The 2024 1st International Conference on Materials Sciences and Mechatronics for Sustainable Energy and the Environment

المؤتمر الدولي الأول لعلوم المواد والميكاترونيات من أجل الطاقة المستدامة والبيئة 2024

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Preface

We are pleased to announce the outstanding success of the **1st International Conference on Materials Sciences and Mechatronics for Sustainable Energy and the Environment (MSMS2E 2024)**, held from **October 1 to 3, 2024**, 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 2024 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, Younes Ziat** and **Yassine Lakhal**, for their outstanding leadership and invaluable contributions, which were instrumental in the organization and success of this international conference.

MSMS2E 2024 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 **الأول لعلوم المواد والميكاترونيكس للطاقة المستدامة والبيئة(MSMS2E 2024)** ، الذي نُظم من 1 إلى 3 أكتوبر 2024 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 2024) 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: يونس زيات و ياسين لكحل** على قيادتهم الحكيمة وإسهاماتهم القيمة التي كانت أساسية في تنظيم وإنجاح هذا المؤتمر الدولي.

لقد كان **MSMS2E 2024** 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.

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The Key Factor Sustainability of Solar Energy: Evidence in Yogyakarta, Indonesia

Dessy Rachmawatie[1]*, Lisya Indrayana[2]

[1]*Magister of Economics, Postgradate School, Universitas Muhammadiyah Yogyakarta, Kasman Singodimedjo Postgraduate School Building 1st Floor of UMY Integrated Campus, Brawijaya Road, Tamantirto, Kasihan, Bantul, Yogyakarta,55183, Indonesia*
[2]*Department of Economics, Universitas Muhammadiyah Yogyakarta, 2nd Floor Ki Bagus Hadikusumo Building, UMY Integrated Campus, Brawijaya Road, Tamantirto, Kasihan, Bantul, Yogyakarta,55183, Indonesia*
*E-mail : d.rachmawatie@umy.ac.id

Abstract. Solar Panels are one of the renewable energies potentially be a turning point in Yogyakarta's electricity issues. The challenges arise about how to run solar projects that are sustainable in society. This study aims to analyze factors becoming the key to sustainable solar panel projects in Yogyakarta. The analyses carried out 19 variables, divided into 5 dimensions (economics, social, regulatory, government and environmental) of sustainable renewable energy. This study was examined using *Multiplications Applied to a Classification Model (MICMAC)* resulting in 5 key variables identified as the key factors for sustainable solar panel projects in Yogyakarta. The result shows that according to *MICMAC* analysis, there are five key variables for solar panel development in Yogyakarta. Namely affordable energy prices, energy price instability, scarcity of energy supply, and two regulatory indicators, the regional regulations that support renewable energy from the Central Government and the regional regulations that supports renewable energy from Regional Governments. These key variables can be considered for sustainable renewable energy development programs, especially for solar panels in Yogyakarta province.

Keywords: Key factors; Renewable energy, Solar panel; Sustainable development; Sustainability

Advancements and Challenges in the Photovoltaic Energy Supply Chain: Insights from a Global Perspective

Hajar RAJI[1], Abdelghani BOUDAOUD[2], Mounaim AQIL[3]

[1] *Laboratory of Studies and Research in Economics and Management Sciences, University Sultan Moulay Slimane, Superior School of Technology, University Campus M'ghila BP:591, Beni Mellal 23000, Morocco.*

h.raji@usms.ma

[2] *Engineering Applied Physics Team (EAPT), University Sultan Moulay Slimane, Superior School of Technology, University Campus M'ghila BP:591, Beni Mellal 23000, Morocco.*

abdelghani.boudaoud@usms.ma

[3] *Engineering Applied Physics Team (EAPT), University Sultan Moulay Slimane, Superior School of Technology, University Campus M'ghila BP:591, Beni Mellal 23000, Morocco.*

mounaim.aqil@usms.ma

Abstract, Energy is the lifeblood of our civilization, and solar energy, particularly photovoltaic (PV) systems, is at the forefront of the renewable energy revolution. As of 2024, the global PV market reached an installed capacity of over 1,000 GW, showcasing its exponential growth and potential. The solar energy PV supply chain is essential in this transition, covering the production, distribution, and installation of PV systems that convert sunlight into electricity. This paper aims to explore the intricacies of the PV supply chain, identifying key components such as raw material sourcing, PV cell and module manufacturing, and logistics. The objective is to provide a comprehensive literature review that highlights technological advancements, market trends, and potential barriers to sustainable growth in the PV industry. Our methodology involves an extensive review of academic journals, industry reports, and market analyses to compile current knowledge and identify gaps in the literature. Preliminary results indicate significant advancements in production efficiency and cost reduction, making solar energy increasingly accessible and competitive. However, challenges such as geopolitical tensions affecting material availability, environmental concerns regarding the lifecycle of PV products, and infrastructure limitations persist. This study underscores the need for innovations in recycling and waste management of PV materials, along with policy support and international cooperation to ensure a resilient and sustainable PV supply chain. By understanding the dynamics and complexities of this supply chain, stakeholders can better navigate and contribute to the growth of the solar energy industry.

Keywords: Photovoltaic Energy, Photovoltaic Supply Chain, Renewable Energy, PV Systems, Sustainable Growth.

Developing Circular Economy Through Sustainable Production of Biofuels Using Electrochemical Systems

Mohammad Zain Khan[1]*

[1]*Electrochemical Research Laboratory, Department of Industrial Chemistry, Faculty of Science, Aligarh Muslim University, Aligarh 202002, UP India*

*Email: dr_mzain.ch@amu.ac.in

Abstract. The transition to a circular economy necessitates innovative approaches to resource management and energy production, with one promising strategy being the sustainable production of biofuels using electrochemical systems. This approach integrates renewable electricity with biomass conversion processes to create a closed-loop system that minimizes waste and maximizes resource efficiency. This research aims to explore the potential of electrochemical systems in the sustainable production of biofuels, evaluating their efficiency, scalability, and environmental benefits. Principal methods involve a comprehensive review of existing literature, focusing on microbial electrolysis cells, electrochemical CO_2 reduction, electrode materials and reactor design advancements, and process optimization techniques. The findings underscore the significant potential of electrochemical systems to contribute to a circular economy, with recent technological advancements enhancing their viability for large-scale implementation. Further research and development are essential to address remaining challenges and fully realize the potential of these systems in achieving environmental sustainability and energy security.

Keywords: Bioelectrochemical systems; Circular economy; Biorefinery; Microbial electrosynthesis; Methanol

Improving power sharing and enhancing the stability of an isolated AC microgrid by implementing droop control and virtual impedance

Abdelaziz Youssfi[1]*, Youssef Ait El Kadi[2],

[1]*Engineering and Applied Physics Research Team (EAP), High School of Technology, Sultan Moulay Slimane University, Beni Mellal, Morocco*
[2]*Engineering and Applied Physics Research Team (EAP), High School of Technology, Sultan Moulay Slimane University, Beni Mellal, Morocco*

*Email: abdelaziz.youssfi@usms.ma

Abstract. The stability and accuracy of power sharing between DGs in isolated microgrids are key points for favoring renewable energy sources within a wider operating margin to extract the maximum available power. The conventional droop control method CDC and the improved virtual impedance droop control CDC-VI are proposed in this work to enhance the stability, improve the speed, robustness and accuracy of power distribution between two parallel DGs feeding tow linear loads of different types connected to the AC bus within an isolated AC microgrid. A Matlab/Simulink simulation is carried out to validate our proposal: robustness, accuracy of power sharing between DGs and stability are well improved by the implementation of the proposed CDC and CDC-VI controllers.

Keywords: Microgrids; Droop Control; Robust Droop Control; Virtual Impedance; Power Sharing

Urbanization, Industrialization and Carbon Emission on the Short and Long-Term Economic Growth: Encouraging Sustainable Cities in ASEAN Countries

Dessy Rachmawatie[1,2]*

[1]*Magister of Economics, Postgradate School, Universitas Muhammadiyah Yogyakarta, Kasman Singodimedjo Postgraduate School Building 1st Floor of UMY Integrated Campus, Brawijaya Road, Tamantirto, Kasihan, Bantul, Yogyakarta,55183, Indonesia*
[2]*Department of Economics, Universitas Muhammadiyah Yogyakarta, 2nd Floor Ki Bagus Hadikusumo Building, UMY Integrated Campus, Brawijaya Road, Tamantirto, Kasihan, Bantul, Yogyakarta,55183, Indonesia*

*E-mail : d.rachmawatie@umy.ac.id

Abstract. The purpose of this research is how influences urbanization, industrialization, and carbon emission on economic growth in Six ASEAN countries (2000-2022). The data used in this research is annual data for the period 2000-2002 taken from the World Bank Data. The estimation tool used in this research is using the *Vector Error Correction Model* (VECM). The research results show that in the short term, urbanization is insignificant, but has a negative and significant in the long term (-0.003). Industrialization is positive and significant in the short term (0.262) and significant in the long term (2.475). Carbon emission is insignificant in the short term but has a negative and significant in the long term (-3.758). These findings research shows that the findings of this research show that cities in six ASEAN countries, especially cities that are industrial cities and urbanization destination areas, must from now on develop and prioritize the use of new and renewable energy sources, because based on the results of this research, these efforts able to have a significant impact on economic growth in the six ASEAN countries in the long term. The importance of the energy transition in the future in increasing economic growth and increasing sustainable cities.

Keywords: ASEAN countries; Carbon emission; Industrialization; Long and short term; Urbanization

Solar Drying Of Agricultural Produce

Rachida Ouaabou[1]*, Lahcen Hssaini[2], Said Ennahli[3], Jalal Isaad[1]

[1]*Laboratory of research and development in engineering sciences, Faculty of Sciences and Techniques Al Hoceima, Abdelmalek Essaadi University*
[2]*National Institute of Agricultural Research, Avenue Ennasr, P.O. Box 415 Rabat Principale, 10090 Rabat, Morocco*
[3]*Laboratory of Food and Food By-Products Chemistry and Processing Technology, Ecole Nationale d'Agriculture de Meknès (ENAM), Meknes 50001, Morocco*
*Email : *r.ouaabou@uae.ac.ma*

Abstract. Solar drying is a sustainable and cost-effective method for preserving agricultural produce, particularly fruits, in regions with ample sunshine. Thus, the present work studies the application of solar drying techniques for Moroccan fruits. Morocco's diverse climatic conditions are well-suited for solar drying, with high levels of solar irradiation throughout the year. The process involves placing freshly harvested fruits on elevated, ventilated drying beds or trays and exposing them directly to sunlight. As the moisture in the fruits evaporates, their shelf life and nutrient content are preserved, making them suitable for long-term storage and transportation. Several factors influence the efficiency of solar drying, including air temperature, relative humidity, the physical properties and bioactive compounds of the fruits. Research has demonstrated that careful optimization of these parameters can significantly enhance the drying rate and product quality. The adoption of solar drying technology can offer numerous benefits to Moroccan fruit producers. It reduces post-harvest losses, minimizes the need for energy-intensive mechanical drying, and allows for the preservation of natural flavors and nutritional value. Moreover, the low operational costs associated with solar drying can improve the economic viability of small-scale farming operations, supporting rural livelihoods and contributing to the country's food security .

Keywords: solar drying; Moroccan fruits; Quality; Storage.

A Bibliometric Analysis of Outdoor Thermal Comfort Research in Smart Cities: Trends and Methodologies

Safae Ahsissene[1]*, Fatima Zahrae Rhziel[1], Naoufal Raissouni[1]

[1]*Remote Sensing, Systems and Telecommunications Research Laboratory, National School of Applied Sciencesof Tetuan, Abdelmalek Essadi University, Tetuan 2121, Morocco*
*Email : safae.ahsissene@gmail.com

Abstract. This study conducts a comprehensive bibliometric analysis to assess how thermal comfort is addressed in smart city research and to categorize the methodologies used, including traditional questionnaires, simulations, temperature measurements, and other approaches. Rapid urban development and climate change have made maintaining thermal comfort in both outdoor and indoor environments increasingly challenging. Understanding thermal dynamics is crucial for sustainable urban planning and effective mitigation strategies.Data from Web of Science and Scopus were combined, yielding 314 relevant papers. After removing duplicates, 207 unique records were analyzed. CiteSpace was utilized to identify key publications, authors, research trends, and emerging topics. Studies were categorized based on their methodologies: questionnaires, simulations, temperature measurements, and innovative approaches.Preliminary analysis shows a significant increase in publications over the past decade, indicating growing interest in thermal comfort within smart cities. The research identified various approaches: 35% used questionnaires, 40% employed simulation tools, 20% relied on direct temperature measurements, and 5% used alternative methods. Key trends and methodological shifts were highlighted, reflecting the evolution of research practices in this field.This bibliometric analysis provides valuable insights into the research landscape of thermal comfort in smart cities. The findings underscore the importance of a multidisciplinary approach that incorporates both conventional and innovative methodologies. These insights can inform future research and urban planning strategies, contributing to the development of more resilient and sustainable urban environments.

Keywords: Climate mitigation; Simulation tools; Smart cities; Sustainable urban planning; Thermal comfort

Kinetic Analysis And Thermal Behavior Of Main Components Of Redwood (Pinus Sylvestris L.)

N. ANTER [1]*, M. Y. GUIDA [1], A. CHENNANI[1], A. MEDAGHRI-ALAOUI [1.2], A. HANNIOUI [1.2]

[1] *Molecular Chemistry, Materials and Catalysis Laboratory, Faculty of Sciences and Techniques (FST-BM), University of Sultan Moulay Slimane (USMS), 23000, Béni-Mellal, Morocco.*

[2] *Department of Chemistry and Environment, Faculty of Sciences and Techniques (FST-BM), University of Sultan Moulay Slimane (USMS), 23000, Béni-Mellal, Morocco.*

*Email : nadia.anter@usms.ma

Abstract. In this scientific study, the thermochemical conversion of redwood (RW) was investigated. Using thermogravimetric analysis (TGA), the thermal behavior of RW samples was examined at four heating rates ranging from 5 to 20 K min^{-1} in an inert atmosphere between 300 and 900 K. The study had two main objectives: first, to determine the kinetic decomposition parameters of RW (Pinus sylvestris L.); second, to analyze the variation of characteristic parameters from TG-DTG curves of RW's main components, such as cellulose, hemicellulose, and lignin. The kinetic analysis was performed using three isoconversional methods (Vyazovkin, Friedman, and Flynn-Wall-Ozawa), the Avrami theory method, and the integral master-plots method to estimate activation energy (Ea), reaction order (n), pre-exponential factor (A), and kinetic model (f(x)) for the thermal decomposition of cellulose, hemicellulose, and lignin. The TG and DTG curves revealed three stages in the thermal decomposition of RW: the first stage corresponds to hemicellulose decomposition, the second to cellulose, and the third to lignin. For the conversion degree range investigated ($0.1 \leq x \leq 0.7$), the mean values of apparent activation energies for RW biomass were 127.60–130.65 KJ mol^{-1} for hemicellulose, 173.74–176.48 KJ mol^{-1} for cellulose, and 197.21–200.36 KJ mol^{-1} for lignin. The corresponding mean values of reaction order (n) were 0.200 for hemicellulose, 0.209 for cellulose, and 0.047 for lignin. The average values of the pre-exponential factor for the three RW components ranged from 0.083×10^{12} s^{-1} to 3.693×10^{16} s^{-1}.The experimental data for RW overlapped with D4, D2, and F3 models in the conversion degree ranges of 10-30%, 30-55%, and 55-70%, respectively.

Keywords: Thermogravimetric Analysis; Redwood; Kinetic Study; Isoconversional Models; Master-plots models.

Comparative study of the performance of packed beds using different types of thermal storage materials

Aicha Eddemani [1]*, Ahmed Aharoune [1], Lahcen Bouirden [1], Ahmed Ihlal [2]

[1]*Thermodynamic and Energetics Laboratory, Physics Department, University of Ibn Zohr, 80090, Agadir, Morocco*
[2]*Materials and Renewable Energies Laboratory, Physics Department, University of Ibn Zohr, 80090, Agadir, Morocco*
*Email : eddemani.aicha@gmail.com

Abstract. In packed bed thermal energy storage systems, the selection of a suitable storage material as a packing material depends on several factors, including specific heat capacity, desired temperature range, heat transfer properties, thermal stability, cost effectiveness and availability. This work presents a comparative study of some thermal storage materials. A numerical method, subsequently confirmed by experimental results, was used to analyse the performance of the studied packed beds, taking into account the thermophysical characteristics of the different storage materials studied. Numerical simulations were carried out during the charging and discharging processes. The results have shown that the thermal stratification and the efficiency of the system are significantly influenced by the materials under investigation.

Keywords: Thermal storage; Packed bed; Solar energy; CFD; Heat storage material.

Is there a relationship between renewable energy consumption and CO_2 emissions in morocco: an empirical investigation using the toda yamamoto approach

Abdelaziz AGUILAL [1]*, Benaceur OUTTAJ [1]

[1] *Laboratory of Economic analysis and Modeling (LEAM)Faculty of Law, Economics and Social Sciences –Souissi Mohammed V University -Rabat, Morocco*

*Email : abdelaziz.aguilal@um5s.net.ma

Abstract. In recent years, Morocco has experienced substantial economic and demographic growth. Despite relatively low levels of greenhouse gas (GHG) emissions, the country remains vulnerable to the harmful effects of climate change, facing increasing challenges related to its natural resources. In response to this risk, Morocco has made significant decisions to address climate change and has developed various sectoral strategies to integrate environmental considerations into multiple sectors such as energy, transport, agriculture, and tourism. This involves a strategic focus on adopting renewable energies as the main catalyst for reducing CO2 emissions, the primary greenhouse gas. This research aims to study the impact of the amount of renewable energy consumed (RE) on carbon dioxide (CO2) emissions in Morocco between 1990 and 2021. The Toda-Yamamoto causality test is applied to highlight the dynamic link between the two variables. A neutral correlation is empirically detected, suggesting that renewable energy has not yet achieved the autonomy to reduce emissions independently. This deviation from conventional hypothetical expectations underscores the need for a nuanced understanding of the complex mechanisms linking the two variables studied. The results of this research have substantial implications for policymakers and economists, offering a critical perspective to reassess existing policies and explore alternative pathways through which renewable energies can effectively reduce CO2 emissions in Morocco. This study can contribute to the discourse on sustainable energy development by highlighting the importance of well-founded policies that consider the multifaceted dynamics between the integration of renewable energies and CO2 emission levels.

Keywords: Causality test; CO2 emissions; Morocco; Renewable energy; Toda yamamoto

Organometallic Complexes Based on Copper (I) for Light Energy Conversion

Afaf EL AZZAOUI*[1], Othmane ESSAHILI[1], Abdelmajid AL MAGGOUSSI [1,2], Mohamed ILSOUK[1]

[1]*Applied Chemistry & Engineering Research Center of Excellence (ACER CoE), University Mohammed IV Polytechnic, Benguerir, Morocco*
[2] *Laboratory of Innovative Materials, Energy and sustainable Development, Department of Physics, Faculty of Sciences and techniques, University Cadi Ayyad, Marrakech BP 2390, Morocco*
* afaf.elazzaoui@um6p.ma

Abstract. In order to meet the requirements of energy sustainability, copper coordination complexes have attracted great deal of attention due to their abundance, low cost and low toxicity, as well as their excellent photostability and high efficiency in electron and energy transfer processes. These characteristics make them promising candidates for various energy-related applications such as Dye-Sensitized Solar Cells (DSSCs), in which they exhibit significant photovoltaic performance, rivalling traditional sensitizers, also in the development of new materials with interesting electroluminescence properties for Organic Light-Emitting Diodes (OLEDs). In this study, a newly developed family of luminous copper(I) complexes, with formula Cu(POP)(NN) (POP = Bis[(2-diphenylphosphino)phenyl] ether, NN = 1,10-phenanthroline), have been synthesized. All complexes were characterized in terms of structure using Fourier Transform Infrared (FTIR), Nuclear magnetic resonance (^{1}H NMR), and single-crystal X-ray diffraction and thermal stability. The Photophysical and electrochemical properties, have been investigated and demonstrate that increasing π-conjugation and donor substituents (-CH_3) on the coordinated ligands has significant effect on the absorption and emission properties, as well as on the HOMOLUMO energy gap of the corresponding complexes.

Keywords: Complexes; Copper; Efficiency; Energy conversion; Quantum Yield

Enhancing Greenhouse Agriculture: A Study on Passive Solar Heating Using Water-Filled Sleeves for Improved Microclimate and Yield

L.Gourdo[1]*, H.Fatnassi[2], A.Chraibi[4], H. Demrati[1], K.Achgar[1] , A.Wifaya[3], R. Bouharroud[3], A.Aharoune[1], L.Bouirden[1]

[1]*Thermodynamics and Energetic Laboratory, Faculty of Sciences, Agadir, Morocco*
[2] *INRA, Univ. Nice Sophia Antipolis, CNRS, UMR 1355-7254 Institut Sophia Agrobiotech, 06900 Sophia Antipolis, France*
[3] *Regional Centre of Agricultural Research, Agadir, Morocco*
[4] *Association Marocaine des Producteurs et Producteurs Exportateurs des Fruits et Légumes*
**Email : lahoucine.gourdo@edu.uiz.ac.ma*

Abstract. Heating agricultural greenhouses is essential, particularly in the winter when the air temperature inside the greenhouse is below the optimal level for plant growth. Solar heating has garnered significant attention due to its numerous advantages, unlike traditional systems that rely on expensive and polluting fossil fuels. This study explores the performance and efficiency of a solar passive water-sleeve heating system installed under a multi-span greenhouse. The aim is to enhance the thermal environment within the greenhouse, thereby improving plant growth and extending the growing season. The research involves the design, implementation, and evaluation of the heating system, which utilizes solar energy to maintain optimal temperatures. The solar passive water-sleeve heating system presents a viable and sustainable solution for greenhouse heating. By harnessing solar energy, it reduces reliance on conventional energy sources, lowers operational costs, and enhances plant growth conditions. This study demonstrates the system's effectiveness and provides a foundation for further research and development in sustainable greenhouse technologies.

Keywords: solar energy, solar heating system, greenhouse, tomato

Synthesis and DFT studies, of epoxidation reactions of halogen derivatives of himachalen with m-CPBA

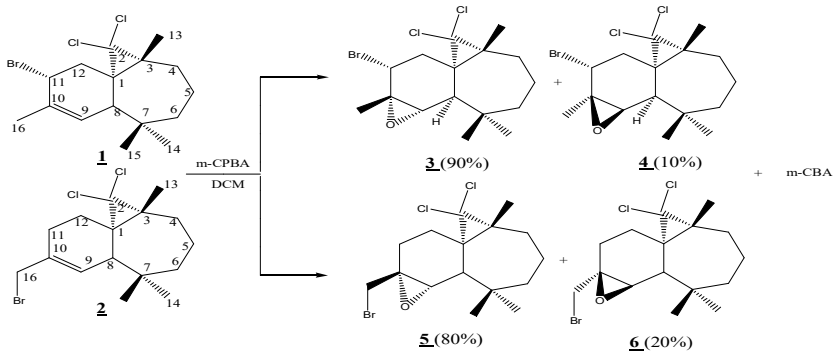
Ilham AIT BRAIM[1*], Anas Ouled Aitouna[2], Abdellah Zeroual[2], Ahmed BENHARREF[1], Ahmed CHEKROUN[1].

[1] *Laboratory of chemistry of natural substances, Faculty of Sciences Semlalia, Cadi Ayyad University, P.O. Box 2390, Marrakech, Morocco.*

[2] *Molecular Modelling and Spectroscopy Research Team, Faculty of Science, Chouaïb Doukkali University, P.O. Box 20, 24000 El Jadida, Morocco.*

*Email : ilhamaitbraim@gmail.

Abstract. Epoxides are widely used in various industrial sectors due to their unique characteristics, making them materials of great commercial importance. The two epoxy formed 3 and **5** were synthesized by epoxidation of himachalene **1** and **2** derivatives by deploying metachloroperbenzoic acid (mCPBA) in room temperature dichloromethane. The compound structures were identified using spectroscopic techniques, including ^{1}H and ^{13}C NMR.



In parallel, a computational analysis was performed using the functional density theory (DFT) at the level wb97xd/6-311+G (d,p), which is consistent with the experimental results obtained.

Keywords: Epoxidation reaction; wb97xd/6-311+G (d,p); DFT calculations; Reactivity.

Opportunities in Implementing Solar Energy Technologies in Moroccan Greenhouses

L.Gourdo[1*], H.Fatnassi[2], K.Achgar[1] , H.Demrati[1], F.Z. Allali[1] , A.Wifaya[3], R.Bouharroud[3], A.Aharoune[1], L.Bouirden[1]

[1]*Thermodynamics and Energetic Laboratory, Faculty of Sciences, Agadir, Morocco*
[2] *INRA, Univ. Nice Sophia Antipolis, CNRS, UMR 1355-7254 Institut Sophia Agrobiotech, 06900 Sophia Antipolis, France;*
[3]*Regional Centre of Agricultural Research, Agadir, Morocco*
*Email : lahoucine.gourdo@edu.uiz.ac.ma

Abstract. The incorporation of solar energy technologies into Moroccan greenhouses shows great potential in revolutionizing agricultural practices. These innovative solutions, by promoting sustainability and resilience, can contribute to achieving a more efficient and environmentally friendly agricultural future in Morocco. This review emphasizes the significance of adopting solar energy to meet the increasing demand for sustainable agriculture and outlines the steps required to encourage widespread adoption. Integrating solar energy technologies into Moroccan agriculture offers a range of benefits. Not only can it enhance productivity and crop quality, but it also provides a means to reduce the environmental impact of traditional agricultural methods. By harnessing solar power, farmers can decrease their reliance on fossil fuels, contributing to Morocco's efforts to combat climate change.

Keywords: Solar energy, Moroccan greenhouses, Climate change.

The impact of climatic variability on water resources in the Ouaoumana River basin in the Middle Atlas of Morocco (November 2021-May 2022)

Omaima Elkbichi[1*], Layati Elhoucein[1], Mohamed Elghachi[3]

[1] *Landscape Dynamics, Risks, and Heritage Laboratory, Sultan Moulay Slimane University, Faculty of Letters and Human Sciences, Beni Mellal, Morocco*
Corresponding author's e-mail address: omaymaelkbichi@gmail.com

Abstract. Today, in the context of climate change and growing demand for water, Morocco's currently available water resources have become very fragile. This study is based on the evaluation and quantification of the water resources of the Ouaoumana River basin, which belongs to the Oum ER-Rabia basin and is located in the Middle Atlas between longitudes 5°43' and 5°50' and latitudes 32°33' and 32°36'. The water resources of the Oued de Ouaoumana watershed, which play several roles (filling the Ahmed El Hansali dam, irrigation, etc) are experiencing numerous disturbances caused by climatic variability, high demand and overexploitation of the water table. To implement our study we will rely on two methodologies, the first a quantitative hydrological methodology based on flow measurements in several points in the River from upstream to downstream during the period (November 2021 - May 2022) to produce hydrometric data and then extract the spatio-temporal variation of flows, and secondly, a statistical methodology for analysing climatic data (rainfall, temperature) from the Taghzoute station, which is located downstream of this River basin, on an annual, monthly and seasonal scale, in order to gain a good understanding of the climatic functioning and the rainfall-discharge relationship in this River basin. These results will contribute to the sound management of the basin's water resources, especially in times of water shortage, and will also preserve the biological diversity of the River, which is now threatened with extinction.

Keywords: River Ouaoumana (Morocco), climatic variability, Water resources , hydrometry , Variability of flows

Spatio-Temporal Variability of Urban Maximum Summer Temperatures in July 2022 in Kasba Tadla, Morocco

Souad Ourabit[1], Mohamed Elghachi[1]

Landscape Dynamics, Risks, and Heritage Laboratory, Sultan Moulay Slimane University, Faculty of Letters and Human Sciences, Beni Mellal, Morocco

Corresponding author's e-mail address: souadourabit1@gmail.com

Abstract. Urban climate is characterized by local modifications of atmospheric conditions, often influenced by urbanization, heat islands, and human activities, creating a distinct thermal environment within urban areas. This study falls within the theme of urban climate and focuses on understanding the spatio-temporal variability of temperature within the city of Kasba Tadla. The objective is to analyze local climatic conditions to better understand the issues related to urban climate in this region. This study analyzed the spatio-temporal dynamics of maximum summer temperatures and the intensity of the urban heat island effect in the city of Kasba Tadla during the hottest month of July. Kasba Tadla is part of the Beni Mellal-Khénifra region of Morocco. Its specific geographical position offers a diverse context for the study of urban climate, with potential influences from local topography, urbanization, and other environmental factors. For the implementation of our study, four thermometers were strategically installed throughout the city to record the temperature every hour. The methodology also included geo-analysis techniques for spatial mapping of temperature and the identification of thermally distinct areas. The collected data provides a detailed temporal basis for analyzing temperature fluctuations. This data will enable an in-depth understanding of the urban thermal dynamics in the region. The expected results will provide a detailed mapping of the spatial distribution of maximum summer temperatures in Kasba Tadla, highlighting their daily temporal variability, specific thermal areas, and potential correlations with local factors such as urbanization and topography. These findings will contribute to a better understanding of the urban climate in the region and could inform adaptation measures to mitigate the effects of urban heat islands.

Keywords: Urban climate, spatio-temporal analysis, Heat islands, Urbanization, City of Kasba Tadla, Morocco

Energy Management Strategy for Hybrid PV and Fuel Cell Systems: A Case Study in Morocco (Essaouira) city

Abssane Sara[1], Outzourhit Abdelkader [2], Amatoul Fatima-Zahra[1,2]

[1] *Department of physique and science. Laboratory of Materials, Energy and Environment, Cadi Ayyad University, Faculty of science Semlalia, Marrakech 40000, Morocco*

[2] *Department of Physique and Science Laboratory of Environmental Science and Sustainable Development, Cadi Ayyad University, High School of Technology Essaouira,44000, Morocco*

Abstract. The global increase in energy consumption, driven by rapid population growth and urbanization, underscores the urgent need for sustainable energy solutions. The reliance on fossil fuels since the Industrial Revolution has significantly contributed to greenhouse gas emissions and global warming, necessitating a transition to renewable energy sources. However, the intermittency of renewable energy sources like solar and wind presents challenges. To address this, integrating energy storage systems such as batteries and hydrogen storage becomes essential. Hydrogen, produced via electrolysis using renewable energy, serves as a clean fuel and an efficient energy carrier. This study develops and simulates a hybrid renewable energy system combining photovoltaic (PV) panels, an electrolyzer, and a fuel cell, aiming to provide a reliable and sustainable power supply for a small community in Essaouira, Morocco. The system's performance is evaluated under various environmental conditions, focusing on hydrogen production and power generation efficiency. The results demonstrate the system's potential to meet the community's energy demands, highlighting the importance of energy management strategy and storage solutions in achieving energy sustainability.

Exploring the structural, electronic, and optical properties of $CaGa_2X_4$ (X = S, Se) chalcogenide spinels for potential solar cell applications: DFT study

Ibtissam Jamaï[1]*, Meryem ziati[2], Naoual Bekkioui[3], Hamid Ez-zahraouy[4]

Laboratory of Condensed Matter and Interdisciplinary Sciences,"Unité de recherche labellisée CNRST" Faculty of Sciences, Mohammed V University in Rabat, Morocco.
*Email : ibtijam98@gmail.com

Abstract. The main purpose of this study is to explore the structural, electronic and optical properties of $CaGa_2X_4$ (X = S, Se) materials for their applications in solar cells, using density functional theory (DFT) calculations in Wien2K software. Structural properties reveal that both compounds possess a cubic phase with the space group Fd-3m (n°227). The stability of both compounds is verified by the negative formation energy. Band structure calculations, using the modified Becke-Johnson potential (TB-mBJ), indicate that $CaGa_2S_4$ and $CaGa_2Se_4$ possess direct band gaps of 1.956 eV and 1.120 eV for $CaGa_2S_4$ and $CaGa_2Se_4$, respectively. Optical properties are examined via absorption, optical conductivity, dielectric function, optical bandgap and Urbach tail. These calculations indicate significant absorption and optical conductivity in the visible range for both materials. Overall, these results suggest that $CaGa_2X_4$ (X = S, Se) chalcogenide spinels are promising as candidate materials for solar cell applications.

Keywords: Density functional theory; Chalcogenide spinel; Structural properties; Electronic and optical properties; Wien2K.

A First-Principles Study of the Indium Halide Perovskites $RbInX_3$ (X= F, Cl, Br, I) for Photovoltaic and Photocatalytic Applications

Mihade El Akkel[1]*, Mounia Achqraoui[1], Hamid Ez-zahraouy[1]

[1] *Laboratory of Condensed Matter and Interdisciplinary Sciences, Unité de Recherche labellisée CNRST, URL-CNRST-17, Faculty of Sciences, Mohammed V University of Rabat, Morocco*

*Email : mihade_elakkel@um5.ac.ma

Abstract. Due to their relevant properties, lead-free halide perovskites have attracted wide attention in the scientific community. This study investigates the structural, mechanical, electronic, optical, and photocatalytic properties of the Indium-based halide perovskites $RbInX_3$ (X= F, Cl, Br, I) based on the density functional theory (DFT) using the WIEN2k package. The results show that $RbInI_3$ exhibits a metallic behavior, while $RbInBr_3$, $RbInCl_3$, and $RbInF_3$ exhibit semiconducting behavior with bandgap energies of 0.67, 1.43, and 2.45 eV, respectively. The high optical absorption and corresponding band gap energies make them good candidates for photovoltaic applications. In addition, the $RbInF_3$ compound exhibits good photocatalytic performance since it satisfies the thermodynamic requirements needed to trigger the water-splitting reaction. This study also allows us to analyze the influence of halogen substitution on the properties of the compound $RbInX_3$. Moreover, it will open the way to the experimental community as it is the first to study the properties of these perovskites.

Keywords: Perovskites; Hydrogen production; Water splitting; Photovoltaic solar cells; DFT

Experimental study of falling film evaporation on a vertical plate

Hayat El Baamrani [1]*, Abdelaaziz Yagourb [2], Ahmed Aharoune [1], Abdallah Boukhris [1]

[1]*Thermodynamics and Energetics Laboratory, Faculty of Science, Ibn Zohr University, BP8106, 80006 Agadir, Morocco*
[2]*Electronic, signal processing and physical modeling Laboratory, Faculty of Science, Ibn Zohr University, BP8106, 80006 Agadir, Morocco*

*Email : hayatelbaamrani92@gmail.com

Abstract. A long experimental device (0.33 x 1.0 x 0.015 m) is used to study the evaporation of a liquid film falling on a plate. The plate is heated by Joule effect using a heating plate to simulate solar heat flux. Heat flux density, mass flow rate and plate length are the operating parameters that primarily influence the thermodynamic state of the liquid film. It is shown that these parameters influence the temperature distribution along the plate and the evaporation rate of the film, as well as the extent of the vaporization surface. Experimental results have enabled us to plot temperature profiles along the plate and determine the parameters influencing evaporation efficiency and the amount of steam produced per hour of experimental set-up used. Particular attention was paid to the operating parameters that can be controlled by the user. The results show that the best performance of the device is obtained when it is used around an operating point linked to these operating parameters. The estimated efficiencies are excellent and very high compared with those obtained in systems of similar dimensions in the literature.

Keywords: Heat and mass transfer; Evaporation; Liquid film; Vertical plate; Experimental study.

Study of the Gravimetric, Electronic and Thermoelectric Properties of $XAlH_3$ (X = Be, Na, K) as hydrogen storage perovskite using DFT and the BoltzTrap Software Package

Ayoub Koufi[1,2*], Younes Ziat[1,2], Hamza Belkhanchi[1,2]

[1]*Engineering and Applied Physics Team (EAPT), Sultan Moulay Slimane University, Beni Mellal, Morocco*

[2]*The Moroccan Association of Sciences and Techniques for Sustainable Development (MASTSD), Beni Mellal, Morocco*

*Email : ayoub.koufi@uit.ac.ma

Abstract. In the context of density functional theory (DFT), this study examines the structural, electronic, gravimetric and thermoelectric properties of perovskite compounds XAlH$_3$ *(X = Be, Na and K)* using the generalized gradient approximation (GGA). Calculations were performed with the BoltzTrap software package integrated into the Wien2k code, enabling analysis of total energy and atomic volume using the Murnaghan equation of state. The results show that the materials behave like conductors due to the overlap of the conduction band and the valence band, with a zero-band gap. NaAlH$_3$ and KAlH$_3$ show increasing electrical and thermal conductivity with temperature, while BeAlH$_3$ exhibits non-linear behavior, peaking at 400 K. These results suggest that XAlH$_3$ materials are promising for hydrogen storage applications and thermoelectric devices, underlining their potential to support a sustainable hydrogen economy.

Keywords: Electrical; Hydrogene storage; Merit factor; XAlH$_3$.

Tensile Effect on Photocatalytic and Optoelectronic Properties of MoS_2 for Hydrogen Production: DFT Study

Mounia Achqraoui[1]*, Houda Jebari [1], Naoual Bekkioui [1], Hamid Ez-Zahraouy [1]

[1] *Laboratory of Condensed Matter and Interdisciplinary Sciences, Unité de Recherche Labellisée CNRST, URL-CNRST-17, Faculty of Sciences, Mohammed V University of Rabat, Morocco*

*Email : mounia_achqraoui@um5.ac.ma

Abstract. The structural, electronic, optical, and photocatalytic properties of MoS_2 compound are investigated by the density functional theory approach using the WIEN2k package. The results revealed that applying the tensile effect can significantly impact the material's properties. MoS_2 is an indirect p-type semiconductor with a bandgap energy of 1.45, 1.45, and 2.04 eV along [100], [010], and [001], respectively. The bandgap decreases as the percentage of applied tensile effect increases. The findings of this work showed that the photocatalytic capacity of MoS_2 is improved with the application of the tensile strain.

Keywords: DFT; Hydrogen production; MoS_2; Photocatalytic; Tensile effect

Development of Polymer-graphite Composites as Electrodes for Methanol-operated Microbial Fuel Cells

Hassan Haddouchy[1*], Mustapha Oukbab[2], Youness Tahiri[2], Saliha Loughmari[3] , Mohamed Oubaouz[2], Abdelilah Chtaini[2] and Salah Eddine El Qouatli[1]

[1]*Laboratory of Physical Chemistry Environment and Material, Moulay Ismail University, Faculty of Sciences and Technologies, Boutalamine 52000 Errachidia , Morocco.*

[2]*Electrochemistry and Molecular Inorganic Materials Team, Faculty of Sciences and Technology, Sultan Moulay Slimane University, Mghilla Campus, BP 523, 23000, Beni Mellal, Morocco.*

[3]*Laboratory of Industrial Engineering and Surface Engineering, Applied Chemistry and Environmental Sciences Team, Sultan Moulay Slimane University, FST-BM, P.B 523, 23 000, Beni-Mellal, Morocco.*

*Email : ha.haddouchy@gmail.com

Abstract. This work focuses on the study of the biocatalyzed electrolytic oxidation of methanol by bacteria in a 1M Na_2SO_4 solution, using a carbon paste electrode modified with a block-styrene polymer. The electrode was obtained by immersing the carbon paste electrode in the polymer for 3 hours, ensuring that the surface of the CPE was uniformly covered with a polymer film. The prepared electrode demonstrated high activity in methanol oxidation. Subsequently, we studied the electrode behavior using voltammetry techniques, employing the Volta Lab PGZ100 potentiostat. The results of these techniques highlighted the existence of a catalytic effect, leading to improved performance in the methanol oxidation process by bacteria.

Keywords: Fuel cells; Methanol; Cyclic voltammetry; optical microscopy.

Exploring the Photocatalytic Characteristics of Perovskite ABX_3 for Optimized Hydrogen Generation

Doha Kabouchi* , El Mehdi Salmani, Hamid Ez-Zahraouy, Abdelaziz Mhirech and Halima Zaari

Laboratory of Condensed Matter and Interdisciplinary Sciences (LaMCScI), Research Unit Labelled CNRST, URL-CNRST-17, Faculty of Sciences, Mohammed V University in Rabat, Morocco

E-mail: doha.kabouchi@um5r.ac.ma

Abstract. Renewable energies stand at the forefront of achieving a sustainable future, with hydrogen playing a pivotal role as a clean energy carrier. In the search for eco-friendly solutions, hydrogen production emerges as a critical area, demanding innovative approaches to enhance its efficiency and sustainability. Therefore, the focus of this study is to explore the potential use of the nanomaterial perovskite ABX3 in enhancing hydrogen production efficiency. This work employs first-principle study calculations to delve into its photocatalytic behavior and interaction with water molecules, aiming to unlock insights into optimizing hydrogen generation. These findings show that this nanomaterial is a promising candidate for hydrogen production and highlight its exceptional catalytic properties that could significantly improve hydrogen efficiency, marking a significant step forward in the development of renewable energy solutions. By improving the efficiency and sustainability of hydrogen production, this research contributes to the reduction of carbon emissions and the advancement of cleaner, greener energy systems, aligning with global efforts to combat climate change and protect the environment.

Keywords: Renewable energies solutions - Hydrogen production - Perovskites ABX_3 -First principle study calculations

Comparative Study of Two ANFIS-Based MPPT Controls under Uniform and Partial Shading Conditions

Mohamed Amine Atillah[1]*, Hicham Stitou[1], Abdelghani Boudaoud[1], Mounaim Aqil[1]

[1]*Engineering and Applied Physics Team (EAPT), Superior School of Technology, Sultan Moulay Slimane University, Beni Mellal, Morocco*

*Email : mohamedamine.atillah@usms.ma

Abstract. In a world where the energy transition to renewable energies is becoming a priority, photovoltaic systems are increasingly important to ensure a sustainable and autonomous power source by exploiting the inexhaustible power of the sun. The power supplied by photovoltaic panels directly depends on climatic conditions, particularly irradiation and temperature. To maximize the energy extracted, it is necessary to use a Maximum Power Point Tracking (MPPT) control. When certain parts of the photovoltaic array are exposed to reduced irradiation, partial shading occurs. This phenomenon results in an uneven distribution of solar energy over the panels, leading to changes in their electrical characteristics. However, the performance of MPPT controls can be disrupted by partial shading conditions, complicating optimal operation. The aim of this work is to study two MPPT controls based on the adaptive neuro-fuzzy inference system (ANFIS) technique with different principles and to analyze and compare their performance in extracting the maximum power available from photovoltaic panels, under uniform and partial shading conditions. The first method combines ANFIS and a fuzzy logic controller, while the second uses ANFIS alone. The comparison will focus on speed, accuracy and stability, as well as the components required for each method. The results show that both methods perform similarly in terms of accuracy and stability, since they are able to extract almost the same power and exhibit the same level of oscillation. However, the second method, which excludes the use of an additional controller, is faster in extracting power and reduces the number of components in the photovoltaic system by eliminating the fuzzy controller, thus improving the system dimensions.

Keywords: ANFIS; MPPT techniques; PARTIAL shading; PHOTOVOLTAIC energy; RENEWABLE energy

DFT and BoltzTrap investigations on the thermal and structural characteristics of the perovskite $MgCuH_3$ and $MgCoH_3$

Ayoub Koufi [1,2], Younes Ziat [1,2], Hamza Belkhanchi [1,2], Abdellah Bouzaid [1,2]

[1] *Engineering and Applied Physics Team (EAPT), Superior School of Technology, Sultan Moulay Slimane University, Beni Mellal, Morocco*
[2] *The Moroccan Association of Sciences and Techniques for Sustainable Development (MASTSD), Beni Mellal, Morocco*

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; Thermal conductivity, Seebeck coefficient; Thermoelectric figure of merit

Impact des projets d'aménagement de la vallée de Bouregreg sur les activites socioéconomiques de l'estuaire du Bouregreg

NOUGA Chaymaa*, Mme CHERKAOUI Essediya & KHAMAR Mohamed.

Civil Engineering and Environment Laboratory (LGCE), Materials, Water and Environment Team, Higher School of Technology of Sale, Mohammed V University in Rabat, Morocco

*Email : nougachaymaa@gmail.com

Abstract. Oued Bouregreg is one of the Moroccan heritage, took its source in the Middle Atlas, after a long course of 23km, it is extended by a wide estuary on the Atlantic coast at 34°N and 6°50' W, bounded by the Sidi Mohammed Ben Abdellah dam. It is known in antiquity by the name of oued SALA. It was not until the thirteenth century that it appeared under the name of «ABIRAKRAK», its Berber name was «ASIF URGRAZ» arabized in «BURGRAG». The latter means in Berber «gravel» and applies to a Berber tribe «RGRAGA» who would have stayed long on the banks of the river. This river became famous because of its intimate connection to the history of the cities Rabat and Salé. The estuary of Bouregreg is an ecosystem of properties encouraging for the practice of socio-economic activities that benefit from its natural wealth, its strategic characteristics as a link between the two cities Rabat and Salé and also to the fact that this environment has ecological characteristics adapted for a large number of individuals. In addition, these activities have undergone a qualitative change after the development. This modification is reduced by the construction of several works (bridges, tower, clubs, restaurants, marina,port...) The aim is to confirm the position of Bouregreg as a link between the two cities and an attraction point for leisure and tourism.

Keywords: Estuary of Bouregreg; Natural resources; Development Projet, Infrastructures

ETAP software based power flow analysis of Electrical Structures of the 225/60/11KV substation in Tinghir

Hicham Stitou[1]*, Mohamed anime Atillah[1], Abdelghani Boudaoud[1], Mounaim Aqil[1]

[1]*Engineering and Applied Physics Team (EAPT), Superior School of Technology, Sultan Moulay Slimane University, Beni Mellal, Morocco*
*Email : hicham.stitou@usms.ma

Abstract. Due to technological development such as computer-based software it is possible to study and analyse complex electrical system problems with a possible solution. The study mainly includes power flow, transient analysis, voltage profile, reactive power control and monitoring, etc. Load flow analysis (LFA), or power flow analysis, is a crucial tool in power system engineering used for modeling and designing electrical power networks. It aims to determine the steady-state operating conditions of a power system to ensure a stable and efficient power balance between generation and load demands. LFA helps design robust power networks, maintains system stability, plans maintenance activities, and assists in the economic dispatch of power generation. It determines key parameters such as phase angle, voltage magnitude, and the flow of active and reactive power, essential for system stability and efficiency. This work focuses on the load flow study in the electrical structures of the 225/60/11KV substation in Tinghir, a predominantly rural subdivision of the Drâa-Tafilalet region of Morocco, using ETAP software.

Keywords: Power system; Power Network; ETAP software; Power Flow Analysis; Short Circuit analysis; Optimal Load flow.

A computational study of the structural and thermal conduct of $MgCrH_3$ and $MgFeH_3$ perovskite-type hydrides: FP-LAPW and BoltzTraP insight

Ayoub Koufi [1,2], Younes Ziat [1,2], Hamza Belkhanchi [1,2], Mohammed Miri [1,2], Noureddine Lakouari [3], El Houssayne Bougayr [1], and Fatima Zahra Baghli [1]

[1]*Engineering and Applied Physics Team (EAPT), Superior School of Technology, Sultan Moulay Slimane University, Beni Mellal, Morocco*
[2]*The Moroccan Association of Sciences and Techniques for Sustainable Development (MASTSD), Beni Mellal, Morocco*
[3]*Consejo Nacional de Humanidades, Ciencias y Tecnologías, Ciudad de México 03940, Mexico*
*Email : ayoub.koufi@uit.ac.ma

Abstract. The structural and thermal conduct of $MgCrH_3$ and $MgFeH_3$ perovskite have been investigated using the full-potential linearized augmented plane wave (FP-LAPW) method and the BoltzTraP package, implemented in the Wien2k code. The calculations involved fitting the Murnaghan equation of state to the calculated total energy and atomic volume. The present analysis includes key ground-state parameters, such as the lattice parameter and its pressure derivative. Where the electrical conductivity of $MgTMH_3$ (TM=Cr and Fe), the thermal conductivity, merit factor, and power factor were discussed in the range of 300-900 K. The obtained outcomes exhibit interesting results to make these compounds as promising materials for thermoelectrical applications.

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

Optimization of Antiperovskite Li_3SO and modification of its structural and optical properties with Fe doping for applications in solar cells

Zakaryaa Zarhri

CONAHCYT- Faculty of Chemical Sciences and Engineering, The Autonomous University of Morelos State, Av Universidad 1001, C.P. 62209, Cuernavaca, Morelos, Mexico.

Corresponding Author: z.zarhri@gmail.com

Abstract. DFT calculations were used to optimize the crystal structure of Li_3SO doped with different concentrations of Fe. The optimized lattice parameters were obtained, and the stability of the doped systems was analyzed in comparison with pure Li_3SO. The results revealed that Fe doping significantly affects the structural and optical properties of Li_3SO. It was found that the introduction of Fe into Li_3SO induces changes in lattice parameters, electron densities and energy gaps, which can have an impact on the absorption and emission properties of electromagnetic radiation. Furthermore, it was observed that the concentration of Fe in Li_3SO influences the structural and optical properties, suggesting that controlled Fe doping can be a strategy to tune the characteristics of antiperovskite materials for their application in the window of the solar cells.

Keywords : Fe-doped Li_3SO, Solar Cells, DFT, Optical Properties.

Comparative Analysis of PWM Schemes for Quasi-Z-Source Inverters

JAOIDE Essaid [1], OUTAZKRIT Mbark [1], EL AAMRI Faicel [2], RADOUANE Abdelhadi [1], MOUHSEN Azeddine [1]

[1] *Hassan First University of Settat, Faculté Sciences et Technique, Laboratoire IRM, Settat, Morocco*

[2] *Laboratory of Materials, Energy and System Control, Hassan II University, Mohammadia, Morocco*

*Email : e.jaoide@uhp.ac.ma

Abstract. The quasi-Z-Source Inverter (qZSI) become one of the most promising power electronic converter topologies for PV applications, due to the excellent ability to handle the wide voltage variations of DC sources in a single-stage topology. The voltage boost and inversion are achieved in a single-stage inverter, unlike traditional two-stage structures. Since been presented, types of switching control for the qZSI have been proposed to achieve wider modulation range, simpler implementation, and lower voltage stress on the switches. The traditional space-vector concept has been modified to be applicable for the qZSI due to its superiority in reducing current harmonics and optimizing voltage utilization. This paper presents a comprehensive comparative analysis of diverse space vector modulation schemes employed in the context of a three-phase qZSI. The objective is to elucidate the fundamental distinctions among these schemes and, ultimately, to deduce an optimal technique. The focus is on achieving a high output voltage while simultaneously minimizing power losses in the switching devices within the inverter.

Keywords: Space vector modulation, Quasi-Z-source Inverter, Voltage stress, Shoot-through ratio, power losses.

Techno-Economic Analysis for Enhanced Ammonia Production: A Case Study of Morocco

Meryem BAHAJ[1]*, Abdechafik ELHARRAK[1], Abdessamad FAIK[1]

[1]*Laboratory of Inorganic Material for Sustainable Energy Technologies (LIMSET),Mohammed VI Polytechnic University (UM6P), 43150, Benguerir Morocco*
*Email : Meryem.bahaj-ext@um6p.ma
Abdessamad.faik@um6p.ma

Abstract. Ammonia (NH_3) is a pungent, colorless gas, and one of the most promising achievements of the 20th century. Around 240 Mt of NH3 was produced globally in 2023, with a forecast of 289 Mt for 2026, making it the second-largest chemical product after sulfuric acid (H_2SO_4).Morocco is the third-largest ammonia importer worldwide, due to its agricultural sector's fertilizer needs. This study evaluates NH_3 purchase and import as well as different production scenarios in the case of Morocco in OCP Group at JorfLasfar. It examines gray ammonia via steam methane reforming, cryogenic air separation, and the Haber-Bosch process, blue ammonia with carbon capture, and green clean ammonia using water electrolysis. Detailed process models were provided, including a techno-economic and sensitivity analysis to evaluate the production of 4 tons of NH3 daily. The results showed that green ammonia offers long-term economic advantages due to zero carbon emissions, despite its higher CAPEX of $2.51/kg NH_3 and higher OPEX of $0.70/kg NH_3. On the other hand, blue ammonia, with an average CAPEX of $1.80/kg NH3 and OPEX of $0.10/kg NH_3, reduces CO_2 emissions by 90% and remains realizable with favorable carbon pricing. Finally, gray ammonia has environmental challenges and long-term costs due to carbon emissions, even its lowest initial CAPEX of $1.05/kg NH3 and OPEX of $0.08/kg NH3.This study gives a detailed analysis for the OCP Group, showing that even though green ammonia requires a higher initial investment and operating cost, it offers remarkable long-term benefits and supports Morocco's transition to sustainable production.

Keywords: Ammonia Production; Cryogenic Air Separation; Haber - Bosch Process; Steam Methane Reforming; Water Electrolysis.

Modeling $Ag_2BeSnTe_4$ kesterite solar energy cells : SCAPS-1D assessment

Gouztal Oumaima[1] , Chrafih Younes[2]

[1] *Lphe-modeling and Simulation Faculty of Science, Mohammed V University in Rabat, Morocco.*

Abstract. This study offers a novel theoretical framework for Tandem solar cell composed of two cells, Cs2AgBiBr6 and Ag2BeSnTe4. The selection and performance augmentation of both cells need to be carefully considered for optimal benefit. To attain optimal outcomes, separate analyses and optimizations are conducted for the top and bottom cells to determine the most advantageous configuration for each.. The estimated perovskite SC spectra are optically filtered onto the lower cells in order to accurately recreate the tandem devices. By varying the bottom layer thickness of the perovskite sub-cell, current matching was accomplished. The findings will pave the way for the next generation of low-energy, high-efficiency solar cells.

Investigation of Structural and Optoelectronic Properties in doped LiMgP and LiMgN Half-Heusler Compounds: A Comprehensive DFT study

Hamza Belkhanchi [1,2], Younes Ziat[1,2] Charaf Laghlimi[2,3]

[1]*Engineering and Applied Physics Team (EAPT), Superior School of Technology, Sultan Moulay Slimane University, Beni Mellal, Morocco*
[2]*The Moroccan Association of Sciences and Techniques for Sustainable Development (MASTSD), Beni Mellal, Morocco*
[3] *ERCI2A, FSTH, Abdelmalek Essaadi University, Tetouan, Morocco*

Abstract. Half-Heusler (HH) compounds have gained significant attention for their promising optoelectronic and thermoelectric applications. In this study, we employ Density Functional Theory (DFT) calculations to investigate the structural, electronic, and optoelectronic properties of doped LiMgP and LiMgN compounds. Various doping elements are introduced to analyze their effects on band structure, density of states (DOS), and optical characteristics, including absorption, reflectivity, and dielectric function. The results reveal tunable band gaps and enhanced optoelectronic performance, demonstrating the potential of these materials for next-generation semiconductor applications. This comprehensive theoretical approach provides valuable insights into material design strategies for optoelectronic and energy-harvesting technologies.

Keywords: Half-Heusler compounds, LiMgP, LiMgN, Density Functional Theory (DFT), Optoelectronic properties.

Numerical investigation on the effect of baffle position and number on thermal stratification in hot water tanks

Ahmed OUEZGAN[a,d,c*], Aziz MAZIRI[a], El Hassan MALLI[a] , Anas EL MALIKI[a], Jamal ECHAABI[a]

[a]Applied Research Team on Composites, Management and Innovation, High National School of Electricity and Mechanics, Hassan II University of Casablanca, Morocco.
[b]Ouezgan Composite Center (O.C.C), Ouezzane, 16200, Morocco.
[c]Technologies and Industrial Services Laboratory, High School of Technology, Sidi Mohamed Ben Abdellah University, Fez, Morocco.
*Ahmed.ouezgan@ensem.ac.ma

Abstract. Energy storage has been received considerable attentions in the recent years, due to the global energy crisis, environmental pollution, population growth and mismatch between energy demand and supply. The use of clean, environmental and sustainable sources to produce energy, especially solar energy, is showing promising potentials as alternative and durable energy to conventional based fossil fuel energies technologies. Nevertheless, these alternatives have low energy density, weather dependent, intermittent and even irregular which make them unreliable and inefficient to be used in large scale. Therefore, energy storage, especially thermal storage, is crucial in the development and expansion of the solar energy technologies. Thermal storage based on sensible heat suffer from inherent limitation related to the development of thermocline in the storage medium which decreases not only the performance of the thermal storage tank but also the entire system including both solar collector and load loops efficiency. A good thermal stratification, where cold water lies at the bottom of the tank and hot water stay at the top with a very thin thermocline zone separating the two zones, leads to increase the efficiency of the collector as more heat can be extracted from it due to large temperature gradient between the sun irradiation and cold water flowing through. On the other hand, a well stratified tank, will reduces or even eliminate the need of using auxiliary heat resources, with immediate consequence in energy bill cost and environmental pollution. The main factor that affect stratification within the tank is the cold-hot fluid mixing induced by the fluid inlet flow. Incorporating baffles inside tank maintains the level of stratification by redirecting the flow and working as an obstacle to hinder mixing. However, the position and number of baffles inside tank play an important role in improving the temperature stratification. Therefore, the objective of the current article is to investigate through a numerical simulation the effect of the position and number of baffles on thermal stratification in cylindrical storage tank during charging and discharging operation modes. The results indicate that placing baffles in the right tank height and using multiple baffles improves and maintains stratification in cylindrical tank in comparison to tank with single baffle placed near the inlet and outlet. The optimum position and numbers of baffles that should be used in similar tank will be present at the conference.

Keywords: Energy storage, Thermal storage, Stratification, Baffles

Advanced Technologies for The Electrochemical Production of Hydrogen

Charaf Laghlimi[1]*

[1] *ERCI2A, FSTH, Abdelmalek Essaadi University, Tetouan, Morocco*
*Email : Charaf.cac.fbs@gmail.com

Abstract. Human gluttony is having a catastrophic effect on the environment. Since the age of industry and the world wars, modern societies have hygienically depleted most of the earth's resources, thus depleting all the resources that will be essential for future generations. The problem doesn't stop there: greenhouse gas emissions have significantly increased the earth's temperature, causing terrible damage to the climate. The production of green energy with no greenhouse effect seems essential to save the planet. Green hydrogen is a suitable and promising way to generate an energy source that produces H_2O molecules instead of CO_2. Green hydrogen is produced by electrolysis of water using a suitable electrical current generated by a non-polluting energy source such as wind turbines. This review covers the latest technologies for electrochemical H2 production, including anion exchange membrane (AEM), solid oxide electrolysis cell (SOEC), polymer electrolyte membrane (PEM) and alkaline water electrolysis (AWE). This article provides a detailed description of the techniques used to produce hydrogen electrochemically, focusing in particular on the technical production processes, the advantages and disadvantages of each technique and the various challenges encountered, which will allow us to propose promising prospects in this field.

Keywords: Alkaline water electrolysis; Anion exchange membrane; Electrolysis; Green hydrogen; Polymer electrolyte membrane.

Series and parallel connected thermal solar energy storage tanks for large-scale storage: Numerical investigation

Ahmed OUEZGAN[a,b,c*] , Aziz MAZIRI[a] , El Hassan MALLI[a] , Anas EL MALIKI[a] , Jamal ECHAABI[a]

[a]*Applied Research Team on Composites, Management and Innovation, High National School of Electricity and Mechanics, Hassan II University of Casablanca, Morocco.*
[b]*Ouezgan Composite Center (O.C.C), Ouezzane, 16200, Morocco.*
[c]*Technologies and Industrial Services Laboratory, High School of Technology, Sidi Mohamed Ben Abdellah University, Fez, Morocco.*
*Ahmed.ouezgan@ensem.ac.ma

Abstract. The Shifting towards clean and sustainable energy resources to produce energy and fill the increasing demand for power has been proved its effectiveness to satisfy economic, human and environmental needs and requirements. Solar energy is clean, free and widely available which makes it very attractive among others renewable energy sources. However, this source is weather dependent, intermittent and irregular during the day and seasons. These drawbacks limit its potential for replacing completely the current energy technologies based frequently on fossil fuels. To overcome these limitations, the use of storage medium to collect and conserve the solar-thermal energy for later use has received huge attention among industrial and academia. Small thermal storage tanks have been introduced into the market since manyyears ago and have widely used in several applications including building heating and air conditioning, domestic hot water applications, greenhouses, and fruits and vegetables transportation. In such applications, the thermal charging-discharging is fast and the storage time where the fluid is stagnant is short. Hence in these conditions, the main factor that destructs the stratification is the mixing between incoming and resident fluid in the tank induced by the temperature gradient between these regions and intensifies with increasing in the inlet fluid velocity. It is well known that improving and maintaining thermal stratification in storage tank improves the efficiency of the tank and the entire system connected to it. Thermal stratification is very complicated and depends to tank shape, size, material, volume and configuration, fluid properties, inlet and outlet locations and numbers, in addition to the operation conditions. Moreover, several interconnected hydrodynamic and thermal phenomena occur and prevail inside the tanks depending on the tank working characteristics. Although, Large-scale storage refers mostly to long-term storage, but this is only a misconception as the long-short terms are related mainly to the operating designed mode rather than storage capacity. In heavy industries, where huge energy is required to be delivered in a short time, to fill the mismatch between the demands and supplied and decrease energy bills, large-scale volume tanks are used with fast charge and discharge periods. Nevertheless, in district domestic heating, these large tanks are charging and discharging during long periods up to 4 months and more. Under this situation, heat losses across the tank walls to ambient, heat conduction between fluid layers and within the tank wall dominate over mixing induced by inlet jet and degrade significantly the level of stratification of the thermal storage. Moreover, the manufacturing of the large tanks are expensive and usually overestimated, which increases the difficulty of their transportation, installation and maintenance. Furthermore, it will be hardly to implement and use them in residential and city building heating applications due to the limited space and common appearance. Therefore, using multiple tanks has the potential to replace these large stores. Multiple tanks can be connected either in series, parallel or in combination. The selection of the right configuration is based on the tank working mode. Hence, the objective of the current article is to investigate numerically the effect of five equal tanks with a total volume 250 m3 , arranged either in parallel or in series on the temperature stratification and storage efficiency of the tank.

Keywords: Large –scale tank; Thermal stratification, Energy storage, Energy storage, Numerical Investigation.

Electrochemical Carbon Capture and Concentration Techniques Inspired By Photosynthesis Reactions For Reduction of CO_2 Emissions

Charaf Laghlimi[1]*

[1] *ERCI2A, FSTH, Abdelmalek Essaadi University, Tetouan, Morocco*
*Email : Charaf.cac.fbs@gmail.co

Abstract. Excessive industrialization has produced huge quantities of CO_2, which has destabilized the global climate, causing destructive phenomena for plants such as drought and flooding. Green plants, from the smallest to the largest, have a highly developed electrochemical system capable of converting CO_2 in the air into organic compounds that can be used by the plant itself (carbohydrates, amino acids, etc.), which is highly beneficial for the ecosystem. This conversion is mainly based on the energy of light and the H^+ electrons and protons produced by the oxidation of H_2O. This article highlights recent advances in technologies for the electrochemical capture and concentration of carbon, inspired in part by photosynthetic reactions. For each technology, successes in the field, current major challenges and potential for improvement are described. The review also presents some innovative and interesting materials for CO_2 fixation. It concludes with an outlook and discussion of future research challenges in the field of electrochemical capture.

Keywords: Electrochemical carbon capture and concentration; Fixing materials; Organic redox; Photosynthesis; Transition metal redox.

The Effect of ETL and HTL Thickness on the Electrical and Optical Properties of OLED Devices

Mohammed EL HALAOUI[1]*, Mustapha EL HALAOUI[1], Lahcen AMHAIMAR[2], Laurent CANALE[3], Bousselham SAMOUDI[1]

[1]*Intelligent System Design Laboratory, Research Team: Optics, Materials and Systems, Faculty of Sciences, Abdelmalek Essaadi University, Tetouan, Morocco*

[2]*Higher School of Applied Arts, Hassan 2 University of Casablanca, Casablanca, Morocco*

[3]*Université Toulouse III–Paul Sabatier, LAPLACE, UMR 5213, (CNRS, INPT, UPS), Toulouse, France*

*Email : mohammed.elhalaoui@etu.uae.ac.ma

Abstract. A simulation was conducted to study a high-performance three-layer green organic light-emitting diode (OLED) structure, consisting of stacked layers of ITO (100 nm) / NPB (X nm) / Alq3: C545T (1%) (30 nm) / Alq3 (95-X nm) / LiF-Al (100 nm). The aim is to optimize the structure under study and enhance the performance of this type of OLED through simulation before moving to the manufacturing phase. We examine the performance of the OLED structure by employing models that incorporate both electrical and optical simulations in Atlas Silvaco. Four devices with varying ETL and HTL layer thicknesses—(15 nm/ 80 nm), (30 nm/65 nm), (45 nm/50 nm), and (60 nm/35 nm)—were studied, while adjusting the interfacial conditions between the layers. Simulation results indicate that variations in ETL and HTL layer thicknesses, and consequently changes in the charge recombination positions, affect the current voltage characteristics, electric field distribution, carrier charge density, charge recombination rate, voltage-luminance characteristics, and luminous efficacy. The device with the thicknesses of (30 nm/65 nm) exhibited the best performance, achieving a maximum luminance of 44,000 cd/m² and a maximum current efficiency of 7.67cd/A, with increasing operating voltage. These results can be used for the practical design and fabrication of this type of OLED, as well as other devices, including phosphorescent OLEDs.

Keywords: OLED, Atlas Silvaco, ITO, luminous efficacy, electrical and optical simulations.

Bacteria Modified Stainless Steel Anode for Glucose Fuel Cell

Salma Zahid, YounessTahiri, Mohamed Oubaouz, Mustapha Oukbab, Aziz Zaroual and Abdelilah Chtaini

Equipe d'Electrochimie Moléculaire et Matériaux Inorganiques, LGI, Faculté des Sciences et Techniques, Université Sultan Moulay Slimane, Maroc.

Abstract. The electrochemical oxidation of glucose on the surface of a stainless-steel electrode was studied in the absence and in the presence of bacteria. The presence of a suspension of bacteria in the electrolytic solution is manifested by the appearance of the anodic and cathodic peaks in the cyclic voltammogram, accompanied by a considerable increase in the electrical current densities, which indicates a strong interaction between the surface of the l electrode and bacteria. The oxidation of glucose shows a redox system on the cyclic voltammogram in the potential interval between - 0.5V and 0 V. This redox system is shifted towards the anodic potential values in the presence of bacteria while the oxidation current densities decrease.

Keywords: Glucose; Electro oxidation; Bacteria; Bio corrosion; Stainless steel; Pseudomonas

Optoelectronic Performance of Epoxy/Silicone Blends with N-Doped CNT Composites and CNT-Modified ZnO/TiO_2 Thin Films: A Study of Surface Morphology and Loading Rate

Hamza Belkhanchi [1,2], Younes Ziat[1,2] Charaf Laghlimi[2,3]

[1]*Engineering and Applied Physics Team (EAPT), Superior School of Technology, Sultan Moulay Slimane University, Beni Mellal, Morocco*
[2]*The Moroccan Association of Sciences and Techniques for Sustainable Development (MASTSD), Beni Mellal, Morocco*
[3] *ERCI2A, FSTH, Abdelmalek Essaadi University, Tetouan, Morocco*

Abstract. The integration of carbon nanotubes (CNTs) into polymeric and thin-film matrices has opened new avenues for optimizing optoelectronic properties in advanced materials. This study investigates the impact of nitrogen-doped CNTs (N-CNTs) on the optoelectronic performance of epoxy/silicone blends and ZnO/TiO_2 thin films. By analyzing surface morphology and the effect of different CNT loading rates, we evaluate the resulting structural, optical, and electronic modifications. Scanning electron microscopy (SEM), atomic force microscopy (AFM), and spectroscopic techniques provide insights into film homogeneity, roughness, and charge transport behavior. The findings reveal a strong correlation between CNT dispersion, loading concentration, and optoelectronic efficiency, highlighting the potential of these hybrid materials for applications in photovoltaics and optoelectronic devices.

***Keywords*:** Optoelectronic properties, N-doped carbon nanotubes, Epoxy/Silicone blends, ZnO/TiO_2 thin films

Topic (2): Materials Sciences in Energy

Innovative phosphate electrode materials: From synthesis to application in pseudocapacitors

F.Z. Moufakkir[1*], H. El Mouahid[1], A. Guessous[1*]

[1]*Laboratory of Materials, Nanotechnology and Environment, Faculty of Sciences, Mohammed V Universityin Rabat, Av. Ibn Battouta, P.O. Box. 1014 Agdal-Rabat, Morocco;*

*Email : fati96.tabit@gmail.com

Abstract. The thin film of $Fe_3(NH_4)H_8(PO_4)_6.\ 6H_2O$ is electrodeposited by a solution of a precursor of Mohr's salt and phosphoric acid. The electrodeposition was carried out using a chronoamperometric method. The electrodeposition reaction takes place in two steps: electrochemical reaction followed by precipitation in a phosphoric medium. The Morphology, crystal structure, purity and thermal properties were studied by scanning electron microscopy combined with energy dispersive X-ray spectroscopy (SEM/EDS), X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), thermogravimetric analysis (TG) and differential scanning calorimetry (DSC), respectively.

Keywords: Chronoamperometric method; Electrodeposition; $Fe3(NH4)H8(PO4)6.\ 6H2O$; thin film; SEM/ EDX/ XRD/ FTIR/ TG/ DSC

Impedance spectroscopy in nanostructured composites based on "(1-x) $AFe_{12}O_{19}$-$xBTiO_3$ (a-ba,pb,sr; b-ba,pb)" after mechanical activation

Kamaludin Abdulvakhidov[1],Zhengyou Li[1],Salim Otajonov[2*],Nurzod Yunusov[2]
Qodir Botirov[2]

[1] *Southern Federal University, Sladkova 178/24, Rostov-on-Don 344090, Russia*
[2] *Fergana State University, Murabbiylar 19, Fergana 100150, Uzbekistan*
Email: otajonov_s@mail.ru

Abstract. In this article, impedance spectroscopy of nanostructured composites "(1 x)$AFe_{12}O_{19}$-$xBTiO_3$ (A-Ba,Pb,Sr; B-Ba,Pb)" during mechanical activation was examined. It was found that the absolute values of the ferroelectric lattice parameters increase after mechanical activation, attributed to topological defects formed during nanostructuring. It was also demonstrated that nanostructuring by mechanical force led to an increase in the hysteresis loop area.

Keywords: impedance spectroscopy, relaxation processes, mechanical activation, nanostructured composites, crystal lattice

Structural behavior of copper monoatomic metallic glass under various cooling conditions

Abdelaziz El kharraz*, Tarik El hafi, Soufiane Assouli, Omar Bajjou, Youssef Lachtioui

Laboratory of Engineering in Chemistry and Physics of Matter (LICPM), Faculty of Sciences and Technics Sultan Moulay Slimane University, B.P 523, 23000, Beni Mellal, Morocco

*Email : abdelaziz.az1994@gmail.com

Abstract. In this work, molecular dynamics simulations used with embedded-atom potential (EAM) to investigate structural behavior of Copper Cu pure metallic glass by analyzing the radial distribution function (RDF), Voronoi tessellation and coordination number. The simulation results confirm that the splitting in the second peak of the radial distribution function (RDF) proving the formation of amorphous phase for cooling rate from 5.10^{12}K/s to 10^{14}K/s under 0GPa, and the glass transition temperature Tg increases a faster cooling rate. The Voronoi tessellation indicated that the percentage of icosahedral-like clusters grows as the cooling rate increases. besides, the coordination number is specified that the local environment and topological structure of zirconium metallic glass change during the cooling process.

Keywords: Zirconium metallic glass; molecular dynamics; radial distribution function; Voronoi tessellation; coordination number; cooling rate

Damaged Steel Pipelines: Composite Wrapping Method and Other System Components for Maintaining Operational Continuity

Korcan ÜNAL[1,2]*, Hande GIRARD[1,3]

[1]*OSTIM Technical University, Faculty of Engineering, Department of Mechanical Engineering 06374 Ankara, Türkiye*
[2]*TANAP Doğalgaz İletim A.S., Sögütözü Mahallesi Sögütözü Caddesi Koc Kuleleri B Blok No:2B/37 Ankara, 06510, Türkiye*
[3]*OSTIM Technical University, Institute of Science and Technology, Department of Aerospace Engineering 06374 Ankara, Türkiye*
*Email : 230804007@ostimteknik.edu.tr

Abstract. Composite wrapping for repairing damaged steel pipelines is a significant and effective rehabilitation method in the oil and gas industry. Specifically, using fiber-reinforced polymer (FRP) materials in composite wrapping has emerged as a viable solution for offshore and onshore pipeline repairs. Composite wrapping involves encasing the corroded sections of steel pipelines with FRP materials, effectively halting further corrosion and enhancing structural integrity. Extensive laboratory and field tests have demonstrated the reliability of this method, showing minimal stress impact on the repaired sections and negligible displacement, even under cyclic operations and sudden pressure changes. This makes composite wrapping not only a temporary fix but also a potential permanent solution for addressing pipeline leaks and damages. The interaction between the composite wrapping and the surrounding soil plays a crucial role in the effectiveness of the repair, particularly for buried pipelines. The properties of the composite materials, such as tensile strength and durability under varying environmental conditions, are critical factors. Overall, composite wrapping offers a promising approach to pipeline rehabilitation, ensuring operational continuity and system integrity. As the industry continues to advance, further research into the material properties and environmental interactions of FRP composites will be essential in optimizing and standardizing this repair method.

Keywords: Composite wrapping; Environmental interaction; Damage; Oil and gas pipeline; Pipeline rehabilitation

MOFs-based materials: A trendy hybrid material for hydrogenation of aromatic nitro compounds

Asmae Laksir[1]*, Marieme kacem[1], Mustapha Dib[1], Rachid Touzani[2], Aziz Boulouiz[1]

[1]*Laboratory of Applied Chemistry and Environment, Mineral Solid Chemistry Team, Faculty of Sciences, Mohammed First University, B.P. 717, 60 000, Oujda, Morocco*
[2]*Laboratory of Applied Chemistry and Environment, Department of Chemistry, Faculty of Sciences, University Mohammed the First, 60000 Oujda, Morocco, Morocco*
*Email : asmae.laksir@ump.ac.ma

Abstract. Metal–organic frameworks (MOFs) represent a class of porous materials comprising metal ions bound by organic ligands to form a three-dimensional structure. They are synthesized using various methods, including solvothermal and microwave... Emerging networks and varieties of material hybrid MOFs encourage innovative applications in the science and technology of material design. The main components of MOFs-based materials combine the exceptional characteristics of their structures, including their high crystallinity, large surfaces, porosity, and the ability as structures for use with functional groups. MOFs-based materials that have attracted much attention due to their potential applications in gas storage, catalysis, and drug administration. Indeed, their porous structure makes it possible to capture and store large quantities of gas, which is crucial for energy and environmental applications. Catalysis is an area where MOFs show considerable potential. For example, they can act as catalysts for the reduction of nitroaromatic compounds, which are common environmental pollutants. However, despite their many beneficial properties, MOFs have some limitations, especially in terms of their stability and the challenges associated with their large-scale production. These obstacles need to be overcome to allow wider use of MOFs in practical applications. The aim of this work is to promote MOFs as hybrid nanostructures on solid materials and to explore their applications in the environmental field. In particular, we highlight their potential as catalysts for the reduction of nitroaromatic compounds. Challenges related to the limited stability of MOFs and large-scale production require special attention to realize their full potential. In conclusion, MOFs represent a class of materials with unique properties that make them suitable for a multitude of technological applications. The development of methods to improve their stability and facilitate their production could pave the way for significant advances in the field of materials and the environment, making technologies more efficient and sustainable.

Keywords: Catalysis; Gas storage; Metal-organic frameworks (MOFs); Porous materials; Solvothermal

Effect of Deposition Time on ZnO Mesoporous Thin Films Properties for Dye-Sensitized Solar Cells Applications

Alphonse Déssoudji Gboglo[1,2,4,5,*], Mazabalo Baneto[1,2], Komlan Segbéya Gadedjisso-Tossou[1,3], Ayayi Claude Ahyi[6], Ognanmi Ako[1,2,4], M. Haris[4], Kekeli N'konou[5], Bruno Grandidier[5], M. Senthilkumar[4], Katawoura Beltako [1,3], Komi Apélété Amou[1,2], Milohum Mikesokpo Dzagli[1,3]

[1]*Centre d'Excellence Régional pour la Maîtrise de l'Electricité (CERME), University of Lomé, 01BP 1515, Lomé, Togo*

[2]*Laboratory on Solar Energy, Department of Physics, Faculty of Sciences, University of Lomé, 01BP 1515, Lomé, Togo*

[3]*Physics of Semiconductor Materials and Components Laboratory, Department of Physics, Faculty of Sciences, University of Lomé, 01BP 1515, Lomé, Togo*

[4]*Department of Physics, Karunya Institute of Technology and Sciences, Karunya Nagar, Coimbatore 641 114, Tamil-Nadu, India*

[5]*Institute of Electronics, Microelectronics and Nanotechnology (IEMN), Univ. Lille, CNRS, Centrale Lille, Univ. Polytechnique Hauts-de-France, UMR 8520, JUNIA-ISEN, F-59000 Lille, France*

[6]*Physics Department, Auburn University, Auburn, AL 36849, USA*

*Email : alphonsedessoudji@gmail.com

Abstract. This study presents the influence of deposition time on the properties of ZnO thin films obtained by chemical bath deposition. ZnO thin films were deposited on glass substrates at different deposition times: 30, 60, 90 and 120 minutes. The effect of deposition time on the morphological, structural, and optical properties of ZnO thin films was studied using X-ray diffraction (XRD), scanning electron microscopy (SEM), Fourier transform infrared spectroscopy (FTIR), and UV-Visible spectroscopy. XRD results show that all the ZnO thin films elaborated are polycrystalline and crystallize in a hexagonal wurtzite structure with average lattice parameters a = 3.247 Å and c = 5.209 Å. The peaks intensity increases as the deposition time increases. The presence of functional groups and chemical bonds characteristic in ZnO thin films was confirmed by FTIR. SEM images reveal that deposition time affects the films morphology. ZnO thin films become more compact as the deposition time increases. The films consist of nanorods with length varying from 25 nm to 60 nm. Optical characterization results show that the ZnO thin films' transmittance decreases with increase in deposition time. Films deposited for 30 minutes exhibit the highest transmittance (68%), while films deposited for 120 minutes exhibit the lowest transmittance (52%) in the visible region.

Keywords: Zinc oxide; Thin films; Mesoporous; Deposition time; Chemical bath deposition; Dye-Sensitized Solar Cells

Functionalized layered double hydroxides: Synthesis, properties and perspectives towards potential applications

Zineb Tchorbo[1]*, Mustapha Dib[1], Kacem Mariem[1], Essaddek Abderrahim[1], Mounsef Neffa[2]
J. M. Doña Rodriguez[3]

[1]*Laboratory of Applied Chemistry and Environment, Mineral Solid Chemistry Team, Faculty of Sciences, Mohammed First University, B.P. 717, 60 000, Oujda, Morocco*
[2]*Laboratory of Bioresources, Biotechnology, Ethnopharmacology and Health, Faculty of Sciences, Mohammed First University, B, P, 717, Oujda 60000, Morocco*
[3]*Fotocatálisis y Espectroscopía para Aplicaciones Medioambientales (FEAM), Department of Chemistry, University Institute of Environmental Studies and Natural Resources (i-UNAT), Edificio Central del Parque Científico Tecnológico, Universidad de Las Palmas de Gran Canaria, Campus Universitario de Tafira, Las Palmas, 35017, Spain*
*Email : zinebtchorbo@gmail.com

Abstract. Layered Double Hydroxides (LDHs), also known as anionic clays, have garnered significant interest in recent years due to their unique structural characteristics, including the uniform distribution of different metal cations within the brucite layer, surface hydroxyl groups, tunable flexibility, and intercalated anions within the interlayer spaces. Additionally, their intriguing properties of anion exchange, adsorption, and porosity enable the intercalation of a wide variety of anions (organic or inorganic). Moreover, LDHs are primarily easy to synthesize through various methods such as co-precipitation, hydrothermal, sol-gel, urea, and reconstruction methods, allowing for the incorporation of diverse functional materials such as polymers, nanoparticles, and biomolecules. Consequently, LDHs and their derivatives have become an important class of layered materials with potential applications in medical fields, catalysis, and especially environmental applications for the removal of removal of toxic pollutants from aqueous solutions. In the present study, functionalized double hydroxides were prepared and characterized by various physicochemical analysis techniques. In addition, the properties of functionalized LDHs have been discussed and prospects for advanced applications explored.

Keywords: Layered Double Hydroxides (LDHs), Functional-LDHs, synthesis, properties, potential applications

pH Effect on Structural, Morphological and Optical Properties of ZnO Mesoporous Thin Films Obtained by Chemical Bath Deposition for Dye-Sensitized Solar Cells Applications

Mazabalo Baneto[1,2]*, Alphonse Déssoudji Gboglo[1,2,3], Ognanmi Ako[1,2,3], Muthiah Haris[3], M. Senthilkumar[3],

[1]*Centre d'Excellence Régional pour la Maîtrise de l'Electricité (CERME), University of Lomé, 01BP 1515, Lomé, Togo*

[2]*Laboratory on Solar Energy, Department of Physics, University of Lomé, 01BP 1515, Lomé, Togo*

[3]*Department of Physics, Karunya Institute of Technology and Sciences, Karunya Nagar, Coimbatore 641 114, Tamil-Nadu, India*

*Email : banetopaul@gmail.com

Abstract. This study presents the influence of pH on the properties of ZnO thin films obtained by chemical bath deposition. ZnO thin films were deposited on glass substrates using precursor solutions of different pH of precursor solution prepared from two bases: sodium hydroxide (NaOH) and ammonia (NH_3). The effect of pH values on the morphological, structural, and optical properties of ZnO thin films was studied using X-ray diffraction (XRD), scanning electron microscopy (SEM), Fourier transform infrared spectroscopy (FTIR), and UV-Visible spectroscopy. XRD results show that all the ZnO thin films elaborated are polycrystalline and crystallize in a hexagonal wurtzite structure. The crystallites size, calculated using the Debye-Scherrer formula, varied from 10.30 nm to 13.39 nm for ZnO thin films obtained with NH_3 and from 14.80 nm to 38.14 nm for those obtained with NaOH. FTIR analysis confirms the presence of functional groups and chemical bonds. SEM images indicate that not only the base affects the films surface morphology but the pH also influences the films morphology through the grains shape. However, the ZnO thin films obtained with NaOH look more mesoporous compared to those obtained with NH_3. Optical characterization results show that whatever the base used, the pH of the precursor solution affects the ZnO thin films' transmittance. Films elaborated with NH_3 exhibit the best transmittance (80%) at pH 8.5, while for films elaborated with NaOH, the best transmittance (81%) is obtained at pH 8 in the visible region.

Keywords: Zinc oxide, Mesoporous; Thin films; pH control; Chemical bath deposition; Dye-Sensitized Solar Cells

First-Principles Calculations Of Structural, Electronic And Optical Properties Of Undoped And Se Doped Sb_2S_3 Using Density Functional Theory

Mustapha MADI[1]*, El Houssine Atmani[1], Ahmed El MANOUNI[1], Najma FAZOUA[1], Imtki Hamza[1]

[1]*Hassan II University, Faculty of Sciences and Techniques, Laboratory of Physics of Condensed Matters and Renewables Energies Casablanca, Mohammedia BP 146, 28806, Morocco*

*Email : madi10mustapha@gmail.com

Abstract. The demand for cheaper, nontoxic and earth-abundant materials as an absorbing layer of solar cell is immensely needed to replace scarce, toxic and expensive one. In this regard, chalcogenide materials have attracted significant attention in the past few years as a next generation showing a great potential for different applications. Antimony sulphide (Sb_2S_3), a chalcogenide binary material is a potential candidate for alternative material in solar cell application, less toxic, abundantly available, stable and efficient. In our present work, the structural, electronic and optical properties of un-doped Sb_2S_3 and Se doped Sb_2S_3 were studied using the Full Potential-Linearized Augmented Plane Wave (FP-LAPW) [1] and the Local Orbital (LO) Method, based on the Density Functional Theory as implemented in Wien2k code. The structural properties have been calculated using and Perdew–Burke–Ernzerhof generalized gradient approximation for solids and surfaces approximation (PBEsol-GGA). Where the Trans-Blaha approximation of the modified Becke–Johnson (TB-mBJ) potential is used for electronic and optic properties to get more reliable results for the fundamental band gap energy value. Our principles calculations show that Se-doped Sb_2S_3 has lower band gap energy compare to pure Sb_2S_3. The optical properties of Se-doped Sb_2S_3 such as dielectric function, extinction coefficient, refractive index, energy-loss function and extinction coefficient, absorption coefficient, reflectivity and transmittance are presented. The results demonstrate that Se-doped Sb_2S_3 has higher optical absorption coefficient in the visible region than pure Sb_2S_3 which are also very close to the experimental results, and approve its potentiality for the photovoltaics applications.

Keywords: *Antimony sulphide*; *DFT*; *Optical properties*; *Selenium*; *Wien2k*

Computational Study of Germanium-Doped $CH_3NH_3PbI_3$ Perovskite: Optical and Electronic Properties and Modulation Potential

Lhouceine Moulaoui[1]*, Abdlhafid Najim[2], Abdelmounaim Laassouli[2], Archi Marouane[1] Omar Bajjou[2], Khalid Rahmani[3], Bouzid Manaut[1]

[1]*LRPSI, Faculty of Polydisciplinary, Sultan Moulay Slimane University, B.P 592, 23000, Beni Mellal-Morocco.*
[2]*Laboratory of Engineering in Chemistry and Physics of Matter (LIPCM), Faculty of Sciences and Technics, Sultan Moulay Slimane University, B.P 523, 23000, Beni Mellal, Morocco.*
[3]*PSES, ERC, Ecole Normale Supérieure, Mohammed V University in Rabat, P. O. Box: BP 5118 Takkadoum Rabat-10000, Morocco*
*Email : moulaoui.h.fpbm@gmail.com

Abstract. In this study, we used the Materials Studio software to calculate the optical and electronic properties of the perovskite CH3NH3PbI3. We doped the lead (Pb) metal with three different percentages of germanium (Ge): 12.5 %, 25 %, and 37.5 %. Pure CH3NH3PbI3 perovskite has a bandgap energy (Eg) of 1.733 eV. The bandgap energies of the doped materials are 1.57 eV, 1.545 eV, and 1.503 eV, respectively. The pure CH3NH3PbI3 structure has a maximum absorption coefficient of $8{,}11.10^4$ cm^{-1} in the wavelength range of 400 nm to 800 nm. This calculation also studied the effects of Ge doping on the bandgap energy, absorption, total density of states, the real and imaginary parts of the dielectric function, refractive index, extinction coefficient, the real and imaginary parts of the optical conductivity, and the loss function. These calculated results are in agreement with experimental results and provide information on the possibility of modulating the electronic and optical properties of CH3NH3PbI3 perovskite through Ge doping, which could have implications for its application in optoelectronic devices.

Keywords: Absorption coefficient, Bandgap energy, CH3NH3PbI3, Density of states, Dielectric function.

Synthesis, structural and optical characteristics of Ni-doped Co_3O_4 layers deposited by spray pyrolysis

Zakaria Barbouch[1*], Abdellatif El-Habib[2], Jamal Zimou[1], Mustapha Beraich[3], Elarbi Laghchim[1], Khalid Fareh[1], Abderrahim Raidou[1], Khalid Nouneh[1], Nadia Elharfaoui[1], Mounir Fahoume[1]

[1]*Laboratory of Materials Physics and Subatomic, Department of Physics, Faculty of Science, Ibn Tofail University, BP 133, 14000 Kenitra, Morocco.*
[2]*ERCMN, FSTT, Abdelmalek Essaadi University, Tetouan, Morocco*
[3]*Laboratory of Materials, Energy and the Environment (LaMEE), Faculty of Science Semlalia. Cadi Ayyad University, P. O. Box 2390, Marrakech 40000, Morocco*
*Email :barbouch.zakaria@uit.ac.ma

Abstract. In this work, the pure and Nickel doped Co_3O_4 nanostructures thin film was successfully grown on glass substrates with optimized parameters. The pur and Nickel doped Co_3O_4 thin films was synthesized by spray pyrolysis technique at fixed temperature of 450 ◦C, Different characterization techniques were used to study the effect of Ni incorporation into the Co_3O_4 compound at different concentrations (0, 1, 3, 5, 7 at. %) on its microstructural, morphological and optical behaviors. The XRD results diagrams showed that all the films had a polycrystalline spinel-like cubic structure. The preferred orientation of the crystallites is towards the (311) plane for all doped and undoped films. Scanning electron microscopy (SEM) images showed a nanocrystalline grain size with a porous structure for the film doped with a concentration of 1% Ni. The optical transmittance decreased with the increase of doping, which indicates that there is a creation of gaps in the structure of the films,

Keywords: Ni doped Co3O4, spray pyrolysis, XRD/UV-Vis/ SEM, Band gap energy

Numerical performance simulation of a $MoSe_2$-based solar cell using SCAPS-1D simulator

M'hamed SEMLAL [a], Mohamed KHUILI [*, a,b] , Nejma FAZOUAN [a], El Houssine ATMANI [a]

[a] *Laboratory of Nanostructures and Advanced Materials, Mechanics and Thermofluids, Faculty of Sciences and Technologies, Hassan II University of Casablanca. Mohammedia, Morocco*

[b] *CRMEF of Beni Mellal-Khénifra, Morocco*

*Corresponding author: m.khuili@usms.ma, Telephone number: +212660061279

Abstract. Due to their low manufacturing cost and simple structure, the 2D Transition metal dichalcogenides material Molybdenum diselenide (MoSe2) have attracted tremendous attentions as an absorbent layer of new solar cells. Simulation studies using SCAPS-1D have already been carried out on this type of perovskite to determine the optimized parameters of this solar cell. In our study, we used TiO2 and In2Te3 as electron and hole-collecting layers respectively. The effects on solar cell performance of temperature, active layer thickness and the density of defects inside and at the interface of this layer are calculated. Our findings indicate that increases in these factors lead to a degradation in device performance. The results, based on power conversion efficiency (η), open-circuit voltage (Voc), fill factor (FF), and short-circuit current (Jsc) curves, show that with optimized parameters, an efficiency greater than 20% and comparable to that of MoS2-based solar cells can be achieved. This research provides theoretical guidance for designing new high-performance solar cells for future studies and manufacturing.

Keywords : Photovoltaics, SCAPS-1D, Solar cells, MoSe2

Role of nano particles in enhancing the behaviour of asphalt concrete: A review

Salman Mustafa Salih Zebari[1], Bakhtyar Qaim Khawaja Al Harki[1] , Nareen N. M.Nadhif[1], Mahmood Huner Dheyaaldin[2]

[1]*Akre University for Applied Sciences AUAS, Akre Technical Institute, Surveying Department, 42004 Iraq*
[2]*Cihan University, College of Engineering, Civil Department, 44001 Iraq*
*Email : salman.mustafa@auas.edu.krd

Abstract. Nowadays, pavement is subjected to increased loads and deteriorates more rapidly than predicted. The paper reviews the role of using nano-particles in improving the behaviour of hot-mix asphalt mixtures. Using nano-particles like nano clay, nano-silica, nano titanium oxide, and graphene in asphalts normally increases the viscosity of binders of asphalt and enhances the fatigue resistance and rutting of asphalt mixtures. The effects of adding different nanomaterials to asphalt mixtures were examined in this study. The objective of the research is to investigate the possibility of improving the resistance and durability of asphalt mixes. This study specifically found to determine how bitumen modification with nanomaterials affected the Marshall properties, resilient modulus, and durability of the asphalt concrete mixture. Moisture susceptibility was determined through the determination of the indirect tensile strength (ITS), and permanent deformation was determined by using the uniaxial repeated load test. The overall review of the available studies has indicated the benefits of nanotechnology in pavement construction; however, using nanomaterials in asphalt mixes is a bit challenging due to the lack of practical implications and proper knowledge. The utilization of nanomaterials significantly enhanced the behaviour of asphalt concrete; furthermore, it provides the possibility of making further durable mixtures with higher resistance to the distress of asphalt pavement.

Keywords: Nanomaterials, Nano Particles, Characterization of Nanomaterials, Modified asphalt binder, Modified asphalt mixture.

Impact of Cs Substitution on the Electronic and Optical Properties of $CH_3NH_3SnI_3$ Perovskite: A Density Functional Theory Study

Abdelhafid Najim[1]*, Abdelmounaim Laassouli[1], Lhouceine Moulaoui[2], Omar Bajjou[1,3], Khalid Rahmani[4]

[1]*Laboratory of Engineering in Chemistry and Physics of Matter (LIPCM), Faculty of Sciences and Technics, Sultan Moulay Slimane University, B.P 523, 23000 Beni Mellal, Morocco*

[2]*LRPSI, Faculty of Polydisciplinary, Sultan Moulay Slimane University, B.P 592, 23000, Beni Mellal-Morocco*

[3]*UNESCO UNISA Africa Chair in Nanosciences & Nanotechnology (U2ACN2), College of Graduate Studies, University of South Africa (UNISA), Pretoria, South Africa*

[4]*PSES, ERC, Ecole Normale Supérieur, Mohammed V University in Rabat, P. O. Box: BP5118 Takkadoum Rabat-10000, Morocco*

*Email : abdelhafid.najim@usms.ma

Abstract. In this work, the electronic and optical properties of pristine MASnI3 (MA=CH3NH3) perovskite and MASnI3 substituted with cesium (Cs) elements were investigated using density functional theory (DFT) calculations. The CAmbridge Serial Total Energy Package (CASTEP) code was then used to construct and optimize these structures and calculate the band structure, total density of states (TDOS), and optical properties. This perovskite material is of significant interest for next-generation optoelectronic devices. Substitution of Cs in MASnI3 perovskite decreases the band gap and alters the TDOS, absorption coefficient, dielectric function, refractive index, optical conductivity, and loss function of the MASnI3 system. The presence of Cs in MASnI3 perovskite significantly affects its electronic and optical properties, suggesting that Cs can be used to control these properties.

Keywords: Absorption; Band gap; CASTEP; CH3NH3SnI3; DFT

Metrological Study of the Gamma Irradiator at CNESTEN's LEGX Calibration Laboratory via Beam Optimization Using Monte Carlo Simulation (MCNP)

T. ZIDOUZ[1,2]*, A. TALBI[2], A. ABARANE[3], A. DIDI[2], E. CHAKIR[1], E. ALIBRAHMI[1], A. ALLACH[2], N. ELIDRISSI[4]

[1] *LPMS, Faculty of Sciences, Ibn Tofail University, Kenitra, Morocco*
[2] *National Centre for Nuclear Energy, Science and Technology, Rabat, Morocco*
[3] *Higher Institute of Health Sciences, Settat, Morocco,*
[4] *Faculty of Sciences, Med V University, Rabat, Morocco*

*Email : taibi.zidouz@uit.ac.ma

Abstract. The Gamma Calibration Laboratory at CNESTEN plays a crucial role in calibrating radioprotection instruments on a national and international scale. Utilizing a Gamma irradiator equipped with Co-60 and Cs-137 sources, along with an X-ray irradiator, the laboratory ensures precision and reliability in radioprotection measurements through its ISO 17025 accreditation. This study aims to optimize calibration methods by characterizing and studying the homogeneity of gamma-ray beams using Monte Carlo simulation (MCNP) to ensure compliance with the technical requirements of ISO 4037 regarding the production of reference fields. The first phase of the simulation involved modeling the geometry and materials of the laboratory components and defining the technical specifications of the radioactive sources. The obtained results were compared with experimental measurements, showing acceptable deviations in the calculated Kerma rates, indicating the model's accuracy. The study also focused on the homogeneity of dose profiles within the collimated beams. The results demonstrated symmetrical energy deposition around the center of the beams, with significant variations in the Kerma rate beyond 4 cm from the central axis. These results allow for improved calibration precision and uniformity, thus enhancing the reliability of radioprotection instruments. The necessary adjustments to ensure this uniformity are discussed, highlighting the importance of Monte Carlo simulation in optimizing calibration procedures.

Keywords: Gamma Calibration, K_{air}, ISO 4037, Monte Carlo Simulation, MCNP, Radioprotection, CNESTEN.

Use of Byproducts and waste materials in the development of asphalt mixture: A review

Salman Mustafa Salih Zebari[1], Bakhtiyar Q. Khawaja AL Harki[1], Heja Ghazi Mohammed Hasan[2] and Nareen N. M Nadhif[1]

[1]*AUAS Akre University for Applied Sciences, Surveying Department, Akre Technical Institute, 42004, Iraq*
[2]*DPU Duhok Polytechnic University, Transportation Department, Technical College of Engineering, 42002, Iraq*
*Email : salman.mustafa@auas.edu.krd

Abstract. Nowadays, the use of by-products and waste materials as alternative eco-materials in the construction of pavement has increased dramatically on a wide range of estimates. The incorporation into the construction industry of by-products and waste materials like the development of mixtures of hot-asphalt concrete offers important environmental and economic advantages. The use of proper materials and accurate engineering can make it more convenient, durable, and cost-efficient for users, and importantly for the environment. To decrease the construction engineers' cost across the world are examining an alternative material to get the same quantity of production (durability, stability, and strength) for a lower cost. This study aimed to examine the usage of various by-product materials in developing the properties of asphalt mixtures. Fillers in the hot mix asphalt fill the void between the aggregates, which are essential for the pavement's stability and strength. However, the fillers are traditionally used (limestone and cement), use of cement is very costly which impacts the construction total cost. While the use of limestone, in addition to the cost, has many problems, the most important of which is stripping the binder from aggregates. The Marshall stability was improved by up to 6% with the amount of fly ash. The use of by-products and waste materials as HMA fillers would save 6-10% on total costs, in comparison with the use of limestone. In addition, when the Silica fume is used as a filler in HMA based on previous studies, Marshall Stability and flow are improved by 23.61% and 4.67%, respectively. However, the percentage of air voids is kept below the agreed limits when density increases.

Keywords: Byproduct materials, Filler, Waste materials, Recycle materials, Hot Mix Asphalt Properties.

Molecular dynamics simulation study of fatigue mechanical properties and microstructural evolution of Al metallic glasses under cyclic loading

S. Bogtob[1*], A. Samiri[1], H. Kourbani[1], A. Hasnaoui[1], K. Sbiaai[1]

[1]*LS2ME polydisciplinary faculty of Khouribga, Sultan Moulay Slimane University of Beni Mellal, BP: 145 25000, Morocco.*

* Email: saidbogtob@gmail.com

Abstract. Because of their high strength, metallic glasses (MGs) offer a lot of potential for use in structural applications. However, they have low fatigue endurance limits and soften under cyclic loadings. In this instance, we simulate tension-compression fatigue tests of Al-MG using molecular dynamics under strain-controlled cyclic loading. The simulation results also reveal that Al-MG exhibits a cyclic saturation stage after the initial cyclic hardening, which is called hardennig phenomenon. The cyclic saturation stage is a dynamic equilibrium of proliferation and annihilation of stacking faults created after the verification of the MG, indicating that the MGs have excellent fatigue mechanical properties. Furthermore, the proportion of stacking faults decreases with increasing strain value, resulting in faster cyclic stability and higher stress amplitude for MGs. These results provide important information for understanding the fatigue mechanisms of MGs from an atomistic point of view and any structural changes created during cyclic deformation. The current work clarifies the basic fatigue mechanisms of MGs, which may help in formulating engineering application methods.

Keywords: Molecular Dynamics, Metallic Glasses, Cycle Deformation, Mechanical Properties, Fatigue Behavior

Electronic and Optical Properties of Double Perovskite Oxide LaFeWO6: A Theoretical Understanding from DFT Calculations

Abdelkebir EJJABLI[1*], Mohamed KAROUCHI[1], Hamza ERRAHOUI[1], Omar BAJJOU[1,4], Khalid RAHMANI[2,3], Youssef LACHTIOUI[1]

[1] *Laboratory of Engineering in Chemistry and Physics of Matter Faculty of Sciences and Technics,Sultan Moulay Slimane University, BP 523, 23000, Beni Mellal, Morocco.*
[2] *Ecole Normale Superieure Mohammed V University, BP 5118, Rabat Morocco.*
[3] *Lphe-modeling and simulation Faculty of Science, Mohammed V University in Rabat, Moroccco.*
[4] *UNESCO UNISA Africa Chair in Nanosciences & Nanotechnology (U2ACN2), College of Graduate Studies, University of South Africa (UNISA), Pretoria, South Africa.*
Email : *Ejjabliabdelkebir@gmail.com*

Abstract. In the field of solar cells and catalysis, double perovskite oxides (DPOs) have emerged as potential candidates in recent years. Through compositional tuning and band gap engineering, a plenty of materials are being developed for pertinent applications in this field of energy. Oxide perovskites possess the advantage of a high carrier lifetime compared to that with halide perovskites, which can be beneficial for energy applications. In this perspective, we have presented theoretical investigations focusing on the different types of double perovskite oxides based on the composition space in a systematic manner. Corresponding electronic and optical properties are discussed along with an outlook on the novel routes to find efficient members in this family. This paper reports the study of electronic and optical properties of double perovskite oxide $LaFeWO_6$ by using the FP-LAPW method within density functional theory. Results of density of states and energy bands are presented. The direct band gaps have been found for the systems by using the GGA-PBE approximation. Calculations of optical properties is also presented by considering the variations of optical parameters as a function of incident photon energy. The results indicate that $LaFeWO_6$ exhibits a suitable band gap (0.71eV) for visible light absorption, along with promising electronic properties, making it a candidate for photocatalytic and photovoltaic (infrared) applications.

Keywords: Double perovskite oxides; Opto-electronic properties; DFT; Bands; photocatalytic

Comparative study on the properties of Zn and In-doped CeO_2 nanostructured thin films grown by spray pyrolysis method: application to electrochromic devices

Abdellatif El-Habib[1]*, Zakaria Barbouch[2], Bilal Brioual[1], Abdessamad Aouni[1], Mustapha Diani[1], Mohammed Jbilou[1] and Mohammed Addou[1]

[1]*Materials, Systems and Energy Engineering Laboratory (MaSEEL), ERCMN, (UAE/U01FST), Abdelmalek Essaâdi University, Tetouan, Morocco*
[2]*Laboratory of Materials Physics and Subatomic (LMPS), Department of Physics, Faculty of Science, Ibn Tofail University, B.P. 133, Kenitra, 14000, Morocco*
*Email : eabdellatif@uae.ac.ma

Abstract. Cerium oxide nanostructured thin films, as well as their variants doped with Zinc (Zn) and Indium (In), were successfully deposited onto both glass and ITO substrates using the spray pyrolysis method. Their structural, morphological, optical, and electrochemical properties were then experimentally studied. X-ray diffraction (XRD) has confirmed the generation of a single-phase polycrystalline cubic fluorite structure of CeO_2. The crystallite size and microstrain of the thin films were found to depend on the type of doping element. Red-shift, peak broadening, and asymmetry in the Raman mode (F_{2g}), as well as a red-shifted energy gap, were confirmed through Raman spectroscopy and UV–Vis–NIR analyses. SEM images reveal nanograin formation in all the films, while EDS analysis confirms the presence of the elements. The electrochemical measurements indicate that doping CeO_2 with Zn and In enhances its electrochemical properties. Furthermore, the doped CeO_2 thin films maintain full transparency during the intercalation and deintercalation of Li^+ ions. Such pivotal findings broaden the potential applications of this oxide, particularly in supercapacitors and electrochromic devices.

Keywords: CeO_2, Doping, Thin film, Spray pyrolysis, Electrochemical properties

A Review of Oxide Layer Formation and Corrosion Dynamics in Reinforced Concrete

Hajar SADEQ[1]*, Abdelkader NASSER[1], Abdelhamid KERKOUR EL MIAD[1] and Najib AMAR[2]

[1]*Mohammed First University Oujda, Faculty of Science Oujda, Laboratory of Materials, Wave, Energy and Environment (LaMOn2E), MEGCE team ESTO, Oujda, Morocco*
[2]*LABNORVIDA laboratory, Oujda, Morocco*
*Email : hajar.sadeq@ump.ac.ma

Abstract. Corrosion is a natural phenomenon that threatens the durability of steel reinforcement in reinforced concrete. Initially, the reinforcement is protected by a layer of iron oxides known as the passivation layer, formed due to the high alkalinity of the concrete medium. This passivation layer acts as a barrier, preventing the progression of corrosion by isolating the steel from corrosive elements. However, the incorporation of corrosion catalysts such as chlorides or carbon dioxide can destroy this protective layer. Once the passivation layer is compromised, reinforcement corrosion begins, leading to the formation of more complex iron oxides, such as rust (Fe2O3). These corrosion products influence the characteristics of the environment around the reinforcement, creating cracks in the concrete and facilitating the penetration of water and other corrosive agents. This process promotes the spread of corrosion within the reinforced concrete structure, accelerating its deterioration. This article provides an in-depth review of the development of the oxide layer on steel reinforcement and its impact on the interface between reinforcement and concrete. It explores the mechanisms by which the passivation layer is formed and the conditions that lead to its failure. Additionally, it examines the environmental and material factors that influence the progression of corrosion, such as concrete quality, humidity, and the presence of aggressive chemicals.

Keywords: Corrosion; Reinforced concrete; Oxide layer; Durability.

Impact of Calcium Doping on the Electronic and Optical Characteristics of Strontium Hydride (SrH_2): A DFT Study

Hamza Errahoui [1]*, Mohamed Karouchi [1], Abdelkebir Ejjabli [1], Aymene Elhaji [1], Abdelmounaim Laassouli [1], Youssef Lachtioui [1], Omar Bajjou [1]

[1] *Laboratory of Engineering in Chemistry and Physics of Matter Faculty of Sciences and Technics,Sultan Moulay Slimane University, BP 523, 23000, Beni Mellal, Morocco.*
*Email : hamzaa.errahoui@gmail.com

Abstract. This study investigates the electronic and optical properties of calcium-doped strontium hydride (SrH_2) using first-principles density functional theory (DFT) calculations via the CASTEP code with the generalized gradient approximation (GGA). We explore the impact of calcium (Ca) doping on the electronic band structure, density of states (DOS), and optical absorption spectra of SrH_2. Our results show that Ca doping significantly alters the electronic properties, notably increasing the indirect bandgap from 1.3 eV to 1.6 eV. The DOS analysis reveals new states near the Fermi level, primarily from Ca 3d orbitals. Moreover, the optical absorption spectra display enhanced absorption in the visible range, suggesting potential for optoelectronic applications. This research highlights the feasibility of tuning the electronic and optical characteristics of SrH_2 through Ca doping, opening the way for advanced materials with tailored properties.

***Keywords*:** DFT calculations, strontium hydride, opto-electronic properties, Density of states, Band gap.

Exploring mechanical and structural properties of monoatomic iron metallic glasses under varying cooling rates and pressures: Insights from molecular dynamic simulation

Soufiane ASSOULI[1*], Tarik EL HAFI[1], Abdelaziz EL kharraz[1], Omar BAJJOU[1], Youssef LACHTIOUI[1]

[1]*Laboratory of Engineering in Chemistry and Physics of Matter, Sultan Moulay Slimane University, Faculty of Science and Technics of Beni Mellal, BP. 523, 23000 Beni Mellal, Morocco*

*Email : dr.assouli@gmail.com

Abstract. This study investigates the formation and mechanical properties of monoatomic metallic glass using molecular dynamics simulations. Iron liquid was subjected to various cooling rates and pressures to understand their effects on the glass transition. The results demonstrate that both cooling rate and pressure significantly influence the glass transition temperature, which increases with higher pressure at a constant cooling rate and with higher cooling rates at a constant pressure. Voronoi tessellation techniques reveal that the prominence of specific Voronoi polyhedra (VPs) such as ⟨0,2,8,10⟩, ⟨0,1,10,2⟩, and ⟨0,0,12,0⟩ is responsible for the splitting of the second peak on the radial distribution function (RDF). The ultimate strength of the metallic glass is found to be inversely proportional to the cooling rate, while the elastic modulus (E) varies inversely with cooling rate and directly with pressure. The optimal cooling rate for achieving a high percentage of icosahedron-like VP and superior mechanical properties is determined to be 5×10^{12} K/s for Fe metallic glass. Furthermore, an increase in mechanical deformation leads to a decrease in the proportion of icosahedral clusters and an increase in applied strain. These findings provide valuable insights into the relationship between cooling conditions, structural characteristics, and mechanical performance of metallic glasses.

Keywords: Iron metallic glass; Cooling rate; Pressure, Microstructure; mechanical properties.

Study the effect pressure of structural, mechanical and optoelectronic properties of $InGeF_3$ using the DFT method

Mohammed Miri [1,2]*, Younes Ziat [1,2], Hamza Belkhanchi [1,2], Youssef Ait El Kadi [1], Ayoub Koufi [1,2]

[1] *Faculty of Science and Technology of Beni Mellal, Sultan Moulay Slimane University, Morocco*

[2] *The Moroccan Association of Sciences and Techniques for Sustainable Development*

*Email: mirimohamed834@gmail.com

Absract. This study explores the structural, mechanical, electronic and optical properties of $InGeF_3$ perovskite under varying pressures using density functional theory (DFT) via the Wien2k code. Elastic constants meet mechanical stability criteria at 0 GPa, with a notable improvement in ductility and hardness under pressure. Electronic analysis reveals an indirect band gap of 1.51 eV at 0 GPa, narrowing to 0.67 eV at 9 GPa, signaling a transition to metallic behavior. The density of states shows the dominance of halogens in the valence band, and significant contributions from indium and germanium in the conduction band. Optical properties, such as absorption and reflectivity, evolve under pressure, with a shift of the absorption spectrum towards lower energies. These findings demonstrate that pressure not only modifies the electronic structure of $InGeF_3$ but also enhances its optical performance, making it a potential candidate for photovoltaic applications.

Keywords: DFT, Pressure, Semiconductor, Stability mechanical, Absorption, Optoelectronic improvement.

Molecular Dynamics Analysis of Atomic Diffusion and Crystallization Behavior of Pure Silver in the Vitreous State under Varied External Pressures

Tarik EL HAFI[1]*, Soufiane ASSOULI[1], Abdelaziz EL KHARRAZ[1], Omar BAJJOU [1], Youssef LACHTIOUI[1]*

[1]*Put author's affiliation here, complete with address, postal code, and country*
[2]*Put author's affiliation here, complete with address, postal code, and country*
*Email : tarik.elhafi@gmail.com; y.lachtioui@gmail.com

Abstract. This study uses molecular dynamics simulations with the embedded-atom method to explore the structural and dynamic properties of silver (Ag) in its vitreous state under external hydrostatic pressures ranging from 0 to 70 GPa during the quenching process. By analyzing crystalline order and fractal dimension, the research uncovers patterns that show how rising pressure affects atomic arrangements. The results indicate that higher pressures lead to more ordered atomic structures, with atomic positions aligning with the face-centered cubic (fcc) lattice structure, emphasizing the system's increased sensitivity to pressure. Additionally, the study reveals that pressure impacts atomic diffusion behavior, with atomic mobility decreasing as pressure increases, illustrating the direct influence of pressure on the dynamics of glassy Ag metal.

Keywords: Silver (Ag) vitreous state; External pressure; Molecular dynamic; Atomic diffusion behaviors; microstructural evolution

DFT study on electronic and optical properties of Ag_2BeSnX_4 (X = S, Se, Te) Kesterites under an external electric field

Jamal GUERROUM[a], Mohamed AL-HATTAB[a]*, Mohamed KAROUCHI[a] Younes CHRAFIH[b], L'houcine MOUDOU[a], Khalid RAHMANI[b,c], Youssef LACHTIOUI[a] ,Omar BAJJOU[a,d]

[a]*Laboratory of Engineering in Chemistry and Physics of Matter (LICPM), Faculty of Sciences and Technics,Sultan Moulay Slimane University,BP 523,23000 Beni Mellal, Morocco.*

[b]*LPHE-Modeling and Simulation, Faculty of Sciences, Mohammed V University in Rabat,Morocco*

[c]*EcoleNormaleSupérieure (ENS), Mohammed V University in Rabat, Morocco*

[d] *UNESCO UNISA Africa Chair in Nanosciences & Nanotechnology (U2ACN2), College ofGraduate Studies,University of South Africa (UNISA),Pretoria,South Africa;*

*Email : jamalguerroum96@gmail.com

Abstract. In this work, density functional theory (DFT) calculations are used to examine the optoelectronic properties of kesterite Ag_2BeSnX_4 (X=S,Se and Te) structure when an external electric field (E_{ext}) is applied. Kesterite structure was built using the Material Studio visualizer module. The band structure, density of states, and optical properties of this structure are then optimized and calculated using the CASTEP code. The E_{ext} effects lead to modulate the band gap and change the total density of states (TDOS), absorption coefficient, dielectric function, optical conductivity, refractive index and loss function. The peaks of TDOS around the fermi level are very weak. In the visible and ultraviolet (UV) ranges, the absorption coefficient increases due to E_{ext} effects. It is found that electronic structures and optical properties of $Ag_2BeSnTe_4$, could be affected by the E_{ext} effects. All these results provide the important information for understanding and controlling the opto-electronic properties by an E_{ext} effects.

Keywords: Kesterites; electronic properties; optical properties; optoelectronic; external electric field.

Elemental Analysis of Eight Medicinal Plants Species Growing in North of Morocco Using Neutron Activation Analysis

AARAB Iliasse[1,2,*], BOUNOUIRA Hamid[2], CHAKIR El Mahjoub[1], BADAGUE Abdelwahab[1,2]; AMSIL Hamid[2], DIDI Abdessamad[2],

[1] *LMPS, Faculty of Sciences, Ibn Tofail University, Kenitra, B.P 242 Kénitra, Morocco.*
[2] *NAA Laboratory, National Center for Energy, Nuclear Sciences and Techniques (CNESTEN), B.P. 1382 R.P. 10001 - Rabat - Morocco.*
*Corresponding author e-mail address: iliasse.aarab@uit.ac.ma

Abstract. This study aimed to evaluate the performance of the k0-standardization method in neutron activation analysis when applied to samples of Moroccan medicinal plants. Irradiation was conducted at the Moroccan Triga Mark II research reactor at CNESTEN. Internal quality control utilized standard reference materials from NIST and WEPAL to ensure accuracy and precision of measurements. Analysis revealed high concentrations of major elements such as Mg, K, Ca, Cl, and Na across 08 medicinal plant species studied. Trace amounts of rare earth elements and toxic elements were also detected. Based on these findings, the medicinal plants were classified according to their profiles of trace elements, macro-elements, rare earth elements, and toxic elements.

Keywords: medicinal plant; neutron activation analysis; K0 standardization method; Triga Marc II reactor

Optimizing CZTS Solar Cell Performance with Advanced Layer Configurations Using SCAPS Simulation

O. Belhaidouri [a], R. Moultif , L. Mouakkir [b]

[a]*Laboratory Of Condensed Matter Physics,Faculty of sciences ben m'sik ,Casablanca ,Morocco*

[b] *Physics departement ,Polymer physics , Mechanical sciences and materials laboratory , faculty of sciences ben m'sik ,Casablanca ,Morocco*

*Email : oussbelhaidouri@gmail.com

Abstract. This investigation delves into the simulation of CZTS (Copper Zinc Tin Sulfide) solar cells with a focus on enhancing performance by tailoring specific material layers. Through the application of comprehensive simulation methodologies, an analysis of the efficiency of CZTS solar cells is carried out, with particular emphasis placed on the employment of a TMD material as the buffer layer, CuO as the hole transport layer (HTL), and ZnO as the window layer. The utilization of SCAPS-1D software in our study allows for the simulation of the basic structure to assess and improve the performance metrics of these solar cells based on CZTS. This process entails the optimization of the absorptive layer thickness in each cell and the precise adjustment of buffer layer. Furthermore, an investigation is conducted into the influence of temperature fluctuations on the performance of CZTS cells, highlighting that changes in temperature impact electron energy levels and, consequently, the bandgap. In order to further enhance the efficiency of solar cells, a detailed analysis is carried out on the work function of the rear contact material. The outcomes of our numerical analyses offer tailored material configurations and thicknesses that aim to enhance efficiency and durability under varying temperature conditions.

Keywords: photovoltaic ; CZTS ; TMD ; HTL ; SCAPS

Quality control method for toothpaste.

Mustapha OUKBAB[1]*, Hassan HADDOUCHY[2], Youness TAHIRI[1], Salma ZAHID[1], Mohamed OUBAOUZ[1], Salah Eddine ELQOUATLI[2], And Abdelilah CHTAINI[1] .

[1]*Molecular Electrochemistry and Inorganic Materials Team, Faculty of Sciences and Technologies, Sultan Moulay Slimane University, Morocco.*

[2] *Physical Chemistry Environment and Material, Moulay Ismail University, Faculty of Sciences and Technologie, Errachidia, Morocco*

*Email: mustapha.oukbab@usms.ma

Abstract. The following work presents a new method to study the quality of different types of toothpastes. Our study is based on a single electrochemical method: cyclic voltammetry (VC). This work examines the condition of various toothpastes, including the concentration of ingredients. The study mainly focuses on the excessive presence of fluoride, considered a corrosive agent for dental alloys. Analysis of the results of the behavior of different toothpastes by cyclic voltammetry reveals catalytic reactions which give good results.

Keywords : Voltamétrie Cyclique ; Alliages dentaires ; Méthode électrochimique .

Synthesis and Characterization of Phosphocalcic Apatites with Phosphite Ions for Biomedical Applications

Noureddine ZELMIMI[1]*, Souhail JERDIOUI[1], Khadra ZEHRAOUI[1]

[1]*Laboratory of Applied Chemistry and Environment, Mineral Solid Chemistry Team, Faculty of Sciences, Mohammed First University, B.P. 717, 60 000, Oujda, Morocco*

*Email : zelmiminoureddine99@gmail.com

Abstract. Phosphocalcic apatites are promising materials for orthopedic and dental surgery, due to their similarity to the mineral phase of bone and their strong affinity to bone tissue. To enhance their physicochemical and biological properties, it is important to prepare apatites with a highly reactive surface. In this work, we synthesized apatites with different amounts of phosphorous acids H3PO3, using a modified double decomposition method. We characterized the synthesized materials by X-ray diffraction, Fourier transform infrared spectrometry, thermogravimetric/differential thermal analysis, and scanning electron microscopy/energy-dispersive X-ray spectroscopy. We also performed a biological study to evaluate the antimicrobial and antifungal activities of the apatites. The results showed that the presence of phosphite ions affected the crystallinity and the structural composition of the apatites. The apatitic phase became less crystallized and more distorted as the phosphite concentration increased and lost its apatitic structure for values above 33% of phosphite ions. The thermal analysis revealed that the phosphite groups stabilized the apatitic structure, as indicated by the shift of the exothermic peaks. The antibacterial activity was tested against four bacterial strains, two Gram-positive (Staphylococcus aureus, Micrococcus luteus) and two Gram-negative (Escherichia coli, Pseudomonas aeruginosa). The results indicated that the addition of phosphite ions improved the antibacterial activity of the apatites, especially against P. aeruginosa. The antifungal activity was evaluated against tow fungal strains, Penicillium digitatum and Aspergillus niger, and a yeast, Candida glabrata. The results suggested that the addition of phosphite ions influenced the antifungal activity of the apatites, but the effect depended on the phosphite concentration, the apatite structure, and the fungal strain. Future research should aim to increase the sample size, optimize the synthesis method, and conduct in vivo tests to confirm the potential of the phosphocalcic apatites with phosphite ions for biomedical applications.

Keywords: Antifungal and antimicrobial activity; biomaterial; double decomposition; phosphocalcic apatitic; phosphite.

Growth and Characterization of Semiconductor ZnO Nanorods for Photovoltaic Applications

O. Haddad [1.2*], A. Ait Hssi[1], A. Soussi[1], N. Labchir[3], K. Abouabassi[1], R. Markazi[2], A. Elfanaoui[1], A. Ihlal[1]

[1]*Laboratory for Renewable Materials and Energies, Ibn Zohr University, BP 8106, Cité Dakhla, 80000 Agadir, Morocco*
[2]*Laboratory of Energy and Sustainable Development, Ibn Zohr University, EST, BP 202, 81000 Guelmim, Morocco*
[3]*Univ. Grenoble Alpes, CNRS, CEA/LETI-Minatec, Grenoble INP, LTM, Grenoble F-38054, France*

*Email : haddad.oumayma19@gmail.com.

Abstract. Metal-oxide semiconductors are highly attracting materials in various applications as solar cells. Among them, zinc oxide (ZnO) which is abundant, stable and non-toxic material. This material is a n-type semiconductor and a promising candidate for solar energy conversion thanks to its good absorption coefficient in the visible range and its direct band gap. Several methods are usually used to prepare ZnO nanorods. In this work, we report the synthesis of doped ZnO nanorods by the electrodeposition technique. The as-electrodeposited Bi doped ZnO nanorods, via two steps at applied potentials of -1 V and -1.4 V for 30 min in acidic aqueous solution (pH = 6), have revealed a good crystallinity with a preferred orientation along the plane (002). Moreover, the transmittance of Bi doped ZnO nanorods is demonstrated that they have high optical transmission (>75%) with a direct band gap energy of 3.5 eV. Then, the PL measurements have showed an increasing in the emission intensity at 670 nm with the increasing of the doping level by Bi from 1% to 6%. This result can be associated to the electron transitions from the bottom of the conduction band to the levels corresponding to the antisite oxygen O_{Zn} defect. Finally, the experimental findings have been compared to DFT calculations in order to have a clear idea about the optical behavior of ZnO nanorods. The reported work on electrochemically synthetized ZnO nanorods is a promising reference for future photovoltaic investigations.

Keywords: ZnO, Bi, nanorods, band gap energy, transmittance, XRD, SEM, UV-visible, PL.

Determination of the Chemical Composition of Ptychotis ammoides Extracts

EL HAJJAMI Kaoutar [1]*, BERRABAH Mohamed [1]

[1]* *Laboratory of Applied Chemistry and Environment, Mineral Solid Chemistry Team, Faculty of Sciences, Mohammed First University, B.P. 717, 60 000, Oujda, Morocco*

[1] *Laboratory of Applied Chemistry and Environment, Mineral Solid Chemistry Team, Faculty of Sciences, Mohammed First University, B.P. 717, 60 000, Oujda, Morocco*

*Email : kaoutar.elhajjami.d23@ump.ac.ma

Abstract. The plant is distinguished by its finely divided leaves and small white or yellowish flowers, with a late dynamic cycle from May to July. It is widely used in traditional medicine for its antidiabetic, antipyretic, antiseptic, antifungal, and antibacterial properties, specifically for treating fever, diabetes, colds, bronchopulmonary diseases, and kidney infections. This study aims to determine the chemical composition of extracts from Ptychotis ammoides, obtained through three distinct methods: maceration, infusion, and hydrodistillation. Plant compounds were extracted using the maceration method with solvents of varying polarities, while infusion was investigated by varying the infusion duration. Finally, the plant's essential oil was extracted using the Clevenger-type hydrodistillation method. These extracts were subsequently analyzed using two chromatographic methods: HPLC/UV and GC/MS.

Keywords: Ptychotis ammoides, Extraction, Essential oil, biological activities.

Application of magnetized water to plant growth and development research

El mostafa EL MESBAHI, A. Elmelouky, Y.Hairch, M.Monkade, R.Elmoznine.

Department of Physic condensed Matter Laboratory, Faculty of Sciences, Chouaib Doukkali University, El-Jadida, Morocco

*Email : elmesbahi.el_mostafa@ucd.ac.ma

Abstract. Water magnetization is a cutting-edge technology, a physical water treatment, which contributes to a more sustainable supply of clean fresh water, and gives tool for mitigating some effects of the climate change in the plant production, and remediating pollution of soil and water. The mechanism of action of water magnetization, the quantum physical and chemical reasons behind it leading to enhanced structural order by hydrogen-bonded networks of water molecules are presented. Practical application possibilities of magnetized water in agriculture, water management and remediation of water and soi are reviewed based on latest researches

Keywords: Magnetic Water Treatment, Agriculture, Magnetized water, Irrigation water treatment

DFT study of the energetic, electronic and structural aspects of hemimellitic and pyromellitic acids

Taoufik GOURTI[1]*, Mohamed LAABD[1], Mahmoud RAHAL[2], Nouh AARAB[1] and Abdallah ALBOURINE[1]

[1] *Materials and Environment Laboratory (LME), Department of Chemistry, Faculty of Science of Agadir (FSA), Ibn Zohr University, Morocco.*

2 Regional Center for Education and Training Professions, Laâyoune Boujdour Saguia El Hamra Region, Morocco.

*Email : gourti.taoufik@gmail.com

Abstract. Benzene polycarboxylic acids (BPAs) present in wastewater and natural waters can have harmful effects on health and the environment. These pollutants are used in a number of fields (pharmaceuticals, oil industry, cosmetics, dyes, printing inks, etc.) as reagents or products. Several studies have been carried out to eliminate them from wastewater, notably by adsorption and photo-degradation. To make these techniques easier and more profitable, it is essential to carry out theoretical research using technological advances. One of the most popular theoretical methods is DFT. This is an approach that better meets current system characterization needs, by minimizing the amount of experimental data required, influencing the duration of the experiment and limiting some areas of experimental conditions. In this study, the optimized geometries of hemimellitic acid (1,2,3-tri-carboxy-benzoic acid) and pyromellitic acid (1,2,4,5-tetra-carboxy-benzoic acid) molecules with energetic and electronic aspects have been obtained using Gaussian 09W at the B3LYP/ (6-31G; 6-31 G+; 6-31 G++) and CAM-B3LYP/ (6-31G; 6-31G+; 6-31G++) levels. Theoretical results from various angles: structural, electronic and energetic, in the gas and aqueous phases, are analyzed to compare the geometric, spectral and electrochemical properties of these pollutants. The results obtained can also be used to predict the various interaction mechanisms between the molecules and the substrates examined.

Keywords: ADSORPTION; DFT; HEMIMELLITIC; ORGANIC POLLUTANTS; PYROMELLITIC.

Theoretical Design of New Organic Materials for Application in Solar Cells: DFT and TD-DFT investigation

SERGENT Chaymae[1]*, KARZAZI Yasser[1].

[1] *Laboratory of Applied Chemistry and Environment, Faculty of Sciences, University Mohammed I, Oujda 60046, Morocco*

*Email : chaymae.sergent.d23@ump.ac.ma

Abstract. The optimization of energy use, particularly from fossil sources, poses a significant challenge for preserving these resources and mitigating the effects of climate change. In this context, the development of sustainable energies, especially solar energy, stands as a major avenue for streamlining energy use in technological, industrial, and economic terms. The advancement of solar cell technology is at the core of the efforts in solar energy production. It is within this framework that this work is situated, focusing on the development of the latest generations of solar cells, specifically organic solar cells (OSC). This study focuses on evaluating the performance of organic solar cells using a new donor material. Density functional theory (DFT) and time-dependent density functional theory (TD-DFT) with the 6-31G(d,p) basis set were employed to predict the excitation energies, open-circuit photovoltage, oscillation strength, absorption spectra, and the energy levels of frontier molecular orbital (HOMO and LUMO). Our results suggest that the studied molecules are promising candidates for organic solar cell (OSC) applications.

Keywords: Solar cells; Energy; OSC; DFT; TD-DFT.

Modeling Hygrothermal Transfer in bio-based Construction Materials using Künzel Model

Mohammed Taibi[1], Younes Abouelhanoune[2], and Fouad Dimane[1]

[1]*LSIA, ENSAH Al-Hoceima, Abdelmalek Essaadi University, Tetouan, Morocco,*
[2] *LSA, EMAO, ENSAH Al-Hoceima, Abdelmalek Essaadi University, Tetouan, Morocco,*
Email: mohamed.taibi12@gmail.com

Abstract. The integration of innovative passive materials in building envelopes is a relevant means to reduce energy consumption and ensure a high level of indoor comfort. Examining the hydrothermal parameters of bio-based construction materials using the Künzel model, a well-established approach for simulating coupled heat and moisture transfer in construction materials, is essential. The numerical validation was carried out using two mathematical models for coupled heat and moisture transfer in porous materials, considering their permeability, sorption capacity, and moisture diffusivity coefficients. These models were chosen not only for their simplicity but also for their predictive ability regarding the properties of our bio-based materials. By adopting a macroscopic approach, we introduce the physical principles of the elementary processes governing moisture and heat.

Keywords: Moisture; Künzel model; bio-based materials; heat transfer; hydrothermal.

Modeling of storage and degradation Lithium-Ion Battery

M. Karim a, M. Tanasehte b, N. Tafsi b, R. Moultif a, A. Hader b,c,*, Y. Ezaier b , I. Tarras b, R. ET Touzi b and F.Z. Kreimech b

a LPMC , Faculty of sciences Ben M'sik . University Hasan II. Casablanca, Morocco
b LBGIM, Ecole Normale Supérieure, University Hassan II. Casablanca, Morocco
cCentre régional des métiers d'éducation et de formation Casablanca- Settat, Morocco
* Corresponding author: ahader73@yahoo.fr

Abstract. Energy storage research attempt to generate sustainable and efficient battery resolutions crossways varied engineering fields. Electric batteries are crucial for converting usable electrical energy from stored chemical energy in electronic systems. Moreover, the emphasis is on the development of environmentally-friendly battery categories able of slow discharge and recharge rates, safeguarding the integrity of electrode while improving durability and performance. Yet, divers complications as heterogeneity and mechanical degradation minimize the endurance and efficacity of battery. This highlights the requirement to introduce mechanics aspects and use numerical simulations to establish performant degradation models. Although these challenges, lithium-ion batteries persist grid storage and the preferred and optimal choice for electric system owing to their extended cycle life and high-power density. Advancing battery technology involves optimizing performance and conquering degradation obstacles over innovative materials and efficient modeling. This paper explains the impact of mechanical strain and thermal noise on electrochemical cycling in battery, by presenting the resulting failure mechanisms and thermal effect in structural batteries. To attain this objective, we propose to use the fiber bundle model as a theoretical simulation for studying the degradation of electrodes.

Keywords: Lithium batteries, Fiber Bundle Model, degradation thickness, cycle, activation energy, jump frequency

Phosphorus Doping Effects on the Optoelectronic Properties of $K_2AgAsBr_6$ Double Perovskites

Abdelmounaim Laassouli[1]*, Lhouceine Moulaoui[2], Abdelhafid Najim[1], Hamza Errahoui[1], Omar Bajjou[1,3], Khalid Rahmani[4], Youssef Lachtioui[1]

[1] *Laboratory of Engineering in Chemistry and Physics of Matter (LICPM), Faculty of Sciences and Technics, Sultan Moulay Slimane University, BP 523, 23000 Beni Mellal, Morocco*

[2] *Research Laboratory in Physics and Sciences for Engineers (LRPSI), Poly-disciplinary Faculty, Sultan Moulay Slimane University, BP 592, 23000 Beni Mellal, Morocco*

[3] *UNESCO UNISA Africa Chair in Nanosciences & Nanotechnology (U2ACN2), College of Graduate Studies, University of South Africa (UNISA), Pretoria, South Africa*

[4] *PSES, ERC, Ecole Normale Supérieure, Mohammed V University in Rabat P. O. Box: BP5118 Takkadoum Rabat-10000, Morocco*

*Email : abdelmounaim.laassouli@gmail.com

Abstract. This study investigates the effects of phosphorus doping on the optoelectronic properties of $K_2AgAsBr_6$ double perovskites using first-principles calculations based on density functional theory (DFT) with the PBE functional, as implemented in the CASTEP code. We examine the electronic and optical characteristics of cubic Fm-3m $K_2AgAsBr_6$, $K_2AgAs_{0.8}P_{0.2}Br_6$, and $K_2AgAs_{0.6}P_{0.4}Br_6$ to elucidate the impact of progressive Phosphorus (P) substitution, chosen for its potential to modify the electronic structure due to its smaller atomic radius and different valence orbital energies compared to As. Our results reveal a systematic narrowing of the band gap with increasing P content, from 0.749 eV for the undoped compound to 0.587 eV for $K_2AgAs_{0.8}P_{0.2}Br_6$ and 0.424 eV for $K_2AgAs_{0.6}P_{0.4}Br_6$. This trend is attributed to the upward shift of the valence band maximum due to the higher energy of P 3p orbitals compared to As 4p orbitals. Analysis of the density of states confirms increased hybridization between P-p and As-p states at the valence band edge. Optical properties, including absorption coefficient, dielectric function, refractive index, and extinction coefficient, demonstrate a consistent red-shift and broadening of spectral features with P doping. Notably, P-substituted compounds exhibit enhanced absorption in the visible light region, with up to a 20% increase in the absorption coefficient at 550 nm for $K_2AgAs_{0.6}P_{0.4}Br_6$ compared to the undoped compound. These findings provide valuable insights into tuning the optoelectronic properties of double perovskites through elemental substitution, paving the way for the design of novel materials for next-generation photovoltaic and optoelectronic devices.

Keywords: Double perovskites, Phosphorus doping, Optoelectronic properties, DFT calculations, Band gap

Theoretical Investigation of Structural and Electronic Properties of SnO_2 Using DFT+U+V Approach

Abderrahim Ait Lhaj[1*], Brahim Ouazik[1], Mohamed El Hasnaoui[1], Hassan Chaib[2]

[1] *Materials and Subatomic Physics, Faculty of Sciences, Ibn Tofail University, Morocco.*
[2] *Materials and Energy Research Group, Polydisciplinary Faculty of Ouarzazate, Ibnou Zohr University, Morocco.*
*Email : abderrahim.aitlhaj@uit.ac.ma

Abstract. In this study, we conduct a theoretical investigation of the structural and electronic properties of SnO_2 using the Density Functional Theory (DFT) with Hubbard U and V corrections. The DFT+U+V approach is an advanced computational technique that incorporates both on-site (U) and inter-site (V) Hubbard corrections to accurately describe electronic correlations in materials. Our optimized crystal parameters, which are a = 4.732 Å, c = 3.345 Å, and u = 0.3056, are in good agreement with experimental data. Furthermore, the electronic energy band gap, which is found to be 3.58 eV by using DFT+U+V approach, is very close to the experimental value, which is 3.56 eV. This significant improvement in the calculation method of the energy band gap, which was found to be 0.58 eV without Hubbard corrections, demonstrates the effectiveness of the DFT+U+V approach in accurately modeling the electronic properties of SnO_2.

Keywords: DFT; DFT+U+V; Energy band gap; SnO_2

Development and preparation of a novel carbon paste sensor modified with NP-ZnO for the simultaneous detection of hazardous metal ions

Abdelaziz Moutcine [1,2*], Charaf Laghlimi [1], Younes Ziat [3], Hamza Belkhanchi [3],

[1] *Faculty of Science and Technology of Beni Mellal, Sultan Moulay Slimane University, Morocco*

[2] *LRSDI, FSTH, Abdelmalek Essaadi University, Tetouan, Morocco*

[3] *Laboratory of Engineering and Applied Technologies, Higher School of Technology, Sultan Moulay Slimane University, Beni Mellal, Morocco*

*Email : abdelazizmoutcine@gmail.com

Abstract. The sensor, designed for the detection of Cd(II), is developed by modifying the carbon paste electrode (CPE) with an inorganic molecule, NP-ZnO. Physical parameters influencing current densities were studied and optimized, yielding optimal conditions: pH = 3, preconcentration time = 5 minutes, and scan rate for cyclic voltammetry (CV) = 100 mV/s. Energy dispersive spectrometry (EDX) combined with electron microscopy was employed to examine the sensor surface. Cyclic voltammetry (CV) and square wave voltammetry (SWV) were used to investigate the electrochemical behavior of lead. Increasing the scan rate from 30 to 150 mV/s resulted in a linear increase in anodic and cathodic peak currents, indicating that the electron transfer from Cd(II) to the CPE/NP-ZnO is an adsorption-controlled process. The CPE/NP-ZnO sensor exhibited a good linear response to cadmium ions in the concentration range of 0.42 mM to 2 mM. CV results showed that the detection limit for Cd(II) is 89 nM.

Keywords: Hazardous metal ions; Electrochemical impedance spectroscopy (EIS); Carbon paste electrode (CPE); Energy dispersive spectrometry (EDX); Scanning Electron Microscope (SEM); Square Wave Voltammetry (SWV).

Strontium substitution effects on the crystal structure, microstructure, optical and electronic properties of $Ba_{2-x}Sr_xMM'O_6$ (M/M'= Ti, Mn, Zr) double perovskites

Abdelaziz EL AAMRANI[1], B. AKHSASSI[2], O. OUZAGUINE[1], A. BOUDDOUCH[3], B. BAKIZ[1], A. TAOUFYQ[1], A. BENLHACHEMI[1]

[1] *Materials and Environment Laboratory (LME), Faculty of Science, Ibn Zohr University, B.P 8106, Cite Dakhla, Agadir, Morocco.*

[2] *CNRS 7334, IM2NP, BP 20132, University of Toulon, University of Aix Marseille, La Garde Cedex, France.*

[3] *Laboratory of Physical Chemistry of Materials (LPCM), Department of Chemistry, Faculty of Science, Chouaïb Doukkali University, El Jadida, Morocco.*

*Email : a.elaamrani@uiz.ac.ma

Abstract. Various studies carried out since the fifties to the present, have revealed that the materials with perovskite structure exhibited a wide variety of physical and structural properties. But probably the reason that determined the intensification of studies on these compounds, is the discovery in recent years, for some of them the colossal magnetoresistance effect. In this work, we report that the compositions in the system $Ba_{2-x}Sr_xMM'O_6$ (M/M'= Ti, Mn, Zr) with $0 \leq x \leq 0.25$, were synthesized by the solid state reaction in polycrystalline form by thermal treatment, in air. Results show that the solid solution system $Ba_{2-x}Sr_xMM'O_6$ (M/M'= Ti, Mn, Zr), remains as cubic perovskite in the marge of $0 \leq x \leq 0.25$, with $Pm\bar{3}m$ (no. 221) or $Fm\bar{3}m$ (no. 225) space group at room temperature. The surface characteristics and microstructure of the samples were studied by SEM images, while micrography and composition were determined by EDS analysis. Vibrational properties of the compounds were studied by FTIR spectroscopy. Furthermore, UV-visible spectroscopy technique was employed to study the optical properties and band gap of the obtained double perovskites.

Keywords: Double perovskite, Synthesis, Crystal structure, Rietveld refinement, Optical properties, Electronic properties.

Recent trends in sustainable eco-friendly materials for chemical detection and removal of emerging contaminants from water

Jalal Isaad[1*], Rachida Ouaabou[1]

[1]*ERCI2A, FSTH, Abdelmalek Essaadi University, Tetouan, Morocco*

*Email: j.isaad@uae.ac.ma

Abstract. Recently, the development of new eco-friendly materials for water treatment has intensified. Designing more efficient and high-performance materials to detect and remove chemical pollutants that are potentially harmful to the environment and human health is crucial. Among these pollutants, heavy metals, dyes, and anions such as cyanide, nitrate, and phosphate are the most dangerous, as they are lethal to humans even at low concentrations. Consequently, it is vital to develop materials capable of detecting and eliminating these pollutants, whose presence in drinking water poses a serious risk to human health. Over the last decade, we have developed new eco-friendly materials for the detection of heavy metals, and cyanide ions and the removal of dyes, nitrates, and phosphates from wastewater. In this conference, we present an overview of these new materials.

Keywords: Eco-friendly material; Chemosensor; Adsorbent; Water; Removal

Study of the performance of a $CH_3NH_3SnI_3$-based solar cell using the SCAPS-1D simulator

M'hamed SEMLAL [a], Mohamed KHUILI [*, a,b] , Nejma FAZOUAN [a], El Houssine ATMANI [a]

[a] *Laboratory of Nanostructures and Advanced Materials, Mechanics and Thermofluids, Faculty of Sciences and Technologies, Hassan II University of Casablanca. Mohammedia, Morocco*

[b] *CRMEF of Beni Mellal-Khénifra, Morocco*

[*]Corresponding author: m.khuili@usms.ma Telephone number: +212660061279

Abstract. In this research, a solar cell featuring $CH_3NH_3SnI_3$ as the active layer and MoS_2 as the hole transport layer (HTL) was designed and analyzed using the Solar Cell Capacitance Simulator in One Dimension (SCAPS-1D) software. The study examined the effects of various factors, including the thickness of the layers, doping concentration, defect and interface density, and temperature, to determine optimal photovoltaic performance such as open-circuit voltage (Voc), short-circuit current density (Jsc), fill factor (FF), energy conversion efficiency (η), and quantum efficiency (QE). The results were then compared to those of similar solar cells utilizing different HTLs in both theoretical and experimental studies.

Keywords: Perovskite, SCAPS-1D, Solar cells, $CH_3NH_3SnI_3$, MoS_2

Structural, electronic and optical properties of La-doped FAPbI3 perovskite : A DFT Study

Anass Kharissi [1], Mohamed karouchi [2], youssef Lachtioui [2], Rachida Moultif [1]

[1]*Laboratory Physics Condensed Matter, Faculty of Sciences Ben M'Sick - Hassan II University, BP 7955, Casablanca, Morocco*

[2]*Laboratory of Engineering in Chemistry and Physics of Matter Faculty of Sciences and Technics,Sultan Moulay Slimane University, BP 523, 23000, Beni Mellal, Morocco.*

*Email : anasskharissi@gmail.com

Abstract. With the aim of investigating the effects of La doping on structural, electronic and optical properties in formamidinium lead iodide (FAPbI3) perovskite from a theoretical study point-of-view first-principles calculations based on density functional theory (DFT-GGA-PBE ultrasoft pseudopotentials.) are done. It shows that doping La onto the Pb site is energetically less prone than, instead of on to FA site. La substitution at the FA site introduces new Gamma-point electronic states within these PEDOT chains, causing a band gap modulation from indirect to direct in this crystal. This change in the electronic band structure is accompanied by a shift to lower energies of density of states and an increase in La--ligand interaction. La doping has a significant effect on the partial density of states at the bottom of conduction band. The coupling of a transition to a direct band gap and superior optical properties places La-doped FAPbI3 as an attractive material toward more advanced optoelectronics applications.

Keywords: Band gap, DOS, PDOS, DFT, Optical Properties, electronic Properties, doped.

Improving Adobe's Mechanical Properties through Sawdust Reinforcement: A Comparative Study of the effect of varying Sawdust Dimensions

Youness Azalam [1]*, Mohammed Benfars[1], Abdelmounaim Alioui[2], Mustapha Mabrouki[1], El Maati Bendada[2]

[1] *Laboratory of Industrial and Surface Engineering Sultan Moulay Slimane FST, Mghila, B.P. 592, Beni Mellal, Morocco, 23000*

[2] *FP, Mghila, B.P. 592, Beni Mellal, Morocco, 23000*

*Email: youness.azalam@usms.ma

Abstract. In a world constrained by economic and environmental concerns due to industrial advancements and their environmental impacts, the construction sector continues to grow, significantly affecting energy consumption and greenhouse gas emissions. Ecological construction, particularly using soil-based materials, offers a viable solution to mitigate these negative impacts while maintaining the mechanical and energy performance of building materials. This research paper examines an adobe construction element reinforced with sawdust of varying dimensions. A comparative study was conducted, altering the length and diameter of sawdust to evaluate its effect on the mechanical performance of the adobe. The results showed that increasing the sawdust dimension from 0,3 cm (thin) to 2 cm (thick) significantly improved the mechanical strength of the adobe. Additionally, other sustainability-related parameters showed improvements, enhancing the overall ecological benefits of the material. This study underscores the potential of using sawdust-reinforced adobe as a sustainable construction material.

Keywords: soil-based material; ecological buildings; sawdust; mechanical performance.

Put the Title of the Paper Here, and Capitalize Each Word without Line Separation

Mohammed Benfars[1]*, Abdelmounaim Alioui[1,2], Youness Azalam[1], Mourad Kaddiri[1], Mustapha Mabrouki[1]

[1] *Laboratory of Industrial and Surface Engineering Sultan Moulay Slimane University Beni Mellal, Morocco*

[2] *Polydisciplinary Faculty Sultan Moulay Slimane University Beni Mellal, Morocco*

*Email : mohammed.fars@usms.ma

Abstract. The roof is the component of the building envelope most exposed to climatic conditions, and it significantly contributes to the total cooling load of buildings in hot climates. Therefore, roof thermal insulation can significantly reduce the substantial energy consumption used for cooling buildings. In this context, the thermal performance and energy efficiency of roofs constructed with traditional concrete blocks used in Morocco, insulated with ecological panels made from plant fibers, were examined through thermal simulations. Using OpenStudio for simulations, we analyze the impact of these panels on indoor ambient temperature and energy demands for cooling. The objective is to promote and evaluate the use of ecological panels to improve thermal insulation and reduce energy consumption under hot climatic conditions. Our results reveal significant variations in thermal performance and energy efficiency depending on the type and thickness of the panels used. These findings provide valuable insights into the potential use of thermal insulation panels to enhance the energy efficiency of conventional buildings and contribute to sustainable construction practices.

Keywords: Thermal simulation; Thermal insulation; Energy efficiency; Ecological panels; Sustainable building

Comparative analysis of energy performance between clay-based and conventional building materials: A case study in Moroccan semi-arid climate

Abdelmounaim Alioui[1,2,*], Youness Azalam[2], Mohammed Benfars[2], El Maati Bendada[1,2], Mustapha Mabrouki[2]

[1]*Polydisciplinary Faculty, Sultan Moulay Slimane University, 2300, Beni Mellal, Morocco*
[2]*Laboratory of Industrial and Surface Engineering, Faculty of Science and Technologies, Sultan Moulay Slimane University, 2300, Beni Mellal, Morocco*
*Email : abdelmounaim.aliouifpb@usms.ac.ma

Abstract. The environmental challenges arising from using traditional construction materials, such as cement, along with their rapid depletion, underscore the necessity of employing environmentally friendly building materials derived from natural resources. In this context, this study presents a comparative analysis of the energy performance of conventional building materials and clay-based materials. Focusing specifically on the Beni Mellal region, adobe bricks reinforced with straw, at weight percentages of 0%, 2%, and 4%, were manufactured. First, the physicochemical properties of the investigated clay were characterized. Subsequently, the thermophysical properties of the fabricated bricks were determined. Annual simulations were conducted using the TRNSYS software, considering a typical meteorological year (TMY) for Beni Mellal City, located in the semi-arid climatic zone. The energy performance of various passive energy efficiency measures was evaluated and discussed, facilitating a thermal analysis to assess the energy needs for heating and cooling inherent to each building material. The results demonstrate that clay bricks, particularly those reinforced with 4% wheat straw, outperform conventional materials in terms of energy efficiency, highlighting their potential for sustainable construction. This study emphasizes the significance of local clay resources and natural reinforcements in enhancing energy efficiency and provides insights into their application in eco-friendly construction practices, thereby contributing to sustainable development goals.

Keywords: Composite material, Adobe bricks, Energy performance, Zero carbon, Thermophysical properties, Eco-friendly construction, Thermal comfort.

Modelling Thermal Properties of Graphene: An Integrated DFT and Boltzmann Transport Equation Approach

Othmane Soubai and Younes Abouelhanoune

EMAO, ENSA Al-Hoceima, Abdelmalek Essaadi Unversity, Tetouan, Morocco
*Email : othman.soubai@etu.uae.ac.ma

Abstract. This work investigates the thermal properties of graphene, a material renowned for its exceptional thermal conductivity and potential applications in nano-electronics and energy systems. Accurate simulation and understanding of graphene's thermal behavior at the nanoscale are crucial for optimizing device performance and reliability. Utilizing Density Functional Theory (DFT) to obtain phonon properties and the Boltzmann transport equation through the OpenBTE package, this research aims to elucidate the mechanisms of heat conduction in graphene. Prior studies have demonstrated the effectiveness of these simulation methods in capturing the thermal transport phenomena in similar materials . The study provides comprehensive insights into how graphene's thermal properties can be tailored and enhanced for improved thermal management in advanced applications. The findings are expected to significantly contribute to the development of graphene-based materials with superior thermal performance.

Keywords: Graphene; Thermal properties; Density Functional Theory; Boltzmann transport equation; Nano-electronics

TiB_2P_2 monolayer: A potential anode material with high storage capacity for Lithium-Ion Battery

A. Etrini[1], S. Oukahou, M. Maymoun, A. Elomrani, K. Sbiaai, and A. Hasnaoui[2]

[1] *LS2ME, Faculté polydisciplinaire, Khouribga, ayoubetrini@gmail.com*

[2] *LS2ME, Faculté polydisciplinaire, Khouribga, hasnaoui59@hotmail.com*

Abstract. Development of high-capacity anode materials is one of the essential strategies for next-generation high-performance Li-ion batteries. Rational design, using density functional theory, can expedite the discovery of these anode materials. Motived by their good stability, high capacity, low diffusion barrier and excellent cyclability, a promising 2D anode material TiB_2P_2 with Dirac cone states was investigated. Based on the adsorption energy of lithium on the monolayer surfaces, we identified the sites that can hold lithium ions with high adsorption energy. Additionally, TiB_2P_2 exhibits good ionic and electronic conductivity, a suitable voltage profile, and high structural stability during the Li-loading process. Importantly, a high storage capacity was found. These criteria highlight the appealing electrochemical performance of the TiB_2P_2 monolayer as a promising anode material for LIBs.

Elaboration of $MnPO_4.H_2O$ thin film on recycled graphite using a Pulsed Potential Electrodeposition method for pseudocapacitors applications

H. El Mouahid, F.Z. Moufakkir, Y. Bou-ouzoukni, A. Guessous

Laboratory of Materials, Nanotechnology and Environment, Faculty of Sciences, Mohammed V University in Rabat, Av. Ibn Battouta, P.O. Box. 1014, Agdal-Rabat, Morocco

*Email : elmouahidhicham@gmail.com

Abstract. For the first time, $MnPO_4.H_2O$ thin films on recycled graphite rods (RGR) as pseudo-capacitor electrodes were obtained by pulsed-potential electrodeposition with constant toff of 10s and a ton comprised between 0.5 and 1.5s. The morphology, composition and crystalline structure of $MnPO_4.H_2O$ thin film on RGR synthesized at ton = 0.5s (the best result) were examined by scanning electron microscopy coupled with SEM/EDS and by XRD. The electrochemical performance of the films was obtained using cyclic voltammetry (CV), galvanostatic charge-discharge (GCD) and electrochemical impedance spectroscopy (EIS) in different electrolytes. The electrochemical results show that, in 3 M NaOH and KOH as electrolytes, the $MnPO_4.H_2O$ thin film in microsphere form has an excellent specific capacitance of about 303.1 and 272.8 Fg^{-1} at 0.5 Ag^{-1}, respectively. However, the retention of capacitance in the KOH electrolyte is more important than in the NaOH electrolyte due to the capacitive behavior of K^+ on the material surface.

Keywords: $MnPO_4.H_2O$ thin film, Pulsed-potential electrodeposition, Pseudocapacitor, Recycled graphite rod.

Vibration Control of Tapering FGM Beam Using Piezoelectric Materials

Khalid El Harti[1]*, Mohamed Touil[1], Rachid Saadani[1], Miloud Rahmoune[1]

[1] *Laboratory of Advanced Materials Studies and Applications, FS-EST, Moulay Ismail University of Meknes, Meknes, Morocco*
*Email : elhartikhalid@gmail.com

Abstract. Piezoelectric materials have many interesting applications thanks to their ability to generate an electrical voltage when subjected to mechanical pressure, and vice versa. In the field of vibration energy recovery, these materials can convert mechanical vibrations into electrical energy. For example, piezoelectric sensors integrated into roads or pavements can generate electricity from vibrations caused by vehicles or pedestrians. In the field of wind turbines, the vibratory control of wind turbine blades can increase the overall efficiency of these systems. In addition, mechanical systems are increasingly incorporating composite materials into the manufacture of structures, and specifically FGM materials. This work focuses on the active vibration control of FGM beams with non-uniform cross-sections, using piezoelectric materials. Euler-Bernoulli beam theory combined with the finite element method is applied to an FGM beam. The equation of motion is generated using Hamilton's principle.

Keywords: Euler-Bernoulli beam theory; Functionally graded materials; Non-uniform beam; Piezoelectricity; Vibration control

Study of the physico-chemical parameters of irrigated soil with different chromium concentrations

Soukayna AZZOUZI[1], Mohamed KHAMAR[1], Abderrahman NOUNAH[1], Essediya CHERKAOUI[1] & Abdelmjid ZOUAHRI[2]

[1]*Laboratory of Civil Engineering and Environment (LGCE), Higher School of Technology of Salé, Mohammed V University In Rabat, Morocco*

[2]*INRA, Regional Center for Agronomic Research of Rabat, Research Unit on the Environment and Conservation of Natural Resources, BP 6356 Rabat-Instituts, Morocco.*

[1]*Put author's affiliation here, complete with address, postal code, and country*

[2]*Put author's affiliation here, complete with address, postal code, and country*

*Email : soukayna_azzouzi@um5.ac.ma

Abstract

The many industrial, domestic, agricultural, medical and technological applications of heavy metals have led to their widespread distribution in the environment, giving rise to increasing concern about their potential effects on human health and the balance of ecosystems. Analysing the transfer of heavy metals in soils from above (in plants) is essential for determining the risks to health and the environment.

Soil contamination by anthropogenic chromium (Cr) is a worldwide problem. Several industrial activities such as leather tanning, wood preservation and metal finishing are the main sources of Cr pollution. Cr penetrates the soil, and the spatial distribution of Cr.

The pH value determines the physical (structural stability, resistance to threshing, etc.), chemical (bioavailability of chromium, assimilability of phosphorus, etc.) and biological (moistening and mineralisation of organic matter, etc.) behaviour of the soil. The electrical conductivity of the soil determines the degree of salinity.

Our aim is to study the effect of chromium at different concentrations on pH (water), pH (kcl), soil electrical conductivity and organic matter. However, we observed a stability in pH, a decrease in electrical conductivity and an increase in organic matter.

Keywords: contamination, chromium, soil.

Alphabetically sorted; Capitalized first word; From a to z; Maximum 5 keywords; Sentence case; Separate by semicolon between keyword

Novel self-assembled monolayer-based HTLs for inverted perovskite solar cell application

Othmane El baz[1]*, Othmane Essahili[1] , Sarah Derbali[1], Abdelmajid Almaggoussi[1,2], Mohamed Ilsouk[1]

[1] *Applied Chemistry & Engineering Research Centre of Excellence (ACER CoE), Mohammed VI Polytechnic University (UM6P), Lot 660 – Hay Moulay Rachid, 43150, Benguerir, Morocco.*

[2] *Cadi Ayyad University (UCA), Avenue Abdelkrim Elkhattabi, B.P 549, 40000, Marrakech, Morocco.*

*Email : othmane.elbaz@um6p.ma

Abstract. Self-assembled monolayers (SAMs) are promising materials for both improving the performance and the stability of perovskite solar cells (PSCs).In general SAMs are known as a good hole transport material, furnishing very effective charge extraction from their interfaces with perovskite, hence lowering recombination losses. The tunable molecular structure further allows one to optimize the energy levels at the interface with the perovskite layer, hence improving overall solar cell efficiencies. Moreover, energy level alignment interface modification by these SAM materials is oriented towards better charge transfer and mainly avoiding various energy barriers. The aim of the present work is to synthesize novel SAMs structures for use as hole transporting materials (HTLs) in PSCs. The resulting synthesized structures are confirmed by Fourier transform infrared spectroscopy (FT-IR) and Nuclear magnetic resonance spectroscopy (^{1}H-NMR) and then used to elaborate self-assembled monolayer films on conductive substrates such as fluorine doped tin oxide (FTO) or indium tin oxide (ITO) coated glasses. The deposited films will be studied by several analyses such as X-ray photoelectron spectroscopy (XPS) and contact angle to investigate their chemical and physical properties and their suitability for application as HTL in PSCs.

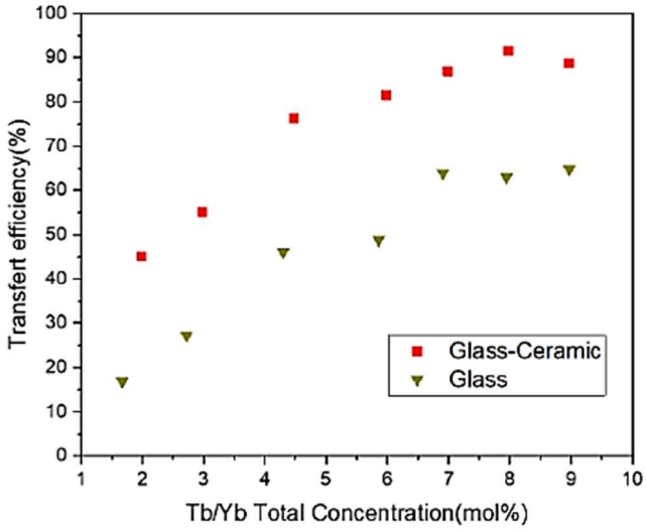
Keywords: Perovskite solar cells; Self-assembled monolayers; Hole transporting material.

Optimizing n-AlInN/p-Si Heterojunction Solar Cell Growth by RF Sputtering via Down-Converting Layers Co-Doped with Tb3+/Yb3+ Rare Earth Ions

Salima EL Amrani[1]*, Mickael Sun[2], M.Reda Britel[1],Adel Bouajaj[1],Sirona Valdueza Felip[2] and Frenando. B. Naranjo[2]

[1]*Laboratory of Innovative Technologies, National School of Applied Sciences of Tangier,Abdelmalek Essaadi University, Tetouan 93000, Morocco.*
[2]*Photonics Engineering Group,University of Alcala, 28871, Alcala de Henares, Spain.*
*Email : salima.elamrani1@etu.uae.ac.ma

Abstract. Nowadays, III-nitrides are widely recognized as highly desirable semiconductors for electronic and optoelectronic devices, thanks to the distinctive properties of these materials. It isworth mentioning that aluminum indium- nitride (AlInN) alloys have become important contenders, showing great potential for photovoltaic applications. This is attributed to their broad direct bandgap energy, encompassing the solar spectrum from 0.7 eV (InN) to 6.2 eV (AlN). Furthermore, their exceptional resistance to high temperatures and resistance to high-energy particles further enhance their suitability for various technological applications. The aim of this study is to optimize the efficiency of the AlInN on silicon heterojunction solar cell growth by the RF sputtering technique. Our approach is focusing on down-conversion process using silica-hafnia glass-ceramic layers co-doped with Tb3+/Yb3+ Rare earth ions. The silica-hafnia glass-ceramics films were fabricated by sol-gel route using the spin coating technique, following a well consolidate protocol and an appropriate thermal treatment. In fact, sol-gel technology provides versatility in fabricating multicomponent materials with controlled composition, shape, morphological and optical properties of the final product. The research presented here has been performed on 70SiO2-30HfO2 silica-hafnia glass-ceramic films activated with 19% rare earth ions: [Tb + Yb]/ [Si + Hf] = 19%. Two main results will be discussed: (a)The investigation into the photoelectrical and photovoltaic properties of AlInN on Si (100) and Si (111) devices reveals that the maximum conversion efficiency of 2.2% has been shown with the sample Al0.28In0.72N on Si (100). (b) The highest quantum efficiency of 190% has been shown with 70% SiO2–30% HfO2 glass-ceramic layers co-doped with 19% mole of Tb3+/Yb3+ ([Yb+ Tb] = 19%) as shown in the figure. which confirms the validity of this system as a down-converting filter to enhance the efficiency of n-AlInN/p-Si heterojunction PV cells.



Keywords: AlInN solar cell; Down-conversion; Heterojunction solar cell; rare earth ions; RFsputtering

Ab initio study of the structural, electronic, and optical properties of $MgTiO_3$ perovskite materials doped with N and P

Abdellah Bouzaid[1,2], Younes Ziat[1,2], Hamza Belkhanchi[1,2], Hamid Hamdani[1], Ayoub Koufi1,2, Mohammed Miri[1,2], Charaf Laghlimi [2,3], and Zakaryaa Zarhri [4]

1 Engineering and Applied Physics Team (EAPT), Superior School of Technology, Sultan Moulay Slimane University, Beni Mellal, Morocco
2 The Moroccan Association of Sciences and Techniques for Sustainable Development (MASTSD), Beni Mellal, Morocco
3 ERCI2A, FSTH, Abdelmalek Essaadi UniversityThe institution, Tetouan, Morocco
4 CONAHCYT- Faculty of Chemical Sciences and Engineering, The Autonomous University of Morelos State, Cuernavaca, Morelos, Mexico

Abstract. This study investigates the electronic, optical, and structural properties of MgTiO3 perovskite materials, whether pure or doped with elements such as nitrogen (N) and phosphorus (P). The investigation utilizes density functional theory (DFT) with the GGA-mBJ approximation as implemented in the Wien2k code. The results show that the band gap energy of doped MgTiO3 is significantly lower than that of pure MgTiO3, which has a band gap of 2.933 eV, at oxygen sites with Y (N, and P). In particular, with N and P, the band gaps drop to 1.74 and 0.65 eV moreover, the Fermi energy (Ef) level shifts towards the valence band (VB) in a p-type semiconductor (SC). Further, we have analyzed the optical characteristics of these systems, including their dielectric function ("ε" _1 and "ε" _2), optical conductivity (σ), absorption coefficient (α), and refractive index (n). Furthermore, doping with N and P increases absorption in the visible spectrum, which raises the photocatalytic activity in the presence of light because the doped materials' valence and conduction bands transition more readily, producing hydrogen. The discoveries above suggest that these materials possess a broad spectrum of applications, encompassing the creation of optoelectronic apparatus.

Topic (3): Mechatronics in Energy

Comparative Study of Controllers for a Wind Energy Conversion System Based on a DFIG

Achraf EL OUALI [1]*, Yassine LAKHAL [1], Mohamed BENCHAGRA [1], Hamid CHOJAA [2]

[1]*Team of engineering and applied physics Higher school of Technology of Beni Mellal, Morocco*
[2]*Industrial Technologies and Services Laboratory, Higher School of Technology, Sidi Mohamed Ben Abdellah University, Fez 30000, Morocco*
*Email : elouali.hraf@gmail.com

Abstract. The aim of this paper is to develop an MPPT control for a variable-speed wind turbine based on a DFIG. Firstly, we model the wind turbine, the doubly-fed induction generator, and the power converter to obtain a reliable simulation model. For this, we use MATLAB/Simulink to simulate the established model. To ensure the wind turbine operates in MPPT mode, it is necessary to use an appropriate controller to follow the maximum power point. This study focuses on comparing different MPPT controllers, including PI, Backstepping, and Sliding Mode Control. The performance of each controller is evaluated using simulations to determine their respective effectiveness.

Keywords: Backstepping; Mppt; Proportional-integral (PI); Sliding Mode Control; Wind turbine modeling.

Metamodeling For Predicting the Behavior of Airfoils of Wind Turbine Blades: An Integration of Artificial Neural Networks

Mohammed Haiek[1]*, Yassine Lakhal[2], Nabil Ben Said Amrani[1], Driss Sarsri[1]

[1]*Laboratory of Innovative Technologies, National School of Applied Sciences of Tangier. B.P. 1818, Tangier, Morocco.*
[2]*Team of engineering and applied physics, Higher School of Technology of Beni Mellal, Morocco*
*Email : haiek.mohammed@gmail.com

Abstract. The aim of this paper is to develop a robust metamodel capable of predicting the behavior of wind turbine blade airfoil profiles, despite variations in the input parameters of computational fluid dynamics (CFD) simulations. We begin the development of this metamodel by specifying the essential geometric parameters for the simulations. Subsequently, an empirical analysis of the airfoil profiles is conducted, and the results of the corresponding simulations are presented. These data are used to train and refine the metamodel, which is based on an artificial neural network. The model fitting process is divided into three main stages: training, validation, and testing, during which we strive to minimize the error function using the Levenberg-Marquardt algorithm. In conclusion, we validate our model by a thorough comparison of the results from the metamodel and the CFD simulations, aiming to optimize computation time.

Keywords: Airfoils of Wind Turbine Blades; Artificial neural network (ANN); Computational fluid dynamics (CFD) simulations; Levenberg-Marquardt algorithm; Metamodel.

Topic (4): Internet of Things & Artificial Intelligence (IoT & AI) in Energy

Optimization of Photovoltaic Power Efficiency Using an IoT-Based Automatic Solar Panel Cleaning System and Anti-Dust Coating

Abed OUBARI[1*], Pr. Khalid NOUNEH[1], Dr. Elmehdi HAMZAOUI[2], Eng. Hafid AMAYOUD[2], Mr. Khalid FATHI[2]

[1] *Ibn Tofail University, Kénitra, Morocco*

[2] *National Centre for Science, Energy and Nuclear Techniques, Rabat, Morocco*

*Corresponding Author E-mail: abed.oubari@uit.ac.ma

Abstract. Several factors, such as dust and bird droppings, can impact the efficiency of solar panels. This study compares the efficiency of three solar panels installed on the same metal structure and exposed to identical environmental conditions. One panel is cleaned daily by an intelligent cleaning system based on the ESP32 microcontroller. The second panel has an anti-dust coating applied to its surface, while the third panel serves as a reference. Sensors connected to the ESP32 collect and record data on current, voltage, power, humidity, temperature, and solar irradiation, which is then stored on Google Sheets. The study found that the intelligent cleaning system and anti-dust coating both helped reduce efficiency losses compared to the reference panel. The intelligent cleaning system required a modest amount of water and energy to operate over the course of the study.

Keywords: Anti-dust coating; Energy conversion; ESP32; IoT; Photovoltaic efficiency

Study of Energy Dissipation and Satisfaction Rates in Mixed Traffic Flow with Lights: A TwoLane Cellular Automaton Approach

Ayoub Laarej [1*], Julio César Pérez-Sansalvador [1,2], Noureddine Lakouari [1, 2], Hamid Ezzahraouy [1, 2]

[1] *Laboratoire de Matière Condensée et Sciences Interdisciplinaries (LaMCScl), URL-CNRST, P. O. Box 1014, Faculty of Sciences, Mohammed V University in Rabat, Morocco.*

[2] *Consejo Nacional de Humanidades, Ciencias y Tecnologías, Ciudad de México 03940, Mexico.*

[3] *Coordinación de Ciencias Computacionales, Instituto Nacional de Astrofísica, Óptica y Electrónica, Puebla 72840, Mexico.*

Abstract. Traffic lights in cities play a crucial role in regulating the complex dynamics of diverse vehicles, giving priority to certain users or vehicles on the road. However, the alternating stop-and-go patterns induced by these lights have an impact on desired speed of vehicles and energy dissipation. In this paper, we examine the impacts of traffic signals, focusing on a two-lane cellular automaton model. Our model accounts for traffic heterogeneity by differentiating vehicles based on speed (slow and fast) and size (large, slow vehicles and small, fast vehicles). In our study, we concentrated on a case in which the lane-changing rules were asymmetric, this regulation stipulates that slower-moving traffic should keep to the righthand lane (or the left-hand lane in countries where driving is on the left) to allow faster vehicles to pass. Although these vehicles occasionally change lanes, they revert to their preferred lane at the earliest opportunity. Hence, we examined two traffic light control strategies: the green wave and synchronized methods. Our findings indicate that both strategies exhibit comparable performance for vehicles in terms of traffic flow parameters. However, differences emerge when comparing the two lanes or vehicle types. Specifically, the slow lane demonstrates a higher traffic flow for slower vehicles and a reduced flow for faster vehicles. When examining satisfaction rates and energy dissipation, notable variations emerge, especially in extremely low densities. The green wave demonstrates marginally superior performance compared to the synchronized traffic light control. This investigation deepens our understanding of the impact of various control strategies on performance. The findings can serve as a foundation for exploring more intricate aspects of traffic management, enhancing the potential for creating efficient and adaptive urban transportation systems.

***Keywords*:** Two lanes, green wave, synchronized traffic light strategy, cellular automata.

Topic (5): Embedded System in Energy

Creation of an optical sensor based on the pCdTe – nCdS and pCdTe – nCdSe heterostructure for detecting polluted air

S.M. Otajonov[1], R.N. Ergashev[1]*, Z. Xaydarov[1], K.A. Botirov[1], M. Bahromov[1], T. Axmedov[1], M. Raxmonkulov[1]

[1]*150100 Fergana, Fergana State University, Uzbekistan*
*Email: rova08@pf.fdu.uz

Abstract: This article discusses the creation of optical sensors for detecting polluted air based on the pCdTe – nCdS and pCdTe – nCdSe heterostructures. It was established that the developed optical sensors, with an automatic control system using Arduino, operate effectively across wide ranges of the IR spectrum. The study found that the increased responsiveness of the optical sensor ensures uniform sensitivity and a high degree of background light suppression. It was demonstrated that using the optical sensor, it is possible to determine the level of dust and smoke in both indoor environments and open land areas.

Keywords: Heterostructure; Ventilation; Sensor; LED; Photodetector