspect of energy efficiency in building in the arid and semi-arid zones of Morocco requires having innovative solutions that can adapt with the Moroccan building tradition. Despite their high thermal mass, it has been observed that traditional earthen buildings like adobe or rammed earth may not have the level of thermal mass to prevent overheating of the indoor environment during periods of significant diurnal temperature fluctuations. This work is a numerical contribution to the thermal performance of PCM-based clay composites, serving in the development of an ecologic construction material suitable for passive thermal regulation. This study is an extension of a previously proposed and validated Python-based enthalpic model, which has been successfully applied to investigate the performance of doped perlite-PCM composites. The model solves the transient, nonlinear heat conduction equation by the finite volume method in a manner that is able to account for the dynamics of the phase change in latent heat storage. Here, the emphasis is transferred from perlite-lightweight-aggregate to clay, which is the main constituent of vernacular Moroccan construction. Two conditions are considered: the baseline composite of clay and micro-encapsulated PCM and the enhanced one, which resulted from the optimization of PCM mass fraction and the addition of conductive additives to enhance the rather low inherent thermal conductivity of both clay and organic PCMs. The imposing superiority in thermal inertia is already manifested in preliminary results, demonstrating distinctive and repeatable phase change plateaus that are not present in simpler formulations. The model predicts the large rise of the energy storage and release powers targeting a high degree of return loss efficiency indispensable for practical use. This work proposes an experimentally validated modelling platform to engineer sustainable, advanced, low-cost building materials using locally available materials. It provides a route for integrations of advanced PCM technologies into traditional earth building in synergy, thus contributing to the reduction of cooling energy requirements and heat comfort in sustainable structures.

Keywords: Phase Change Materials (PCMs) ; Clay Composites ; Moroccan Building Tradition ; Enthalpy Method ; Energy Efficiency.

plasmonic resonance phenomena effect in structural and optical properties of Fe modified Li3SO Antiperovskite structure

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Abstract. We used density functional theory calculation (DFT) to optimize the crystal structure of Fe doped Li3SO at different concentrations. Using the relaxation method, the optimized lattice parameters were obtained, and the stability of the doped systems was analyzed in comparison with pure host material. The results show that Fe doping can significantly alter the structural and optical properties of the antipervskite. And that the introduction of delocalized iron impurities induces changes in the lattice parameters, electron densities and energy gaps of Li3SO, which can have an impact on the absorption and emission properties of electromagnetic radiation in the visible light range. Also, it was observed that the concentration of Fe doping influences the structural and optical properties, suggesting that controlled Fe doping can be a strategy to tune the physical properties of this materials for better use in optoelectrical applications.

Bibliometric analysis of contemporary research on charge transfers between medium voltage power distribution circuit

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Abstract. This research work delves into the realm of contemporary investigations concerning charge transfers occurring within medium voltage power distribution circuits. Such transfers primarily arise from maneuvers executed exclusively by energy suppliers and often result in power interruptions. Another facet of this study involves the identification of analogous research endeavors conducted in disparate geographical regions, with a particular emphasis on the localized context of Cuernavaca, Morelos. Furthermore, this article engages in interdisciplinary discourse, employing logical analogies to establish a conceptual topology. This conceptual framework can be instrumental in the identification, through logical connectors, of instances where a charge transfer within an electrical power distribution system implies a power interruption. This, in turn, contributes to the optimization of energy utilization, a critical consideration within the purview of smart cities.

Predicting Heavy Metal Adsorption From Water Using Machine Learning Algorithms

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Abstract. Heavy metal contamination in water is a serious environmental concern due to its toxicity, persistence, and bioaccumulation potential in living organisms. Among the various treatment techniques, adsorption using activated carbon remains one of the most effective and economical methods for removing metal ions such as Cu(II), Zn(II), Ni(II), Pb(II), Cd(II), Cr(VI), and As(V). Optimizing this process through conventional experimentation, however, is often time-consuming and resource-intensive. In this study, a predictive framework based on machine learning was developed to estimate the amount of metal adsorbed (Qe, in mg/g). A large dataset comprising 1,480 experimental records was assembled, incorporating key adsorbent textural parameters (BET surface area, pore diameter, pore volume), operational variables (pH, temperature, initial concentration, dosage, contact time), and intrinsic ionic properties (ionic radius, hydrated radius, electronegativity). Five supervised learning algorithms were implemented and evaluated: Decision Tree, Random Forest, Extra Trees, Gradient Boosting, and XGBoost. Among them, Gradient Boosting exhibited the highest predictive performance (MSE = 1.12, RMSE = 1.05, R^2 = 0.981), followed closely by XGBoost (MSE = 1.64, RMSE = 1.28, R^2 = 0.965). The results highlight the significant potential of machine learning approaches in accurately simulating adsorption behavior, offering a valuable alternative to labor-intensive experimentation and contributing to the design of more efficient water treatment systems.

Keywords: Adsorption, Heavy metals, Machine learning, Water treatment, Predictive modeling

DFT approach for improving the electronic and optical properties of $KZnF_3$ perovskite: Impact of copper doping

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Abstract. This study investigates the structural, electronic and optical properties of cubic perovskite $KZnF_3$, in its pure state and doped with copper (Cu) at a concentration of 12.5%, using the full-potential linearized augmented plane wave (FP-LAPW) method within the framework of density functional theory (DFT) which is implemented in the Wien2k code. Density-of-state (DOS) analysis reveals that doping significantly alters electronic properties, notably through the emergence of 3d-Cu impurity states near the Fermi level, resulting in a shift towards the valence band and a decrease of the band gap to 2.72 eV. Optical properties were also analyzed through dielectric functions (real and imaginary parts), absorption coefficient, optical conductivity, refractive index and reflectivity. Cu doping enhances absorption in the visible spectrum, increases electron polarization and optimizes charge carrier mobility, boosting the material's performance in optoelectronic devices. These results highlight the key role of doping in engineering perovskite properties for advanced applications, including photovoltaic technologies, optical sensors and next-generation electronic systems.

Keywords: $KZnF_3$; Wien2k code; Absorption coefficient; Optical conductivity.

Optimization of Recycled Copper Purity: Pretreatment and Fire Refining Approach for Industrial Applications

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Abstract .In response to growing global copper demand, recycling has emerged as a key pillar for sustainable development. This study proposes a cost-effective and practical method for improving the purity of recycled copper, specifically tailored for small-scale industrial foundries. The process combines a pre-treatment stage with fire refining at an optimal temperature of 1120 °C. Three types of copper scrap were analysed, including bare wires (Berry) and heterogeneous scrap (Cliff). The pre-treatment eliminated 23% of impurities and enabled a final copper purity of up to 99.99% (4N), with electrical conductivity exceeding 86% IACS, reaching 88% in some cases. These results meet ASTM industrial standards and open potential applications in industrial boiler manufacturing. The method offers a sustainable recycling solution while reducing the environmental impact of copper recovery.

Assessing $Mg_{84}Cu_{16}$ as a novel PCM for high-temperature energy storage: Focus on thermal stability and material compatibility

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Abstract. The development of efficient latent heat storage materials for high-temperature thermal energy systems is essential to improving the performance and reliability of concentrated solar power (CSP) plants. This study evaluates the thermal resilience and chemical compatibility of the $Mg_{84}Cu_{16}$ eutectic alloy, which has emerged as a promising phase change material (PCM) due to its high thermal conductivity and favorable melting properties. Accelerated cycling tests (30 cycles between 300–550 °C) were performed to assess the alloy's structural and thermophysical stability. Post-cycling characterization using SEM-EDS and DSC showed negligible degradation in microstructure and thermal performance, with melting point and latent heat remaining stable at ~488°C and ~232 J/g, respectively. Furthermore, static corrosion tests with stainless steels (SS304, SS316) and Inconel at 550 °C for 240 hours demonstrated moderate compatibility with stainless steels and excellent resistance in Inconel. To the best of our knowledge, this is the first study to evaluate the corrosion resistance of $Mg_{84}Cu_{16}$ under prolonged high-temperature exposure (550°C for 240 h), providing new insights into its long-term compatibility with containment materials. These findings confirm that $Mg_{84}Cu_{16}$ maintains structural and thermal stability under operational conditions, making it a strong candidate for high-temperature latent heat storage systems in industrial energy applications.

Keywords: Phase change material; Mg-Cu alloy; Latent heat storage; Thermal stability; Corrosion compatibility.

Characterization of Cancerous Tissue by Electrochemical Method

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Abstract. Non-muscle-invasive bladder cancer (NMIBC) presents a significant challenge in terms of diagnosis, follow-up and recurrence monitoring. Current methods for follow-up, such as cystoscopy and cytology, are invasive, time-consuming, and often associated with discomfort for patients. Hence, there is a pressing need for the development of non- invasive, cost effective and efficient techniques for NMIBC monitoring. In this study, an electrochemical simplified method for the follow-up of NMIBC is proposed, offering a promising alternative to conventional approaches. The method is based on the detection of cancerous cells using a carbon paste electrode (CPE). This electrode showed considerable activity for the detection and characterization of cancerous cells, which are manifested by the appearance of two redox peaks, and a remarkable increase in specific capacitance. The effect of the presence of iron ions in the electrolytic medium showed a very considerable difference in voltammograms. Fenton reaction was manifested by two-redox peaks characteristic of the presence of cancer cells.

Keywords: BC; CPE; CB; EIS; non-invasive follow up; SWV.

DFT and BoltzTrap Investigations on the Thermal and Structural Characteristics of the Perovskite MgCuH3 and MgCoH3

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Abstract. This research investigates the structural and thermoelectrical characteristics of perovskite $MgMH_3$ (M = Cu and Co) using the Meta-GGA, within the framework of density functional theory (DFT), to do this, we use the BoltzTrap package implemented in the Wien2k code, we analyze the calculated total energy and atomic volume using Murnaghan equation of state along with insights into band structure and densities of states. The analysis of the band structures for $MgCuH_3$ and $MgCoH_3$ indicates their behavior as conductors, with the conduction band overlapping the valence band, resulting in a gap equal to 0 (ev). Furthermore, thermoelectrical properties (including electrical conductivity (σ), thermal conductivity (κ), merit factor (Zt), and power factor (PF)) variations across temperatures ranging from 300 to 900K, were evaluated using the BoltzTrap package, revealing intriguing aspects. The electrical conductivity (σ) of $MgCuH_3$ reduces, but $MgCoH_3$ increases with rising temperature. The thermal conductivity (κ), responsible for heat transfer, increases linearly with temperature. The Merit factor (Zt) indicates that, whereas $MgCoH_3$ decreases between 300 and 600 K but increases between 600 and 900 K, and $MgCuH_3$ increases with increasing temperature. The Power factor (PF) indicates that $MgCoH_3$ (PF) decreases between 300 and 700 K but increases between 700 and 900 K and $MgCuH_3$ increases with increasing temperature.

Keywords: Electrical conductivity; Seebeck coefficient; Thermal conductivity; Thermoelectric figure of merit