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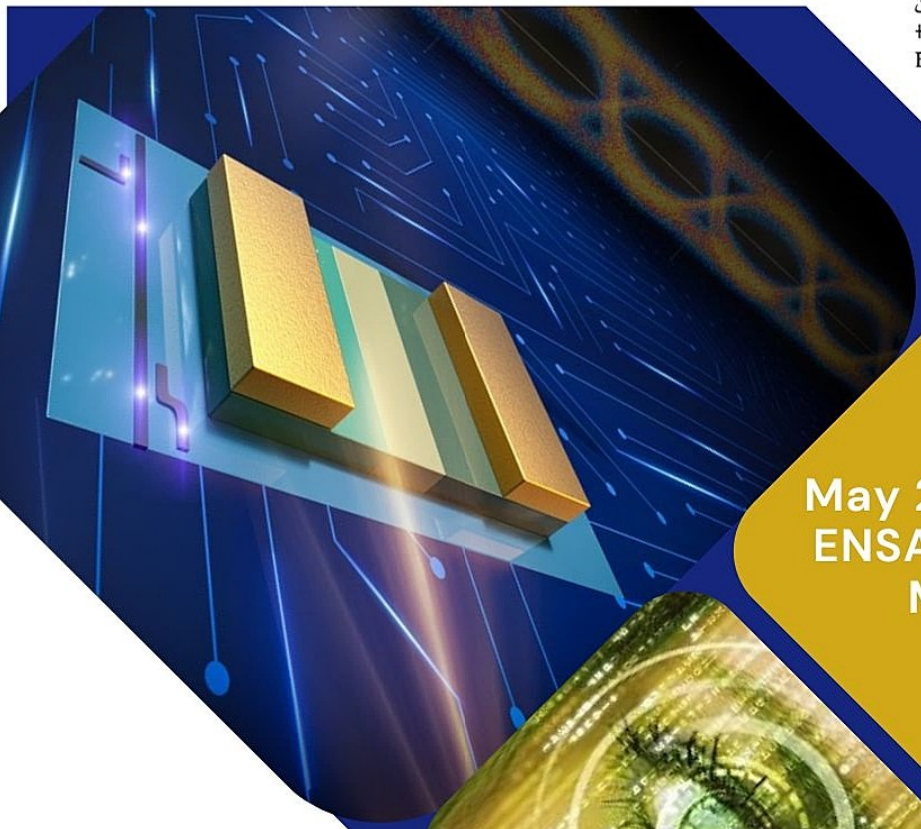

May 21 & 22, 2025
ENSAJ, El Jadida, Morocco

The 19th International Symposium on Advanced Organic Photonics (ISAOP-25)

Scope:

Organic and hybrid photonic materials

Organic optical devices (optical waveguides, optical fibers, organic semiconductor devices)

Nanotechnology and environmental technology, smart materials

Organic and hybrid solar cells

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E-mail:
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International Symposium on Advanced Organic Photonics

21-22 May 2025, El Jadida, Morocco

At National school of applied sciences, EL JADIDA

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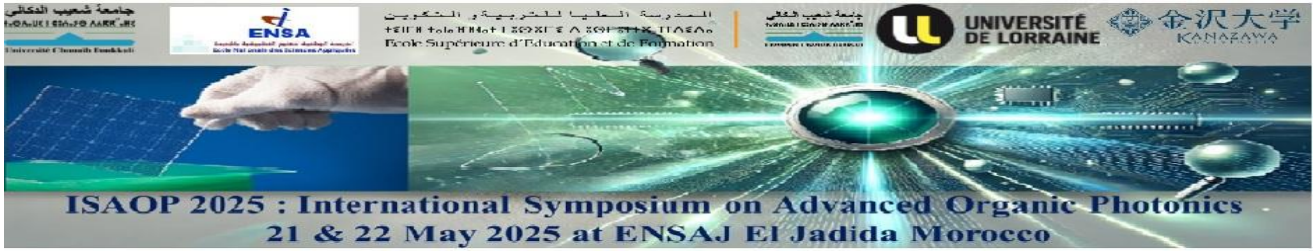
Organic and hybrid photonic materials



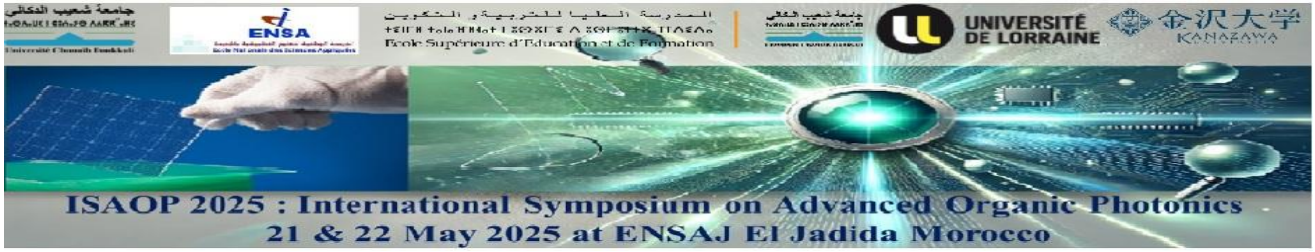
Application of a thin TiO_2 layer as a transducer for the development of a biosensor for anti-COVID-19 antibody detection with docking study

Otmane SADEK*, Samira TOUHTOUH, Abdelowahed HAJJAJI

Laboratoire des Sciences de l'Ingénieur pour l'Energie, Ecole Nationale des Sciences Appliquées d'El Jadida, BP 1166, EL Jadida Plateau 24002, Maroc
**Corresponding authors: otmansadek@gmail.com (O. Sadek*)*

La maladie à coronavirus 2019 (COVID-19) est une maladie infectieuse humaine émergente causée par des syndromes respiratoire coronavirus 2 (SRAS-CoV-2), Détecté à Wuhan (la chine), En décembre 2019, il s'agit d'un virus de la famille de coronavirus ; il a ensuite été renommé coronavirus 2 (SRAS-CoV2) par le Comité international de taxonomie des virus. A cause de l'augmentation rapide de la contamination des personnes par ce virus, l'épidémie de COVID-19 est classée par L'Organisation mondiale de la Santé (OMS) comme une pandémie le 12 mars 2020. Les tests actuellement utilisés pour le diagnostic sont principalement basés sur la PCR et qui présentent plusieurs inconvénients notamment la lenteur et la nécessité de déplacer les personnes vers les hôpitaux qui les exposent à une contamination par le virus. Pour répondre à cette problématique, l'objectif de ce travail est d'utiliser une couche mince de TiO_2 optimale comme transducteur pour la réalisation d'un biocapteur pour la détection rapide des anti-COVID-19 d'une manière sensible, rapide sans contaminer les autres personnes.

Keywords: Titanium dioxide (TiO2); Titanium tetraiso-propoxide (TTIP); Sol-gel; material characterization



Copper oxide nanoparticles-decorated cellulose acetate: Eco-friendly catalysts for reduction of toxic organic dyes in aqueous media

El houceine BENHADRIA, Lahoucine BAHSIS, El-Houssaine ABLOUH, Najoua LABJAR, Souad EL HAJJAJI

LS3MN2E, CERNE2D, ENSAM, Mohammed V University in Rabat, Morocco, Université Cadi Ayyad, 4162 Safi, Morocco

Materials Science, Energy and Nanoengineering Department (MSN), Mohammed VI Polytechnic University (UM6P), Lot 660 – Hay Moulay Rachid, Benguerir 43150, Morocco

LS3MN2E, CERNE2D, faculty of sciences, Mohammed V University in Rabat, Morocco

* Corresponding author: benhadria.smc@gmail.com (E. Benhadria)

In this study, we aimed to gain insight into the potential of catalytic reduction using copper oxide nanoparticles decorated cellulose acetate as a biosupport (CuxO@CA) for the removal of specific pollutants. The prepared catalyst was submitted to a series of spectroscopy techniques for characterization purposes. The results of the catalytic tests on methylene orange (MO) and methylene blue (MB) solutions suggest that the elimination efficiency may be influenced by several factors, including the catalyst dose and the concentration of the pollutant. Kinetic studies were also carried out, and the value of the rate constant Kapp derived from the pseudo-first-order kinetics was found to be highest for the prepared catalyst in a very short reaction time. The CuxO@CA catalyst was tested on a combination of MO/MB dyes, and the results indicated that it exhibited the highest catalytic activity in reducing and degrading these organic dyes in aqueous solutions, which is an encouraging outcome. Furthermore, the prepared catalyst demonstrated promising catalytic performance and exhibited the potential for recycling multiple times without significant loss of activity, which could be advantageous for large-scale production and practical use in water treatment.

Keywords: Cellulose acetate, Copper oxide nanoparticules, Methylene orange, Methylene bleu

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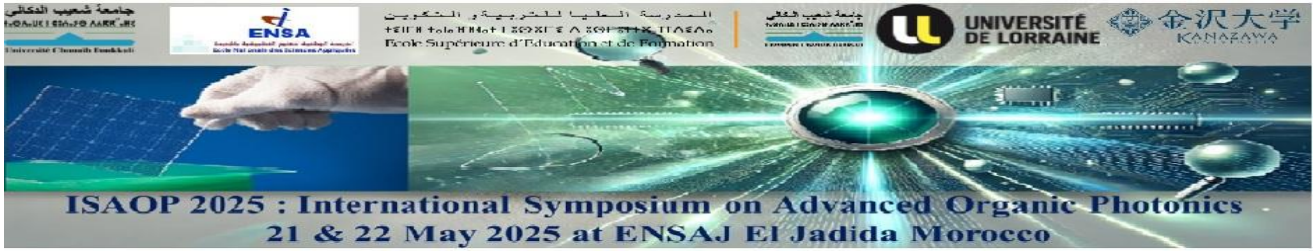

Eco-Friendly Innovations in Organic Photonics for Next-Generation Technologies

Dr MURUGESH.V

1 JCT college of Engineering and Technology
** Corresponding author: drmurugeshv@gmail.com Dr MURUGESH.V*

The transition to sustainable technologies necessitates energy-efficient and eco-friendly solutions in optics and electronics. Organic photonics offer a promising pathway, leveraging carbon-based materials for flexible, low-cost, and biodegradable photonic devices. This paper presents a study of advanced organic photonic materials and their application in solar cells and sensors, evaluating key performance parameters such as optical absorption, efficiency, and environmental stability. Results show competitive performance with lower environmental impact compared to conventional inorganic systems.

Keywords: Organic Photonics, Sustainable Technologies, Organic Solar Cells , Photonic Devices , Green Electronics

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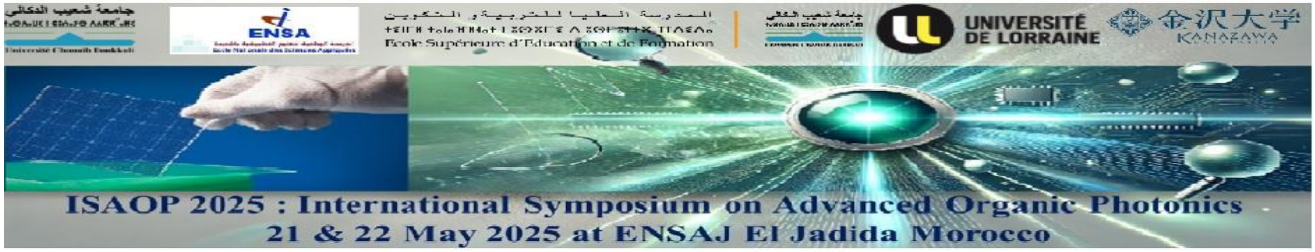


Elucidating the Factors Governing the Regio- and Stereoselectivity of 1,3-Dipolar Cycloaddition Reaction of Fused Pyrrole-2,3-diones with Nitrones: A MEDT and Docking Approach

Soukaina AMEUR, Zineb OUAHDI

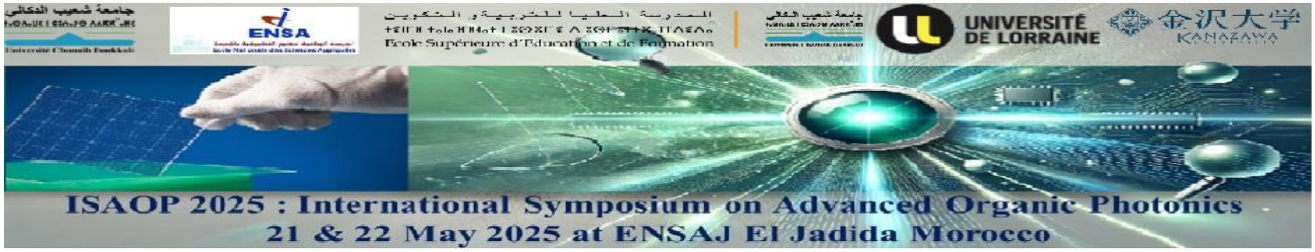
Molecular Modeling and Spectroscopy Research Team, Faculty of Science, ChouaïbDoukkali University, P.O. Box 20, 24000. El Jadida, Morocco

2Bioorganic Chemistry Team, Department of Chemistry, Faculty of Sciences ChouaïbDoukkali University, P.O. Box 24, 24000. El Jadida, Morocco

* *Corresponding author: ameursoukaina8@gmail.com* (Soukaina AMEUR)

The 1,3-dipolar cycloaddition between 1H-pyrrole-2,3-diones and nitrones was investigated using Molecular Electron Density Theory (MEDT) and Density Functional Theory (B3LYP/6-311G(d,p)) in gas phase and polar solvents. The reaction proceeds via a concerted but asynchronous mechanism, involving two transition states: endo and exo. The endo transition state is more stable, due to reduced steric hindrance and favorable electrostatic interactions between the nitrone and the 1,3-dicarbonyl group. Regioselectivity and preferred cyclization were rationalized through activation energy calculations and frontier molecular orbital analysis. A topological study based on the Electron Localization Function (ELF) offered further insight into the reaction mechanism. In parallel, molecular docking studies were carried out to evaluate the binding affinities of three ligands toward a biological target. Ligand L-1 exhibited the highest affinity (−6.9 kcal/mol), followed by L-2 (−5.0 kcal/mol), while the reference compound AZT showed the lowest (−3.9 kcal/mol). These results suggest L-1 as a promising anti-HIV candidate. Overall, this work highlights the effectiveness of theoretical approaches in understanding reactivity and supporting drug discovery.

Keywords: MEDT, DFT, ELF, 1,3-Dipolar Cycloaddition, ELF, ADME, Molecular Docking, Anti-HIV Drug Design.



Hybrid Nanoparticle Synthesis by Supercritical Hydrothermal Synthesis and Its Application to Optics

Tadafumi ADSCHIRI, Akira YOKO

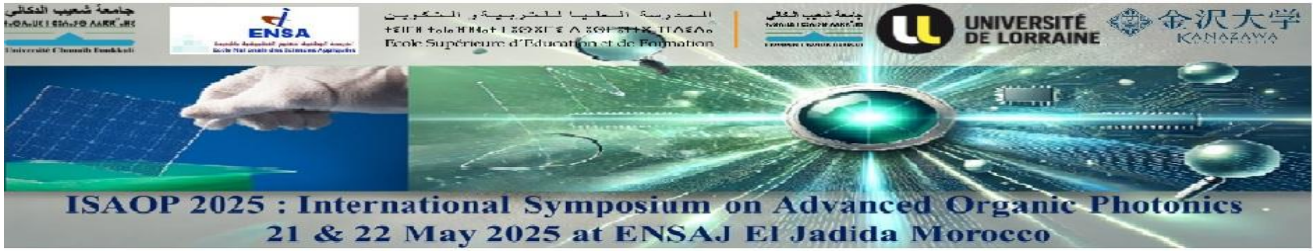
Advanced Institute of Materials Science, Tohoku University, Japan.

* *Corresponding author*: Tadafumi.ajiri.b1@tohoku.ac.jp

In this presentation, we will introduce nanoparticle synthesis technology using supercritical hydrothermal synthesis and its application to phosphor materials and optical materials. About 30 years ago, we invented a distribution-type nanoparticle synthesis method using supercritical water as the reaction field. This method is called supercritical hydrothermal synthesis, and many commercial processes are already in operation. This method enables not only continuous mass synthesis of nano-sized particles but also hybridization with organic molecules. This enables perfect dispersion of nanoparticles (NPs) in organic solvents with extremely high concentration, through the precise design of organic modifiers on the surface of nanoparticles to achieve super high affinity between NPs and the solvents. This nano fluid can be used for immersion lithography or heat transfer medium for optical devices. The organic modified NPs enables the creation of transparent hybrid polymers with improved affinity to polymers. Anti-reflective films could be made from materials with a high concentration of zirconia dispersion. GdVO3 nanoparticles can be used in CT and MRI, and can be observed in visible light by doping with fluorescent atoms such as Eu, Tb, Dy, and Ce. The size can be controlled to several tens of nanometers for EPR effect, and the surface organic molecules can be modified with cancer antibodies. By setting the size of the nanoparticles to 1 or 2 nm, strong luminescence was observed upon X-ray irradiation, even though they are organically modified CeO2 nanoparticles. In addition, ferromagnetism, which is not usually observed, was also observed. Nanocarbons made from biomass as well as inorganic nanoparticles can be synthesized at the supercritical hydrothermal synthesis field, and when lignin was used as a starting material, nanocarbons of several nm in size and strong luminescence were observed.

Keywords: Supercritical, hydrothermal, nanoparticles, hybrid material.

References:



Near-IR Photoconductivity of Electrodeposited PEDOT/Fullerenol

Alexey TAMEEV*, Oxana GRIBKOVA, Ildar SAYAROV, Varvara KABANOVA, and Alexander NEKRASOV
Frumkin Institute of Physical Chemistry and Electrochemistry of the Russian Academy of Sciences 31-4, Leninsky prospect, 119071 Moscow, Russia
* *Corresponding author*: * tameev@elchem.ac.ru

The electronic structure, morphology, spectroelectrochemical, electrochemical properties and near-IR photoconductivity of the composite films of poly-3,4-ethylenedioxythiophene (PEDOT) with fullerenols studied for the first time we have reported recently [1, 2]. Water soluble fullerenols are of Na+-containing fullerene with hydroxyl groups ($Na_4[C_{60}(OH)_x]$, where x ~ 30) (NaFl) and K+- containing fullerene with 5 carboxyl groups (KPCF), absorption bands of which are in the UV-visible range shorter than 600 nm.

The PEDOT/fullerenol films exhibit photoconductivity under irradiation in the 700nm–900 nm bandwidth. Electrically conductive PEDOT in semi-oxidized and oxidized states possesses electron levels of polarons and bipolarons that are located inside the band gap and provide ab-sorption of the polymer in the near-IR range. We attribute the photocurrent to an increase in the concentration of photogenerated charge carriers since fullerene can provide rapid exciton separation by the transfer of photoexcited electrons from PEDOT to fullerene molecules as the transfer is energetic favorable according to positions of their electronic states. The higher photocurrent in PEDOT- NaFl compared to PEDOT- KPCF shows that the photoconductivity associates with the influence of the fullerene structure on the degree of PEDOT doping and the morphology of the resulting layers. NaFl creates more favorable conditions for the formation of PEDOT chains and, as a consequence, a more uniform and denser layer of the composite with NaFl than with KPCF.

Keywords: Electrochemical synthesis and investigations were supported by the Ministry of Science and Higher

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Education of the Russian Federation (grant No. 125012200626-9); Photophysical investigations were supported by the Russian Science Foundation (grant No. 23-19-00884).

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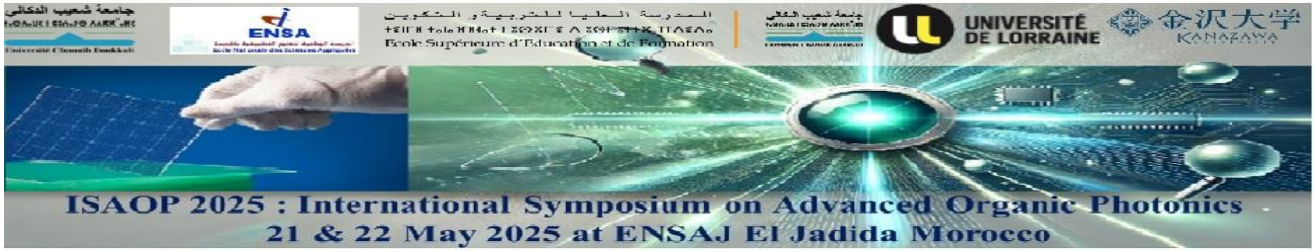


Nitration of Benzimidazole Derivatives: Synthesis, Characterization and Evaluation of Biological Activities

Abouelhaoul EL ALAMI, Assiya ATIF, Fatima YOUSSOUFI1, Houssine AIT SIR, Mustapha SOUFYANE

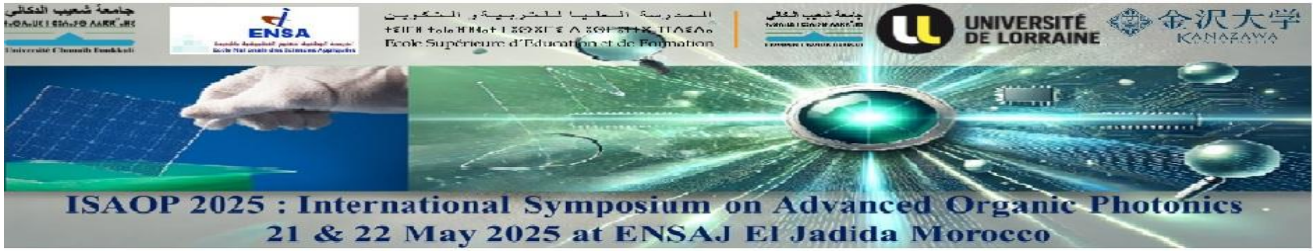
Bioorganic Chemistry Team, Faculty of Sciences, Chouaib Doukkali University, El Jadida, Morocco.

** Corresponding author: abouelhaoul.elalami103@gmail.com*

In this work, a new series of 4,6-dinitrobenzimidazole derivatives were synthesized and evaluated for their biological activities. In a one-step process, the reaction between substituted benzimidazoles **1(a-e)** and nitric acid (in excess) in sulfuric acid at low temperature (0–10 °C) for 1 hour, gives the desired 4,6-dinitrobenzimidazoles **2(a-e)** in good yields. The structures of the synthesized 4,6-dinitrobenzimidazoles **2(a-e)** have been established using physicochemical analyzes and various spectroscopic techniques such as (1H NMR, 13C NMR, mass spectrometry and FTIR-ATR). Further, all the synthesized compounds were evaluated for their anticancer activity. The results of the anticancer screening showed that the compounds **2b**, **2c** and **2d** possess average activity against cancer cell lines (HT29, HCT-116 and U87).

Scheme

Keywords: Synthesis, 4,6-dinitrobenzimidazole derivatives, biological activities, anticancer activity.



Photoluminescence Enhancement and Energy Transfer in Znq_2 Thin Films Co-Doped with DCM

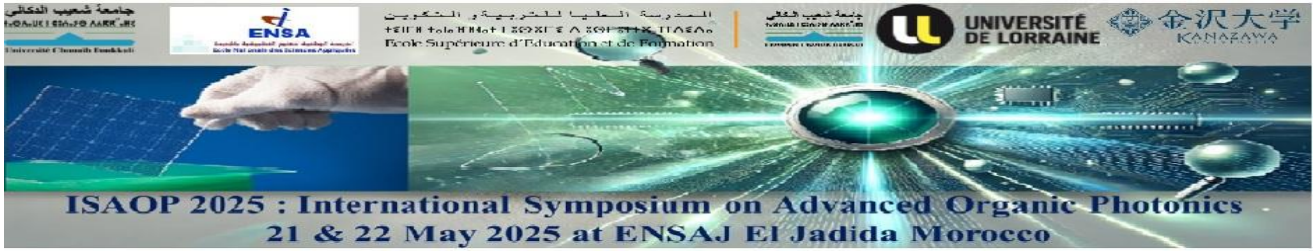
Amina LAOUID, Amine ALAOUI BELGHITI, Krzysztof WISNIEWSKI, Przemyslaw PLOCIENNIK, Abdelowahed HAJJAJI, Anna ZAWADZKA
Institute of Physics, Faculty of Physics, Astronomy, and Informatics, Nicolaus Copernicus University in Torun, Grudziadzka 5, PL 87-100, Torun, Poland
Engineering Science for Energy Lab, National School of Applied Sciences, Chouaib Doukkali University of El Jadida, El Jadida, 24000, Morocco
Centre for Modern Interdisciplinary Technologies, Nicolaus Copernicus University in Torun, Wilenska 4, PL 87-100, Torun, Poland
Institute of Engineering and Technology, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University, Grudziadzka 5, PL 87-100, Torun, Poland

** Corresponding author: laouidamina9@gmail.com*

Metal-organic complexes, such as zinc bis(8-hydroxyquinoline) (Znq_2), have gained significant attention in recent years due to their excellent thermal stability, high photoluminescence efficiency, and promising applications in organic light-emitting diodes (OLEDs), sensors, and other optoelectronic devices. When fabricated as thin films, these materials offer enhanced control over their structural, optical, and electronic properties. In this work, we present a comprehensive experimental study on the photoluminescence behavior of Znq_2 thin films co-doped with various concentrations of DCM (4-(dicyanomethylene)-2-methyl-6-(4-dimethylaminostyryl)-4H-pyran), a well-known laser dye characterized by strong emission in the orange-red spectral region. This study presents a novel experimenta investigation into the photoluminescence properties of Znq2 thin films co-doped with varying concentrations of DCM. Thin films were deposited on glass substrates using vacuum evaporation under high vacuum conditions. Photoluminescence measurements were conducted at both room temperature and across a temperature range from 77 K to 300 K, with intervals of 25 K, under high vacuum conditions. Real-time decay time measurements were employed to study the lifetime of the samples. The results demonstrate significant doping-induced changes in the photoluminescence intensity, indicating a complete energy transfer from Znq2 to DCM. This transfer resulted in a shift of the photoluminescence peak towards the orange wavelength region associated with DCM. Notably, the lifetime analysis revealed a single decay time component of approximately 4.47 ns for undoped Znq2, while doped samples exhibited dual decay time components.

These findings underscore the influence of doping on the optical properties of Znq2, positioning it as a promising candidate for optoelectronic applications.

Keywords: Photoluminescence, Decay time, thin film, Physical vapor deposition, AFM.



Self-Assembly of Perovskite Nanocrystals and Transfer Printing via Controlled Surface Wettability

Kaoru TAMADA*, Yuto KAJINO, Yuko AIDA, Yusuke ARIMA

Institute for Materials Chemistry and Engineering (IMCE), Kyushu University

**Corresponding author:* tamada@ms.ifoc.kyushu-u.ac.jp (Kaoru TAMADA)

Lead halide perovskite (LHP) nanocrystals (NCs) have shown great potential in advanced photonics and optoelectronic applications due to their nearly unity photoluminescence (PL) quantum efficiency, narrow emission bandwidth and tunable spectral wavelength. However, LHP NCs are unstable to heat and polar solvents, making it difficult to fabricate spatially uniform ultrathin films over large device areas. In this study, we demonstrated a 2D assembly of various LHP NCs by simple spin-coating on macroscopic surfaces and also multilayered film formation by repeated spin-coating cycles [1]. The key process is careful purification of NCs for assembly (i.e., removing excess ligands), and complete vacuum drying between spin-coating cycles. The optimized methodologies realize strong NC-NC lateral interactions and also vertical stacking and long stability of the self-assembled structures. Another challenge in this study is contact printing of LHP NC films [2]. Traditional lithography techniques are difficult to apply to LHP NC films due to their instability. To solve this problem, solvent- and heat-free contact printing technique were applied for the transfer and microfabrication of LHP NC self-assembled monolayers. The key process is precise control of substrate wettability. To realize the multi-step transfer of NC films, it is necessary to increase adhesion forces between the NCs and substrates at each step. On the other hand, fabrication of spatially uniform LHP NC selfassembled monolayers by spin-coating requires some affinity between LHP NCs and the substrates. To meet these two requirements, the initial substrate for spin-coating was modified with a mixture of fluoroalkyl silane and alkyl silane, and the substrate for the final film transfer was modified with hexamethyldisilane. This back-to-basics approach provides a simple and reliable process for the integration of LHP NCs into advanced nano-optoelectronic devices.

Keywords: Perovskite Nanocrystals, self-assembly, monolayer, contact printing, wetting

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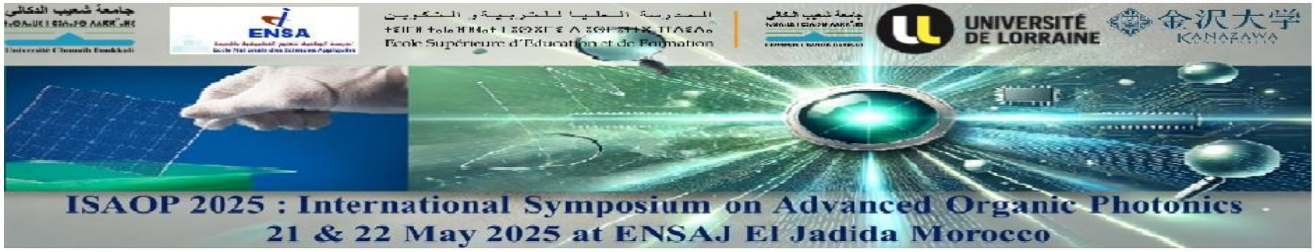

Superconducting and pining vortex properties of mixed state in deuterated κ-(BEDT-TTF)2Cu[N(CN)2]Br organic superconductor.

Omar SLIMAN, Ahmed TIRBIYINE, Jamal ELQARS, A.Bourdyme, Mohammed BELLIOUA, N.El ghazal, Hassan ELOUADDI, Youssef AIT AHMED, Mohammed ID ELAMEL.

Laboratory of Materials, Electrical Systems, Energy and Environment, Faculty of Applied Sciences Ait Melloul, Ibn Zohr University, Agadir, Morocco.

Laboratory of Physics of Condensed Matter and Nanomaterials for Renewable Energy, Faculty of Sciences, Ibn Zohr University, Agadir, Morocco

Health Sciences and Technologies Laboratory, Higher Institute of Health Sciences (ISSS), University Hassan 1st, Settat , Morocco.

Laboratory of Materials Physics and Systems Modelling, Physics Department, Faculty of Sciences, Moulay Ismail University, Meknes, Morocco

** Corresponding author: sliman.omar@edu.uiz.ac.ma (Omar SLIMAN)*

The organic compound κ-(BEDT-TTF)2Cu[N(CN)2]Br under study, is made up of layers of planar organic molecules. At very low temperature below Tc=11.6 K, it behaves as type II superconductor that exhibits a mixed state[1]. By replacing the eight hydrogen atoms of the compound with deuterium atoms, the molecule is fully deuterated, and the compound κ-(ET)2Cu[N(CN)2]Br is denoted κ-D8-Br[2]. If the external magnetic field surpasses the low magnetic field, the full Meissner state is destroyed, and vortices penetrate into the sample marking a mixed state[3]. In this work we have studied the magnetic hysteresis loop at low magnetic field to access the lower magnetic field and the full magnetic penetration field at T=2K[3]. The analysis of hysteresis loop at intermediate magnetic field allows us to determine the critical current density Jc and the pining force Fp at the same temperature, both in rapid and slow cooling of the sample through the structural transformation that occurs near 80K[1]. The investigation of Jc and Fp reveals important insight on the dominant pining mechanism[4]. Our results show that the cooling rate near 80K has a significant influence on the superconducting and pining properties. The magnetic phase can be improved, and superconductivity can be degraded by fast cooling.

Keywords: organic superconductor, hysterisis loop, critical current density, pining force, cooling rate.

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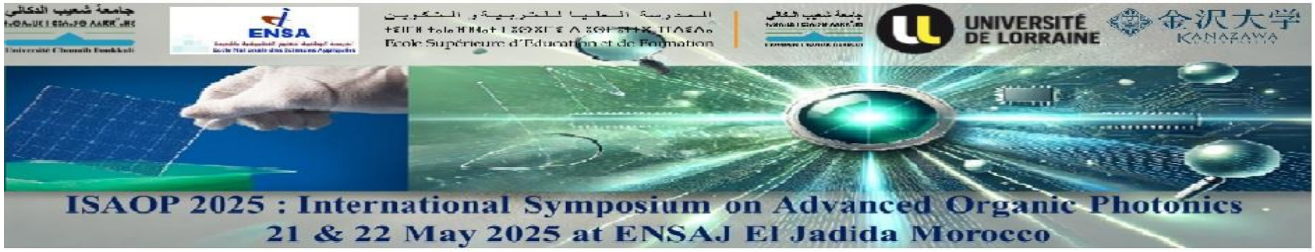


Sustainable Adsorption of Methylene Blue from Aqueous Medium by Hydrochar-Based Activated Carbon from *Chamaerops humilis* Fruit Pulp

Nouhaila GADDA, Houda LABJARF, Najoua LABJAR, Youssra EL HAMDOUNI, Najoua SOUAD LAGMIRI, Hamid NASRELLAHD, Ayoub CHERRATE, Ghita Amine BENABDALLAHA, Souad EL HAJJAJI

Laboratory of Molecular Spectroscopy Modelling, Materials, Nanomaterials, Water and Environment, CERNE2D, ENSAM, Mohammed V University in Rabat, Morocco;

(IRSM) Laboratory, Higher Institute of Management Administration and Computer Engineering, ISMAGI, Rabat, Morocco;

Higher School of Education and Training, Chouaib Doukkali University, El Jadida, Morocco;

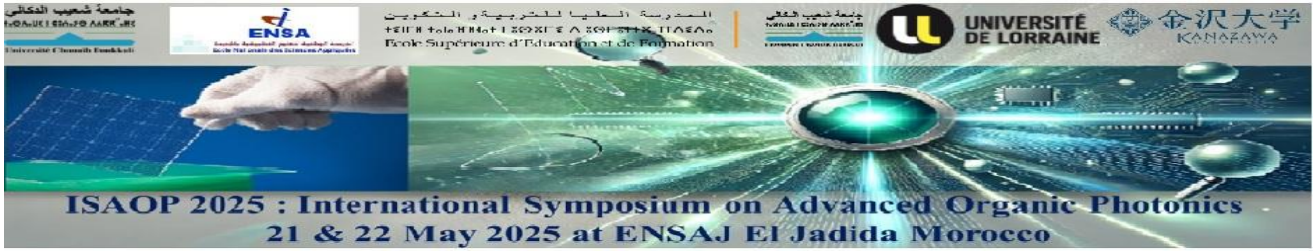
Forensic Institute of Gendarmerie Royale, Rabat, Morocco;

Laboratory of Membranes, Materiels and Environnement, Faculty of Sciences and Technologies of Mohammedia, Hassan II University of Casablanca, Morocco;

* Corresponding author: najoua.labjar@ensam.um5.ac.ma

This study valorized *Chamaerops humilis* fruit pulp as a sustainable precursor to produce hydrochar-activated carbon (CHHAC) through hydrothermal carbonization and subsequent chemical activation. The produced substance was characterized for its application in the elimination of methylene blue (MB) dye in water. The focus has been given on systematic optimizing of the experimental parameters like, adsorbent dosage, pH, contact time and stirring speed in order to enhance adsorption process. The Response Surface Methodology (RSM) was used to determine best conditions and the adsorption mechanism. The surface characteristics, structural morphology, and functional groups involved in the adsorption process were comprehensively studied by BET analysis, SEM-EDX, and FTIR spectroscopy. Reusability and regeneration studies were also performed for long-term applicability. This study illustrates how agricultural-waste-derived carbonaceous materials can open new avenues for sustainable wastewater treatment technologies.

Keywords: *Chamaerops humilis, Hydrochar-activated carbon, Methylene blue, Adsorption, Wastewate Treatment*



Synthesis and Anticorrosion Activity of 2-methyl-5-(2-methyl-1Hbenzo[d]imidazol-5-yl)-1,3,4-oxadiazole

Assiya ATIF*, Rachid HSISSOU, Abouelhaoul EL ALAMI, Fatima YOUSSOUFI, Houssine AIT SIR

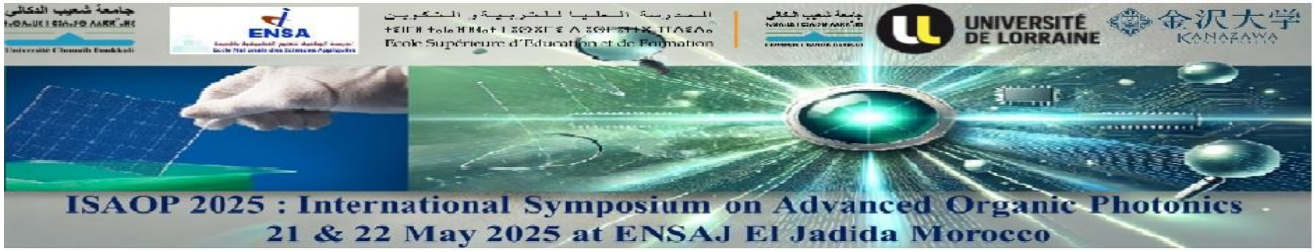
Bioorganic Chemistry Team, Laboratory of Bioorganic Chemistry, Faculty of Sciences, ChouaibDoukkali University, 24000 El Jadida, Morocco.

Laboratory of Organic Chemistry, Bioorganic and Environment, Chemistry Department, Faculty of Sciences, Chouaib Doukkali University, El Jadida, Morocco

**Corresponding author: assia.atif@gmail.com*

1,3,4-oxadiazoles, five-membered heterocycles consisting of two carbon atoms, two nitrogen atoms, and a single oxygen atom, are attracting major attention in various fields of medicinal chemistry and pesticides, but also in polymer and materials science. The procedure was chosen which consists of reacting (5-(hydrazinecarbonyl)-1Hbenzo[d]imidazol-2-yl)methylium with acetic acid in the presence of phosphoryl trichloride at reflux to obtain 2-methyl-5-(2-methyl-1H-benzo[d]imidazol-5-yl)-1,3,4-oxadiazole. The application and physicochemical study of this molecule as a potential corrosion inhibitor for C38 steel in hydrochloric acid (1M HCl) showed that it is a good inhibitor.

Keywords: *1,3,4-oxadiazoles, phosphoryl trichloride, corrosion inhibitor, C38 steel*



Synthesis of 2,5-bis(2-(trifluoromethyl)-1H-benzimidazol-5-yl)- 1,3,4-oxadiazole

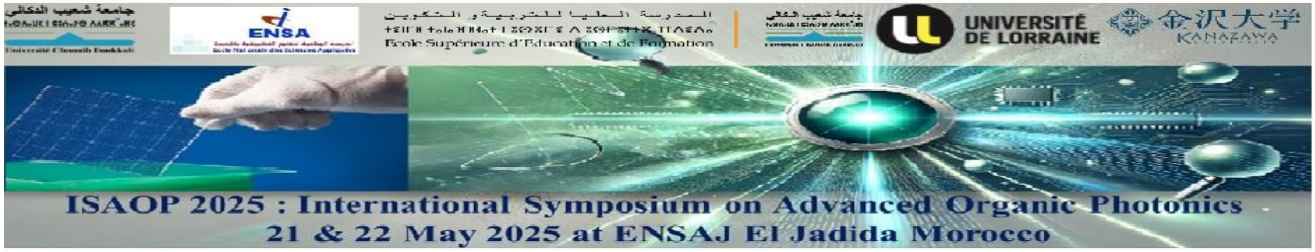
Assiya ATIF*, Abouelhaoul EL ALAMI, Fatima YOUSSOUFI, Houssine AIT SIR

Bioorganic Chemistry Team, Laboratory of Bioorganic Chemistry, Faculty of Sciences, ChouaibDoukkali University, 24000 El Jadida, Morocco.

**Corresponding author: assia.atif@gmail.com*

1,3,4-oxadiazoles, five-membered heterocycles consisting of two carbon atoms, two nitrogen atoms, and a single oxygen atom, are attracting major attention in various fields of medicinal chemistry and pesticides, but also in polymer and materials science. we proceeded to the synthesis of 2,5-bis(2-(trifluoromethyl)-1H-benzimidazol-5-yl)-1,3,4- oxadiazole by reacting 2-(trifluoromethyl)-1H-benzimidazole-5-carboxylic acid with hydrazine hydrate in polyphosphoric acid at reflux . After treatment, the precipitate obtained is then recrystallized from ethanol. The compound is obtained with a yield of 86% and a melting temperature greater than 300°C.

Keywords: *1,3,4-oxadiazoles, polyphosphoric acid, hydrazine hydrate, synthesis*



Synthesis of a Fruit Shell-Based Adsorbent for Methylene Blue Removal: Optimization Using Central Composite Design (CCD)

Asmae SANAD, Meryem BENSEMLALI, Meryeme JOUDI, Abdellatif AARFANE, Mina BAKASSE, and Hamid NASRELLAH

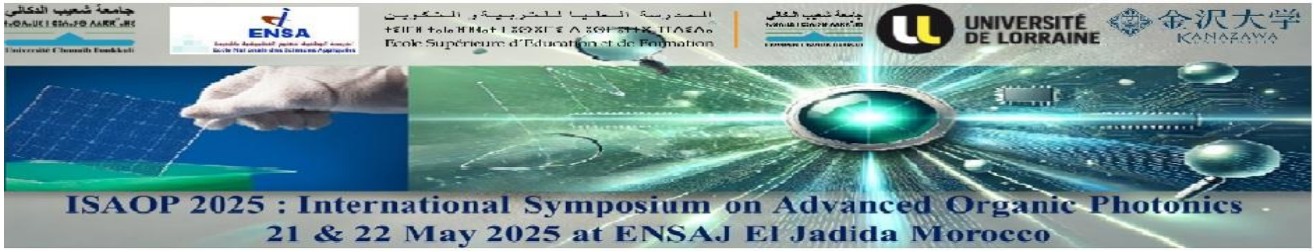
Laboratory of Organic Bioorganic Chemistry and Environment, Faculty of Sciences, University Chouaib Doukkali, El Jadida, Morocco.

Laboratory of Chemistry of Coordination and Analytics, Faculty of Sciences, El Jadida, Morocco.

Higher School of Education and Training, University Chouaib Doukkali, El Jadida, Morocco

In response to the growing concern over water pollution caused by industrial dyes, this study investigates the synthesis of a low-cost adsorbent derived from fruit shells, an abundant agro-waste material. The biosorbent was chemically activated and characterized. Its efficiency in removing methylene blue (MB), a commonly used cationic dye, was assessed under various experimental conditions. To optimize the adsorption process, a Central Composite Design (CCD) was employed to evaluate the influence of five key factors: solution pH, adsorbent dose, initial dye concentration, contact time, and temperature. The results revealed significant interactions among these parameters, with optimal conditions leading to maximum MB removal efficiency. This work highlights the potential of fruit shell-based biomaterials as sustainable and eco-friendly alternatives for dye-contaminated wastewater treatment.

Keywords: methylene blue; Adsorption; Experiment design; Wastewater treatment.



Synthesis, Characterization and Biological Activity of New 4-Trifluoromethyl Substituted 2-(1*H*)-Pyridinone

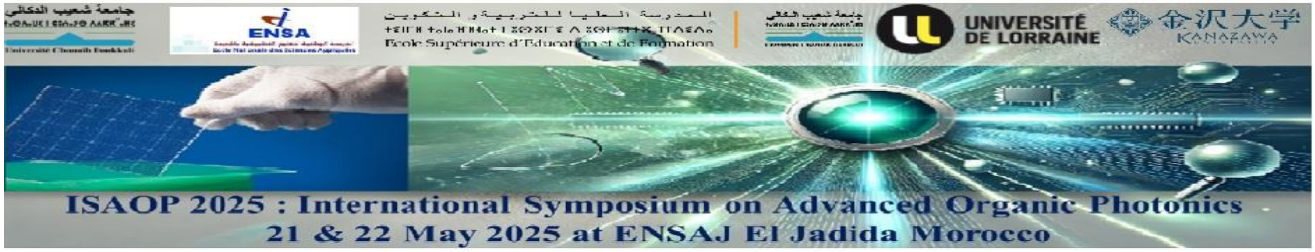
Fatima YOUSSOUFI*, Abouelhaoul El ALAMI, Assiya ATIF, Hamid SDASSI, and

Mustapha SOUFYANE

Bioorganic Chemistry Team, Faculty of Sciences, Chouaib Doukkali University, El Jadida, Morocco.

**Corresponding author:* *fatimayoussoufi1995@gmail.com*

Our objective is to develop a new synthesis a new functionalized fluorinated pyridine-2-one 3 from a trifluoromethylated enaminodiketone 1. The obtained compound 3 was synthesized in good yield by a nucleophilic substitution and intramolecular cyclisation reaction of the enaminodiketone 1 in the presence of the ethyl glycinate hydrochloride 2 using the Michael 1,4-addition/elimination approach. The structure of the synthesized 4- trifluoromethyl-(1*H*)-2-pyridinone 3 was established using physico-chemical analyses and various spectroscopic techniques such as ATR-FTIR, 1H NMR and 13C NMR and Mass spectrometry. The results of the analyses are in good agreement with the proposed structure of the synthesized compound. Synthesis of trifluoromethylated pyridin-2-(1H)-one **3.**



Synthesis, Characterization and Evaluation of Biological Activity of New Trifluoromethyl Substituted Pyrazoles

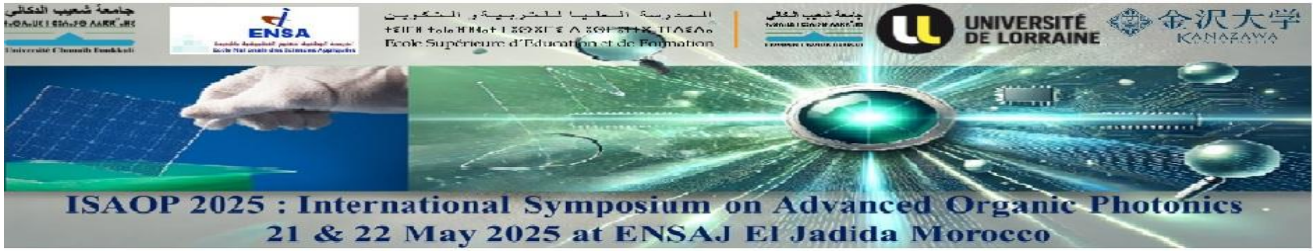
Fatima YOUSSOUFI*, Abouelhaoul El ALAMI, Assiya ATIF, Hamid SDASSI, and

Mustapha SOUFYANE

Bioorganic Chemistry Team, Faculty of Sciences, Chouaib Doukkali University, El Jadida, Morocco.

**Corresponding author:* *fatimayoussoufi1995@gmail.com*

This work has the objective of synthesizing a new fluorinated pyrazoles 3, 5a and 5b from a highly functionalized precursor (diethylaminomethylenehexafluoroacetylacetone) called DAMFA 1. The formed products 3, 5a and 5b were synthesized in good yield by the *N-N* exchange reaction of DAMFA 1 with mono and di-substituted nucleophiles 2 and 4 using the Michael 1,4-addition/elimination approach. The structures of the synthesized pyrazoles 3, 5 and 5b were established using physico-chemical analyses and various spectroscopic techniques such as ATR-FTIR, 1H NMR and 13C NMR and Mass spectrometry. The results of the spectral data are in good agreement with the proposed structure of the synthesized compound.



Synthesis, Characterization and Evaluation of the Antimicrobial Activity of A New Series of Benzimidazoles Phosphonates

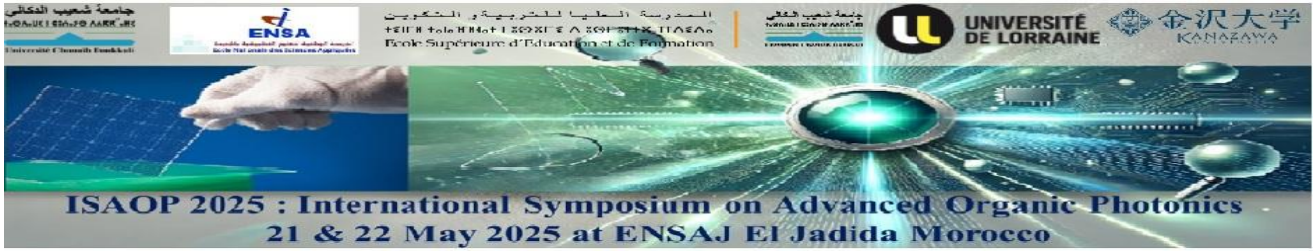
Fatima YOUSSOUFI*, Abouelhaoul El ALAMI, Assiya ATIF, Hamid SDASSI1, and

Mustapha SOUFYANE

Bioorganic Chemistry Team, Faculty of Sciences, Chouaib Doukkali University, El Jadida, Morocco.

**Corresponding author:* *fatimayoussoufi1995@gmail.com*

This work aims to synthesize a new series of benzimidazoles phosphonates and to study their biological activities. The formed benzimidazoles phosphonates compounds 3(a-j) were synthesized in good yields according to an efficient route under solvent-free conditions from the prepared starting materials of 2-substituted benzimidazoles 1(a-j). The structures of the synthesized compounds 3(a-j) were established using physico-chemical analyses and various spectroscopic techniques such as ATR-FTIR, 1H NMR and 13C NMR and Mass spectrometry. Moreover, the formed products were evaluated for their antimicrobial activity. The results of the antimicrobial profile revealed promising activities against microbial strains (*Staphylococcus aureus*, *Escherichia coli*, *Pseudomonas aeruginosa*, and *Candida albicans*).



Synthesis, Characterization, *In Vitro* and *In Silico* α-Amylase Inhibitory Activity of Novel 2,6-di(1,3,4-oxadiazol-2-yl)pyridine derivatives Compounds

Assiya ATIF*, Mohamed MARGHICH, Nour Elhouda DAOUDI, Abouelhaoul EL ALAMI, Tarik HARIT, Fatima YOUSSOUF1, Houssine AIT SIR, Abdelali BITAR.

Bioorganic Chemistry Team, Laboratory of Bioorganic Chemistry, Faculty of Sciences, ChouaibDoukkali University, 24000 El Jadida, Morocco.

Nutritional Physiopathology, Neurosciences and Toxicology Team, Laboratory of Anthropogenetic, Biotechnology and health, Faculty of Sciences, Chouaib Doukkali University, 24000 El Jadida, Morocco.

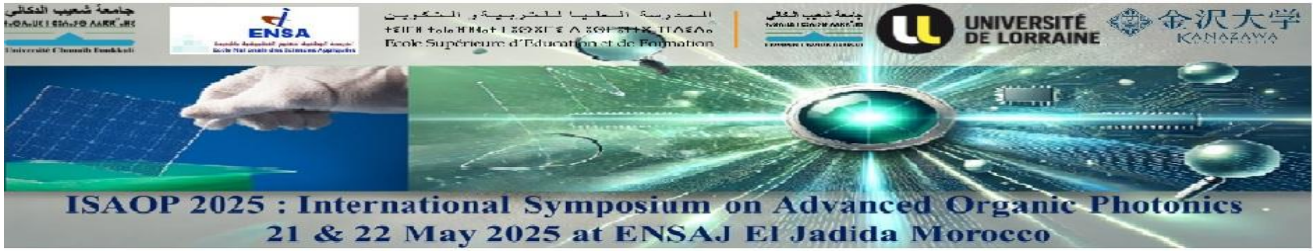
Higher Institute of Nursing Professions and Health Techniques, Oujda 60000, Morocco.

Laboratory of Bioresources, Biotechnology, Ethnopharmacology and Health, Department of Biology, Faculty of Sciences, Mohammed First University, 60000 Oujda, Morocco.

Laboratory of Applied Chemistry and Environment–ECOMP, Faculty of Sciences, Mohammed First University, 60000 Oujda, Morocco

**Corresponding author: assia.atif@gmail.com*

α-Amylase enzymes play a major role in the management of postprandial hyperglycemia. Therefore, inhibition of the α-amylase enzyme is a crucial therapeutic approach for the management of postprandial hyperglycemia and diabetes. The present study aims to synthesize and characterize a novel bis-1,3,4-oxadiazole and evaluate its antidiabetic potential. The inhibitory activity of pancreatic α-amylase was evaluated in vitro, complemented by in silico simulations to explore their binding interactions with the enzyme active sites. New bis-1,3,4-oxadiazole derivatives demonstrated dose-dependent inhibition of α-amylase, particularly 2,6-bis(5-(pyridin-2-yl)-1,3,4-oxadiazol-2-yl) pyridine dose which exhibited the most potent activity with an IC50 value of 0.084 ± 0.015 mg/mL

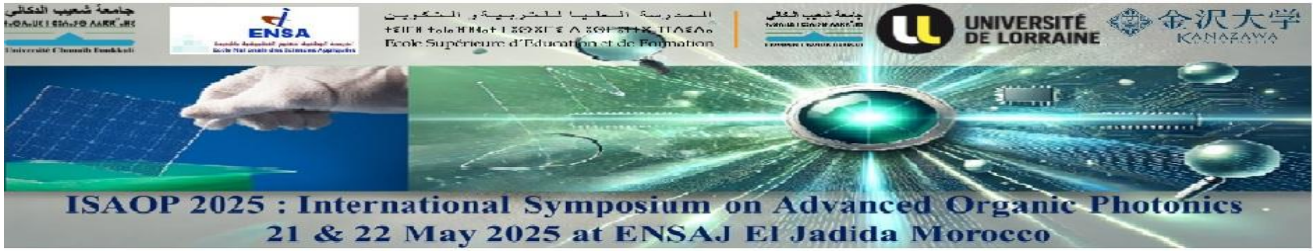


Synthesis, Structural Characterization and Evaluation of the Anticorrosion Properties of a New Benzimidazole Compound: 5-Bromo-1,3-dihydro-4,6,7- trinitrobenzimidazol 2-one

Abouelhaoul EL ALAMI*, Fatima YOUSSOUFI, Assiya ATIF, Houssine AIT SIR and Mustapha SOUFYANE
Bioorganic Chemistry Team, Faculty of Sciences, Chouaib Doukkali University, El Jadida, Morocco.
**Corresponding author: abouelhaoul.elalami103@gmail.com*

In this work, the new benzimidazole derivative, 5-Bromo-1,3-dihydro-4,6,7 trinitrobenzimidazol-2-one (BTB), was synthesized, characterized by (1H NMR, 13C NMR, mass spectrometry and IR-ATR), and evaluated as a corrosion inhibitor for N80 carbon steel in a 1 M HCl medium. The comprehensive study of BTB's inhibitory action was conducted through mass loss measurements and electrochemical analyses, including potentiodynamic polarization curves and electrochemical impedance spectroscopy. The results of electrochemical studies revealed a remarkable corrosion inhibition efficiency, exceeding 95% at 298 K in presence of 10-3M of BTB in solution. Additionally, density functional theory (DFT) calculations were integrated for a theoretical investigation of the inhibitor's reactivity and its interaction with the iron surface. The combined analysis of experimental and theoretical results highlighted that the inhibition potential of the tested inhibitor depends on its electron donation/acceptance capacity. The findings indicate that BTB has the potential to serve as a good corrosion inhibitor for N80 steel in a 1 M HCl medium.

Keywords: Synthesis, 5-Bromo-1,3-dihydro-4,6,7-trinitrobenzimidazol-2-one, Corrosion inhibitor, N80 carbon steel, Experimental studies, Theoretical studies.



The Magnetic Proprites of a VI3 Bilayer

Y. Chegrane1*, A. Boukhal2
Laboratory LPMC, Theoretical Physics Group, Faculty of Sciences, Chouaib Doukkali University, El Jadida, Morocco.
Laboratory LPMC, Theoretical Physics Group, Faculty of Sciences, Chouaib Doukkali University, El Jadida,Morocco.

**Corresponding author: chegrane.youssef@ucd.ac.ma*

We study the effects of exchange interaction inter-layer, anisotropy, temperature and external magnetic field on the VI3 bilayer, to extract the following physical properties: magnetization, susceptibility, and phase diagrams all to describe the magnetic behavior of this lattice structure. We found isolated critical points for specific parameters of the system, and that the system exhibits first- and second-order phase transitions.

Keywords: VI3 Bilayer; Ferromagnetic; Phase diagram.

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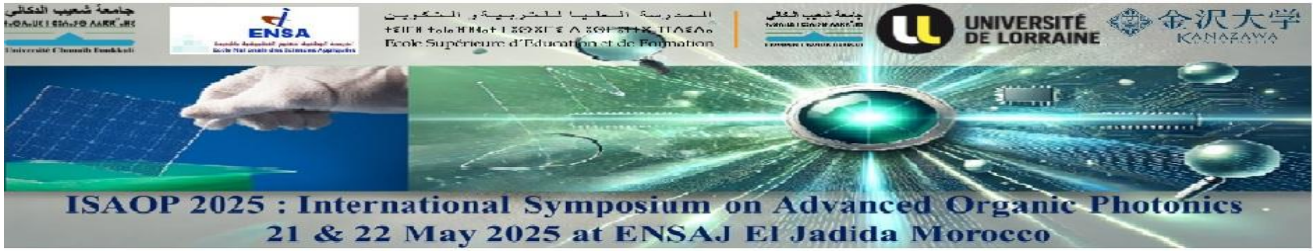
Organic optical devices (optical waveguides, optical fibers, organic semiconductor devices)



Bridgman Growth, and Correlation Between Thermal and Optical of ZnSeTe Crystals

Ali ABOUAIS, Mohammed BOUMHAMDI, Rebin KHALID, Amine ALAUOI BELGHITI, Karol STRZAŁKOWSKI, Abdelowahed HAJJAJI

Engineering Science for Energy Lab, National School of Applied Sciences, Chouaib Doukkali University of El Jadida, El Jadida 24000, Morocco

Institute of Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University in Toruń, ul. Grudziądzka 5, 87-100 Toruń, Poland

**Corresponding author*: Abouais.a@ucd.ac.ma

Zinc selenium Telluride, a type II-VI semiconductor with a tunable bandgap, is attracting considerable interest due to its diverse applications, including nuclear radiation detectors and industrial process monitoring. This study investigated the thermal and optical properties of ZnSe1-xTex ternary semiconductors obtained by the vertical Bridgman-Stockbarger growth method over a manganese content range from 0 to 1. The composition of the samples was determined using the energy dispersive analysis (EDS) technique. X-ray diffraction (XRD) was used to characterize the crystalline structure of the material. Transmission spectroscopy was utilized to measure the bandgap energy of the studied samples. The experimental findings showed that the bandgap energy of the ZnSeTe samples varied from 2.66 eV for x = 0 to 2.2 eV for x = 1. The empirical relation between band-gap energies and composition ratio accorded with a bowing parameter b (b = 0.53 eV). Thermal studies were also carried out using the photopyroelectric calorimetry (PPE) technique [1]. The thermal diffusivity and effusivity values were extracted from the experiment, allowing the calculation of the specimens' thermal conductivity using the Adachi model [2]. The results show that the energy gap increases with the increase in Te concentration. Moreover, the thermal diffusivity and conductivity of the studied materials decrease as the Te content in ZnSe1-xTex increases till x=0.4 and increase with the increase of Te. Based on these measurements, it can be concluded that the incorporation of Te into ZnSe crystals has a significant impact on their optical and thermal properties.

Keywords : Semiconductor alloys; Crystal growth; Gap energy; Thermal conductivity, Lattice disorder.

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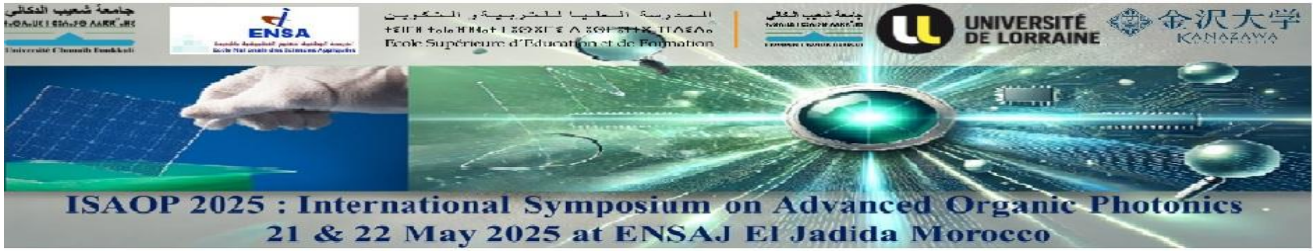

Compositional Effect on Optical and Thermal Properties of Cd1 XZnxTe Mixed Crystals Grown by Bridgman Technique

Mohammed BOUMHAMDI*, Jacek ZAKRZEWSKI, Amine ALAOUI BELGHITI, Ali ABOUAIS, Khalid REBIN, Karol STRZAŁOWSKI, and Said LAASRI

Chouaib Doukkali University of El Jadida, National School of Applied Sciences, Engineering Science for Energy Lab, El Jadida, Morocco.

Institute of Physics, Faculty of Physics, Astronomy, and Informatics, Nicolaus Copernicus University in Toruń,

Grudziadzka 5, PL 87-100 Torun, Poland

** Corresponding author: Med.boumhamdi@gmail.com*

Cadmium telluride-based materials are one of the most promising semiconductor materials being considered to create convenient X-ray and γ-ray detectors. For these materials, it is possible to change electronic properties, lattice parameters, and band gap energies by adjusting the composition of the mixed crystals. The change of band gap energy gives the desired optical properties and emission in the spectrum's entire visible and UV range. The crystal investigated in this work is the cadmium Zinc telluride (Cd1-xZnxTe) with sulfide content of $0 \leq x \leq 0.9$. The samples were grown from the melt using the vertical Bridgman Stockbarger method. The crystals are characterized using two photothermal methods, each associated with a different nature of generating the photothermal signal. The piezoelectric photothermal spectroscopy (PPS) enables measurements in the front and reverse configurations and applies a piezoelectric detector to measure the photothermal signal. It is sensitive to the surface preparation of the sample [1] and enables the determination of the optical properties of the materials. The photopyroelectric technique (PPA) is a contact method that directly measures heat oscillations [2] and allows for the determination of thermal properties (thermal diffusivity and effusivity). Transmittance was measured, and Energy Gap values were extracted for all compositions of the crystals. From piezoelectric spectra, a strong influence of surface preparation on the characteristics of the spectra can be observed. It varies with the modulation frequency, which allows us to estimate the thickness of the defective surface layer and develop an appropriate surface treatment method.

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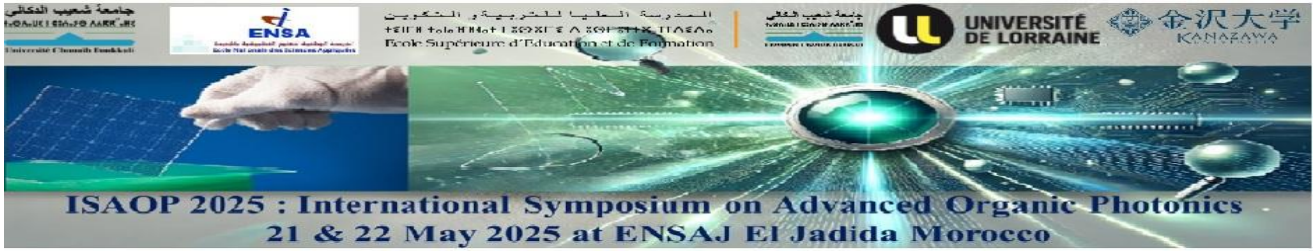


Effects of Zn doping on optoelectronic properties and the transition from p-Type to n-Type in CuO thin films synthesized by M-SILAR

Hafsa DIYAGH *, Latifa ZNAIDI, Ismail BENAICHA, Abdellatif El-HABIB , Nadia HERFAOUI, Ahmed RMILI, Smail AMRAOUI, Khalid NOUNEH*

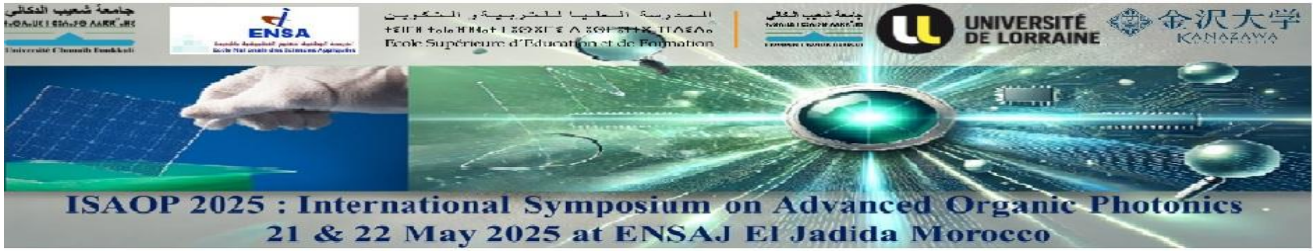
Materials and Subatomic Physics Laboratory, Faculty of Sciences, Ibn Tofail University, Kenitra, Morocco

Materials, Systems and Energy Engineering Laboratory, faculty of sciences and techniques of tangier, Abdelmalek Essaadi University, Tetouan, Morocco

* Corresponding author: khalid.nouneh@uit.ac.ma

In this paper, we invistigates the effects of zinc (Zn) doping on structural, optical, and electrical properties of copper oxide (CuO) thin films synthesized using the Modified Successive Ionic Layer Adsorption and Reaction (M-SILAR) method. Zn concentrations of 0%, 2%, 4%, 6%, 8%, and 12% were doped into CuO films that were deposited on glass substrates. X-ray diffraction and Raman spectroscopy analyses revealed the polycrystalline nature of the thin films and confirmed that Zn ions were incorporated into CuO without altering its monoclinic phase, along with a reduction in crystallite size as the Zn concentration increased. Notably, no Cu2O or other impurities were detected. Scanning electron microscopy and atomic force microscopy revealed changes in morphology, including nanorod shapes, and indicated decreased surface roughness and grain size, with the smallest grains observed at 8% Zn doping. The optical band gap increases from 1.55 eV to 1.62 eV at 8% Zn doping. Halleffect measurements indicated p-type conductivity up to 8%, with 6% Zn identified as the optimal doping level, achieving the highest carrier concentration and mobility. However, at 12% Zn doping, a transition to n-type conductivity occurred, accompanied by increased defects. Therefore, the incorporation of small concentrations of Zn ions into CuO enhances its electrical properties, suggesting that Zn-doped CuO could be suitable for photovoltaic applications.

Keywords: CuO thin films, M-SILAR method, Defect structures, Band gap tuning, p-type to n-type transition.



Illumination of chiral medium by Whittaker-Gauss Beams

F. Iraoui, F. Khannous, A. Belafhal*

Laboratory LPNAMME, Laser Physics Group Department of Physics, Faculty of Sciences, Chouaïb Doukkali University P. B 20, 24000 El Jadida, Morocco

** Corresponding author. E-mail : belafhal@gmail.com*

The propagation of light beams in anisotropic optical media has attracted considerable interest because of its crucial role in the development of optical devices and nonlinear optics. Many devices exploit the anisotropic properties of the media to modulate the electric field. Among these anisotropic media, chiral structures have attracted particular attention because of their ability to influence the polarization and energy distribution of light beams through their chiral activity. Recently, there has been growing interest in the propagation of laser beams in a chiral system [1-3]. Using the Collins diffraction integral, which is the generalized Huygens-Fresnel integral and the transfer matrix ABCD, we derive the analytical expression for the Whittaker-Gauss beams (WGBs) passing through a chiral medium. From the formula obtained, the propagation properties of these beams in a chiral medium are analyzed using illustrative numerical examples. The results obtained could be useful for the application of WGBs in beam shaping and optical micromanipulation.

Keywords: Collins diffraction integral; Huygens-Fresnel integral; Matrix ABCD; Whittaker-Gauss beams.

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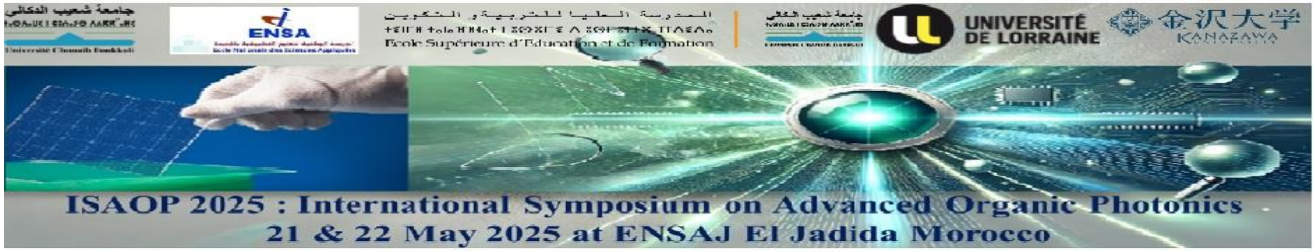

Light manipulation devices using organic EO polymers from visible to NIR

Akira OTOMO, Takahiro KAJI, Toshiki YAMADA

National Institute of Information and Communications Technology

**Corresponding author:* akira_o@nict.go.jp

In recent years, it has become important to improve the performance of light manipulation devices as optical beam steering and forming for light detection and ranging (LiDAR) and free-space optical (FSO) communication. An optical phased array (OPA) is a device in which the optical phase modulators are arranged in an array, and has a function of optical beam steering and forming without any mechanical moving parts (Fig. 1). It can be used not only for LiDAR and FSO communications, but also for undersea optical wireless communications, 3D-AR smart glasses, 3D light field displays, and many other applications from visible to near-infrared (NIR), as shown in Fig. 2. Although OPAs using liquid crystal or Si photonics phase shifters have been demonstrated, the speeds of these OPAs are not sufficient for most applications. Electro-optic (EO) polymers are suitable materials to make the optical phase modulators faster than 100 GHz. Therefore, we expect that the OPA using EO polymer as optical phase shifters realizes an optical beam steering device with ultra-high-speed scanning. However, conventional EO polymers have been developed for devices in the NIR optical communication wavelength band such as the C-band and O-band, and they cannot be used in the short wavelength range due to their large absorption. On the other hand, transparent EO polymers in the short-wavelength region have small EO coefficients and modulators using them have been thought to be inefficient. We successfully developed a high-performance EO polymer for visible light, and a modulator using the EO polymer for visible red light gives that the modulator's figure of merit, $V\pi L$ is 0.52 V·cm, which is more than twofold better than that for the typical C-band EO polymer modulators [1]. We also developed a poled-film transfer process [2] and applied it for fabricating large-scale channel OPAs and inorganic waveguide hybrid OPAs using EO polymers.

Keywords; EO Polymer, Optical Phased Array, Light Manipulation, Modulator

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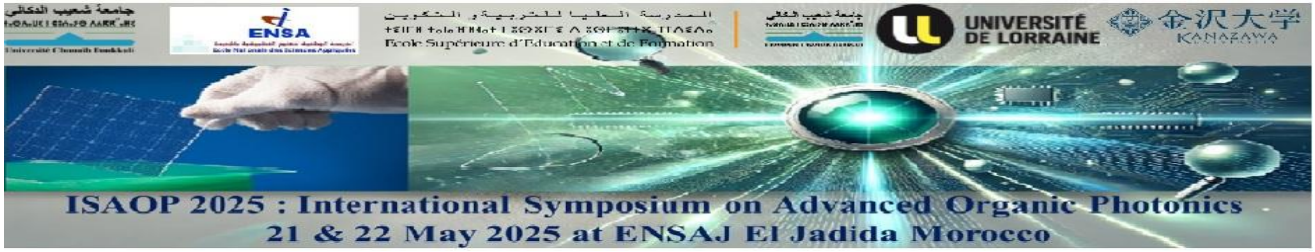

Protein-Based Neuromorphic Devices Emulating Visual Receptive Fields for Illusion Detection

Yoshiko OKADA-SHUDO

Department of Engineering Science, The University of Electro-Communications, Tokyo, 182-8585, Japan

*Corresponding author: yoshiko.okada@uec.ac.jp

Photo-responsive organic materials offer promising capabilities for developing compact and energy-efficient vision systems. In this study, we demonstrate a protein-based optical filtering device that emulates two types of visual receptive fields: retinal ganglion cells and primary visual cortex (V1) simple cells, using the photoactive protein bacteriorhodopsin (bR). The DOG (Difference-of-Gaussian) filter, based on circular and donut-shaped patterns derived from the DOG function, mimics retinal ganglion cells' center-surround receptive field structure. Using oval patterns based on the Gabor function, the Gabor filter replicates the orientation-selective characteristics of V1 simple cells. The filters were fabricated by inkjet printing bR suspension (2.5 g/l) to create patterns on ITO electrodes (resultant thickness: nm/layer). The front and rear electrodes define the excitatory and inhibitory regions, respectively, and are separated by an electrolyte layer containing KCl and HEPES buffer (pH 8.2), as shown in Figure 1. A masking layer on the inhibitory side regulates photocurrent amplitude, enabling lateral inhibition entirely optically. The devices perform spatial convolution of input images by scanning them across the filter and recording light-induced current responses. No external power or digital computation is required during operation, realizing an energy-efficient, all-optical implementation of early visual processing. To demonstrate functionality, we challenged the detection of visual illusions, particularly focusing on the Café Wall illusion, which involves spatial alignment and luminance contrast. A Café Wall pattern was scanned across each device. The Gabor filter output displayed twisted cord-like features, characteristic of the Fraser illusion—a representative orientation-based visual illusion. In contrast, the DOG filter enhanced edges and revealed contrast polarity changes due to center-surround interactions, contributing to the perception of brightness modulation consistent with the Café Wall illusion. This study presents the first realization of biomimetic visual receptive fields entirely based on photo-sensitive protein materials capable of detecting visual illusions. Integrating sensing and pre-processing within the organic material marks a new direction in neuromorphic photonics, with potential applications in low-power, bio-inspired visual systems.

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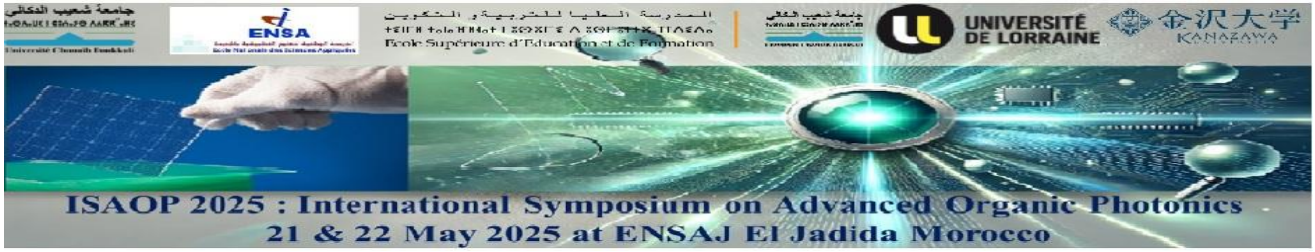
New technologies and applications for optical communication and signal transmission



Anisotropic Polarization Analysis and Humidity Dependence of Dielectric Properties of Polyimides for 5G/6G Wireless Applications

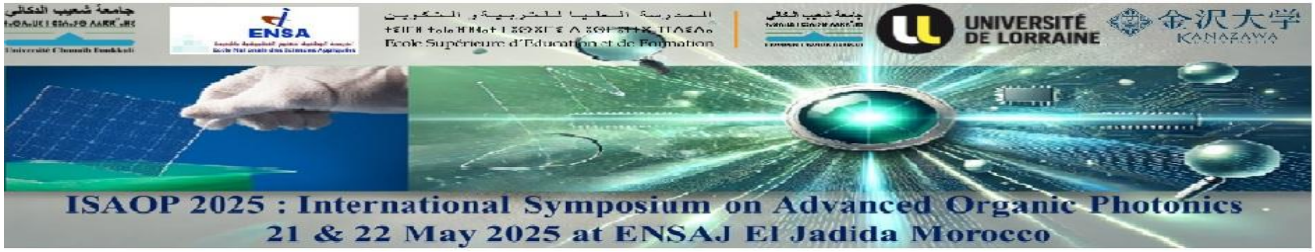
Shinji ANDO*, Ririka SAWADA, and Haonan LIU

Department of Chemical Science and Engineering, Institute of Science Tokyo, Ookayama 2 12-1, Meguro-ku, Tokyo 152-8552, Japan.

**Corresponding author:* ando.s.aa@m.titech.ac.jp

Polyimides (PIs) have been expected to be used as optical waveguide materials and lowdielectric insulators for optoelectronic and 5G/6G wireless communication applications. In our study, dielectric constants (*D*k) and dissipation factors (*D*f) of 15 types of PIs were measured in the transverse electric (TE011) mode at 10−20 GHz, and the relationships among the dipolar orientational (*P*d) and electronic (*P*e) polarizations, as well as *D*k and *D*f, were quantitatively investigated.[1] The total polarization per unit volume, namely *P*t ($\propto$ *D*k), shows a positive linear correlation with *P*e, which indicates that *P*t is mainly dominated by the *P*e evaluated from average (*n*av) or in-plane refractive index (*n*TE) in the NIR region (1310 nm). Besides, we have found that the *D*f of PIs is highly anisotropic and linearly proportional to *P*d in the in-plane direction (*P*d(TE)), which points out that they are closely related to the in-plane component of dipole moment (μTE) and their relaxational motions at 10 GHz. Furthermore, the *D*k and *D*f of all PIs increased linearly with respect to the relative humidity (RH) of the environment, and their slopes (*h*Dk and *h*Df), *i.e.*, the RH sensitivities of *D*k and *D*f showed a proportional relationship with each other. In particular, a perfluorinated PI[2] and highly fluorinated PIs exhibited extremely low *h*Dk and *h*Df values owing to the low polarizability and high hydrophobicity of fluorine. Intriguingly, commercial PIs derived from *s*BPDA dianhydride also showed low *h*Dk and *h*Df due to their dense molecular packing[3] which prevents permeation of water. Most recently, the *D*k and *D*f of 11 types of PIs were systematically measured between 25 and 330 GHz using Fabry-Pérot resonators.[4] As the frequency increased, all the PIs exhibited a continuous decrease in *D*k and a consistent increase in *D*f. Notably, no distinct peaks were observed over the entire frequency range, and the PIs containing –CF3 groups in the diamine moieties exhibited a rapid increase in *D*f with frequency over 50 GHz. Although this originates from a large periodic motion accompanied by a phase disturbance extending over the main chain,[5] it can be overcome by a judicious design of fluorinated diamines. Consequently, highly fluorinated PIs are promising for future telecommunication and wireless technologies.

Keywords : Polyimides, Dielectric constant, Dissipation factor, Anisotropic property, Polarization analysis, Humidity dependence, 5G/6G wireless application, Optical properties in NIR region



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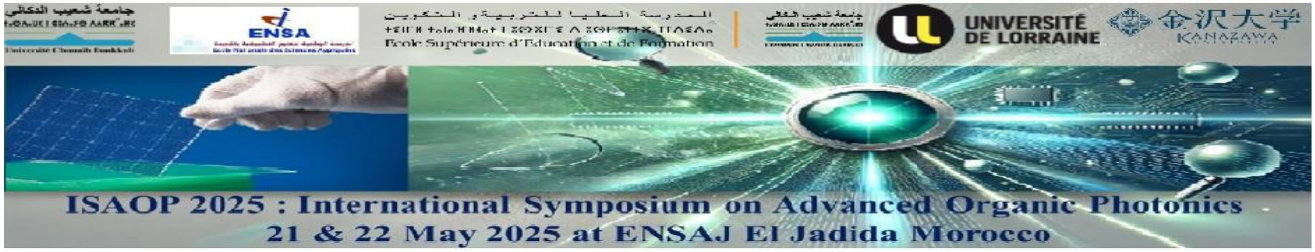


Application of Innovative Environmental Technologies for the Treatment and Reuse of Wastewater from Construction Sites and Industries: Physico Chemical Characterization and Performance Evaluation

Soukaina BAKKASS*, Naoual SEMLALI AOURAGH HASSANI, Mohammed Karim BEN HACHMI, Abdellatif AARFANE, Hamid NASRELLAH

Hydraulic Systems Analysis Laboratory, Mohammedia School of Engineers, Mohammed-V University in Rabat Morocco

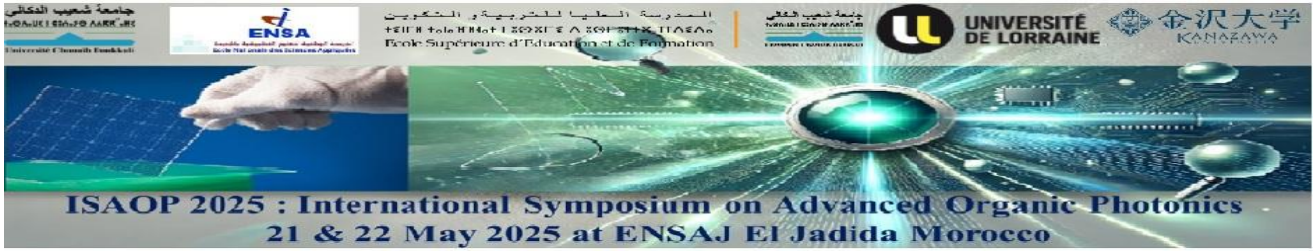
University Chouaib Doukkali, Higher School of Education and Training in El Jadida Morocco

University Chouaib Doukkali, Faculty of Sciences, Laboratory of Organic Bioorganic Chemistry and Environmental in El Jadida Morocco

**Corresponding author: soukaina_bakkass@um5.ac.ma*

The issue of wastewater management in the construction industry is attracting growing attention due to the heterogeneous and potentially polluting nature of liquid discharges generated by various industrial operations. This study aims to characterize the wastewater produced by a construction related industry and to assess the effectiveness of innovative environmental technologies for its treatment and reuse. A comprehensive physico-chemical analysis was conducted on samples collected from an industrial site, focusing on key pollution indicators such as pH, suspended solids (SS), chemical oxygen demand (COD), and the presence of hydrocarbons. Several treatment processes were tested, including technologies based on natural filtration and advanced physico-chemical methods. The results demonstrate significant performance in reducing pollutant loads, paving the way for the partial reuse of treated water for non-potable industrial applications. This research highlights the potential of environmental technologies as a strategic lever to enhance water and environmental sustainability in the construction sector.

Keywords: Wastewater management, Pollution, Wastes water Treatment, construction sector.



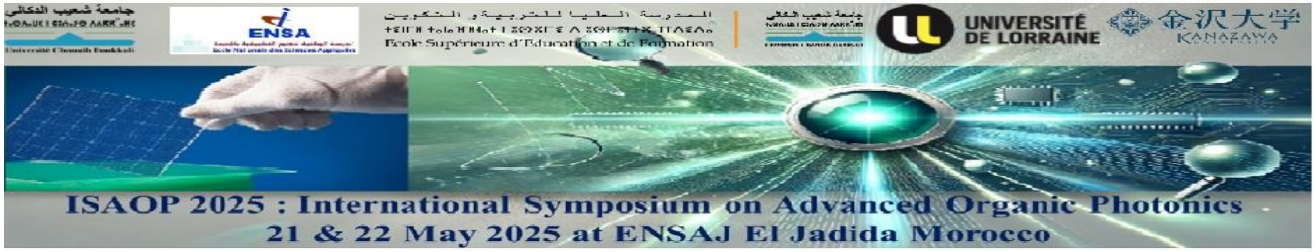
Correction 1 Methods for CC: Enhancing Accuracy in Lithium-Ion Battery State of Charge Estimation

Abdelhakim TABINE, El mehdi LAADISSI, Anas Elachhab, Souhaib BOUZAID, Chouaib ENNAWAOUI, Abdelwahed HAJJAJI
LabSIPE , National School of Applied Sciences, Chouaib Doukkali university, El Jadida, Morocco.

**Corresponding author:* tabine.a@ucd.ac.ma

This paper analyzes the FPSOC method, an innovative approach for accurately estimating the state of charge (SOC) of lithium-ion batteries, factoring in temperature variations. The study tests pulse current charging techniques such as positive pulse, negative pulse, and alternating current. FPSOC performs well across a temperature range of -10°C to +60°C and various current profiles. The model achieves exceptional accuracy with root mean square error (RMSE) values from 0.52% to 1.03%, outperforming the traditional Coulomb Counting (CC) method. It also shows strong performance under varying initial SOC conditions, with errors up to six times lower than the CC model. This research is the first to integrate temperature variations into SOC estimation. FPSOC proves to be a superior method for SOC monitoring in applications like electric vehicles and energy storage systems.

Key words: Lithium-ion battery, SOC estimation, temperature variation, polynomial fitting algorithm, error analysis, RMSE, **Pulse Current.**



Corrosion inhibition of steel C38 in hydrochloric acid (1M) by a novel 1,2-bis (2-(1 H benzo (bisimidazol-2-yl) thio) ethoxy) ethane

Nabil LAHRACHEA, Najoua LABJARA*, Said JEBBARIB, Mohamed OMARID, Ali BARHOUMIE, Mohammed BENMESSAOUD, Hamid NASRELLAHG, Abdelouahed DAHROUCHH, Souad EL HAJJAJIH

Laboratory of Molecular Spectroscopy Modelling, Materials, Nanomaterials, Water and Environment, CERNE2D, ENSAM, Mohammed V University in Rabat, Morocco;

Laboratory of Bio-organic Chemistry, Department of Chemistry, Faculty of Sciences, Chouaib Doukkali University, El Jadida, Morocco;

Multi-laboratory LC2A, N °182 Industrial zone, Mohammedia, Morocco.

Agro-industrial, Environmental and Ecological Processes Team, Faculty of Science and Techniques of Beni Mellal, Sultan Moulay Slimane University, Beni Mellal, Morocco;

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

Laboratoire d'Énergétique, Matériaux et Environnement-CERNE2D, Ecole Supérieure de Technologie Mohammed V University in Rabat, Morocco;

Laboratory of Organic Bioorganic Chemistry and Environment, Faculty of Sciences, University Chouai Doukkali, Morocco

Laboratory of Molecular Spectroscopy Modelling, Materials, Nanomaterials, Water and Environment, CERNE2D, Faculty of Science, Mohammed V University in Rabat, Morocco;

**Corresponding author: najoua.labjar@ensam.um5.ac.ma*

Hydrochloric acid (1 M) is an aggressive medium that attacks C38 steel and its protection against corrosion by a newly synthesized compound, such as 1,2-bis (2-(1 H benzo (bisimidazol-2-yl) thio) ethoxy) ethane. To characterise the synthesised organic molecules, we used Proton nuclear magnetic resonance (1H-NMR), Carbon-13 nuclear magnetic resonance (13C-NMR) and infrared spectroscopy (IR). Two techniques are used in the electrochemical study: Potentiodynamic polarization investigation (PDP) and Electrochemical Impedance Spectroscopy (EIS). The isothermal adsorption study was made using Langmuir study, Temkin and Langmuir models. The theoretical study was made using DFT quantum physical chemistry calculations: Monte Carlo simulations and molecular dynamics simulations. Surface analysis of the MS coupons was studied by scanning electron microscopy (SEMEDX) which was later analysed by Energy Dispersive X-Ray. Our results have shown that the protective layer that bonds with C38 steel surface is stable. This layer can form an obstacle that prevents aggressive agents from penetrating the substrate surface. In this study we use experimental techniques: polarization curves and impedance spectroscopy to study the deterioration protection of C38 in a 1.0 M HCl by the synthetized molecule 1,2-bis (2-(1 H benzo (bisimidazol-2-yl) thio) ethoxy)

ethane. However, they are unable to provide atomicscale information to understand how this organic molecule inhibits metal corrosion. Inhibitory properties are linked to the interaction and adsorption phenomena between this product and the surface of our substrate. The performance of the inhibitor is a function on its electronic structure and that of the C38 steel substrate. Quantum theoretical physical chemistry, Monte 36 Carlo technique and molecular dynamics simulations procedure are ideal for this work. We obtained the following results:

- We have obtained a maximum of inhibitory power of 97.94 % at a concentration of 10-4 mol/litre

- Molecules are adsorbed according to the Langmuir isotherm.

- This inhibitor acts as a mixed-type protector due to its phytochemical properties.

- The polarisation curves obtained show that the protector is of mixed cathodic and anodic type with a cathodic predominance. H+ cation is discharged onto the C38 surface using an activation mechanism and the hydrogen reduction mechanism is not affected.

- The (PIS) curves show a decrease in the capacitance of the double layer, which is proven by

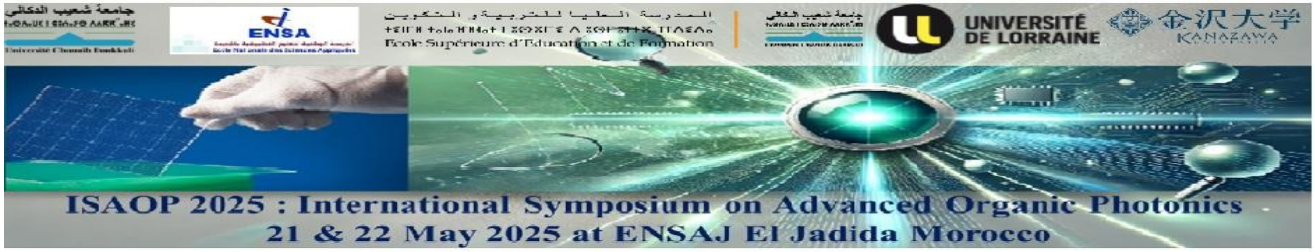
adsorption of bisbenzimidazole-2-thione on the C38, thus forming a protective layer.

- The Energy Dispersive X-ray images show that the area of the steel introduced in the medium containing the inhibitor is uniform compared to that introduced in the corrosive solution without the protector, thus showing the adsorption of bisbenzimidazole-2-thione on the area of C38.

- The main adsorption centres are S, N and O, which form aromatic rings in the protector structure.

Keywords: 1,2-bis (2-(1 H benzo (bisimidazol-2-yl) thio) ethoxy) ethane (BOZS2-yl), steel

C38, EIS, PDP, DFT, 1H-NMR, 13C-NMR, IR, simulations (DM) and SEM-EDX.



Factors Driving Lithium-Ion Battery Aging: 1Current Intensity vs. Temperature 2 Effects

Abdelhakim TABINE*, El Mehdi LAADISSI, Hicham MASTOURI, Anass ELACHHAB, Abdelowahed HAJJAJI

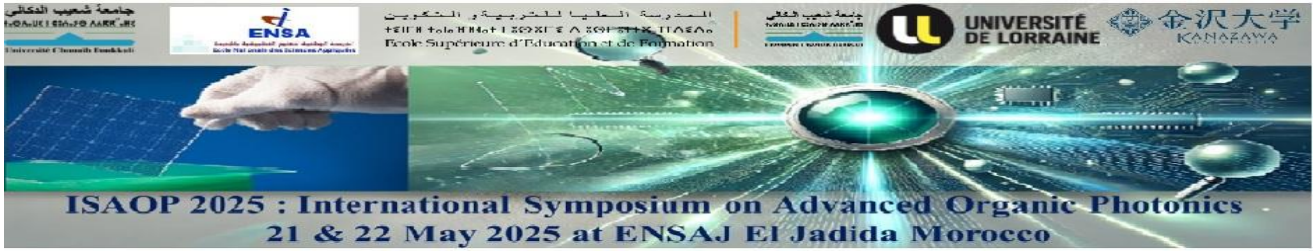
LabSIPE , National School of Applied Sciences, Chouaib Doukkali university, El Jadida, Morocco.

University Mohammed 6 Polytechnic (UM6P) Benguerir, Morocco.

**Corresponding author: tabine.a@ucd.ac.ma*

The aging of lithium-ion batteries has a profound effect on their performance, safety, and overall lifespan. Factors such as temperature and current intensity during charge and discharge cycles are crucial drivers of capacity loss and safety concerns, including overheating and thermal runaway. This study explores how these variables impact battery aging, showing that higher charge/discharge rates cause faster degradation compared to temperature increases. Under moderate conditions (25°C, 1C), a 30% capacity loss was observed after approximately 2100 cycles, serving as a benchmark for battery lifespan. The results emphasize the importance of following the manufacturer's recommended operational limits to improve both durability and safety. Future studies should consider additional factors, like mechanical stress and humidity, to develop methods for enhancing battery performance and prolonging their life.

Key words: lithium-ion batteries, aging factors, performance, capacity loss ,extreme temperatures , Current Amplitude.



Illumination of chiral medium by Whittaker-Gauss Beams

F. Iraoui, F. Khannous, A. Belafhal*

Laboratory LPNAMME, Laser Physics Group, Department of Physics, Faculty of Sciences, Chouaïb Doukkali University, P. B 20, 24000 El Jadida, Morocco

** Corresponding author: belafhal@gmail.com*

The propagation of light beams in anisotropic optical media has attracted considerable interest because of its crucial role in the development of optical devices and nonlinear optics. Many devices exploit the anisotropic properties of the media to modulate the electric field. Among these anisotropic media, chiral structures have attracted particular attention because of their ability to influence the polarization and energy distribution of light beams through their chiral activity. Recently, there has been growing interest in the propagation of laser beams in a chiral system [1-3]. Using the Collins diffraction integral, which is the generalized Huygens-Fresnel integral and the transfer matrix ABCD, we derive the analytical expression for the Whittaker-Gauss beams (WGBs) passing through a chiral medium. From the formula obtained, the propagation properties of these beams in a chiral medium are analyzed using illustrative numerical examples. The results obtained could be useful for the application of WGBs in beam shaping and optical micromanipulation.

Keywords: Collins diffraction integral; Huygens-Fresnel integral; Matrix ABCD; Whittaker-Gauss beams.

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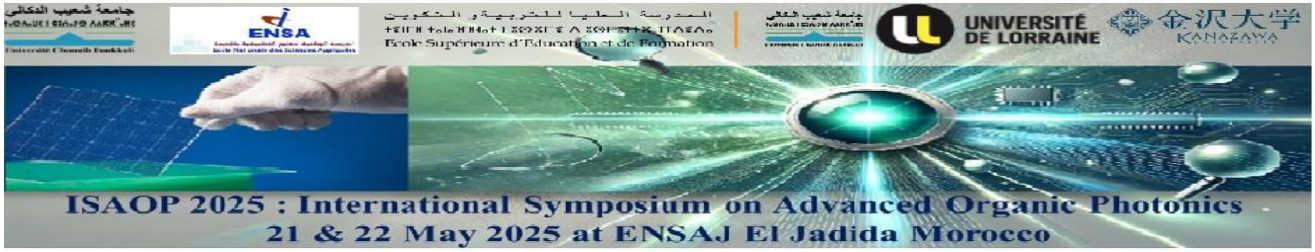
New concepts in Organic and Plastic materials and devices for photonic applications



Characterization of Oriented Polymer Films with Embedded Carbon Micro-Coils: Electrical Behavior

Rei Furukawaa,*, Onur Cem Namli b, Nao Mochizukia, Yusuke Nakashimaa,
University of Electro-Communications
Yeditepe University
**Corresponding author: furukawa@ee.uec.ac.jp*

This study investigated the absorption of electromagnetic (EM) waves by micron-scale carbon microcoils (CMCs) dispersed in a polymer film. Unlike other carbon materials, the helical structure of CMCs allows for discrete EM absorption, offering potential for various engineering applications. To understand this mechanism, CMCs were aligned within the polymer film using directional casting. Scanning electron microscopy (SEM) revealed that larger CMCs aligned more readily, while smaller ones remained randomly oriented. Electrical impedance measurements indicated sufficient conductivity for AC evaluation. The Cole-Cole plot, showing a negative curve, suggested the film behaved as an RC series circuit, implying a network-like connection of the dispersed CMCs, rather than individual inductance as initially expected.

Keywords:
carbon, graphite, PMMA film, orientation, electrical conductivity, alternating current impedance

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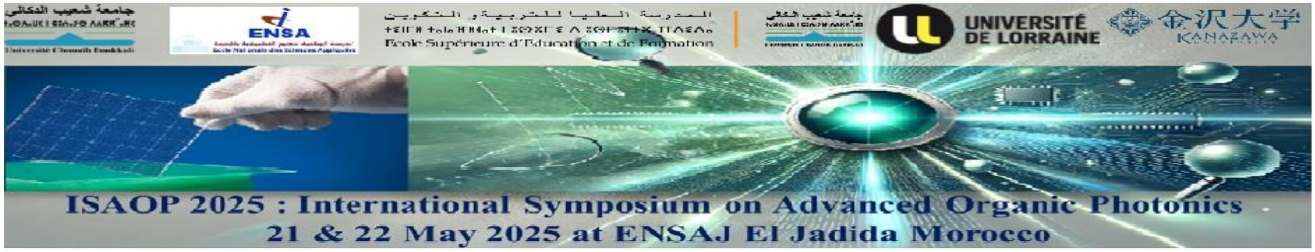
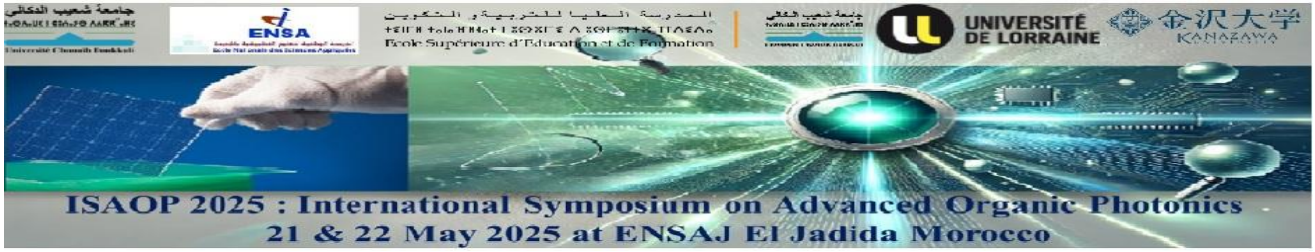


Hearth ash and fly ash filtration efficiency in industrial wastewater treatment and conductivity analysis monitoring

El Mokhtar EL HAFID*, Abdelhadi MORTADI, El Ghaouti CHAHID, Said LAASRI
Laboratory of Engineering Science for energy (labSIPE) ENSA, Chouaib Doukkali University, El Jadida, Morocco.
Laboratory Physics of Condensed Matter (LPMC). Chouaib Doukkali University, El Jadida, Morocco.
Polydisciplinary faculty of Sidi bennour, Chouaib Doukkali University, El Jadida, Morocco.
**Corresponding author: elhafidi.e@ucd.ac.ma*

This research explores the effectiveness of hearth ash, fly ash, and sand as filtration media in a vertical infiltration-percolation system for industrial wastewater treatment, combined with complex conductivity analysis. Conducted on liquid discharges from a steel manufacturing facility in Jorf Lasfar, Morocco, the study focuses on removing pollutants such as heavy metals, suspended solids, and high organic loads from untreated effluents. The filtration setup, composed of hearth ash, fly ash, and sand layers, achieved notable pollutant reductions: 88% in chemical oxygen demand (COD), 78% in biochemical oxygen demand (BOD_5), and 74% in suspended solids (SS), meeting Moroccan irrigation water quality standards. The high silic content and adsorption capacity of hearth ash played a key role in pollutant retention. Monitoring was carried out using impedance spectroscopy, which examined electrical properties such as conductivity. Variations in the conductivity spectrum indicated pollutant neutralization, while an equivalent circuit model of complex conductivity revealed two distinct relaxation mechanisms, demonstrating the system's efficiency in adsorption and potential for optimization. The findings validate hearth ash as an effective and sustainable filtration medium, offering a cost-efficient solution for wastewater treatment. This approach integrates traditional filtration with advanced monitoring techniques, enhancing reliability and real-time operational control. By repurposing industrial by-products and mitigating environmental impacts, the study contributes to the advancement of sustainable water management strategies.

Keywords: Infiltration-percolation; industrial wastewater; impedance spectroscopy; heavy metals.



Newly Designed Drug Delivery System Using Nano-Prodrugs without Carrier and the cellular pharmacodynamics

Hitoshi KASAI

IMRAM, Tohoku University, Sendai/Miyagi, 980-8577, JAPAN

**Corresponding autho: kasai@tohoku.ac.jp*

In this presentation, we propose a new concept, termed "pure nano-drugs" (PNDs), which are comprised of drug ingredient and are delivered into cells in a carrier-free state without using polymer. As the model of PNDs, the nanoparticles of SN-38 cholesterol succinate [Fig.1] or dimer of SN-38 derivatives with SS bond as linker which is the derivatives of SN-38 having the high anticancer activity were fabricated with less than 100 nm in size by the reprecipitation method [1] developed at our laboratory. Aqueous dispersion of the nanoparticles has been shown to exhibit an extremely effective anti-cancer activity not only in vitro experiments [2][3] but also in vivo experiments[4], when compared to irinotecan, a prodrug of SN-38 and a widely used water-soluble anticancer monomer. In addition, interestingly, unlike conventional polymer micelle nanodrugs, our nanodrug has hydrophobic surface, which allowed them to penetrate cancer cells[5], where they then dissolved in the call and exerted their pharmacological effects. These phenomena were confirmed by observations using fluorescence microscopes using unprecedented FRET-based nanoparticles. Further details will be announced on the day.

Keywords: Nano-drugs, The reprecipitation method, Anti-cancer activity, FRET

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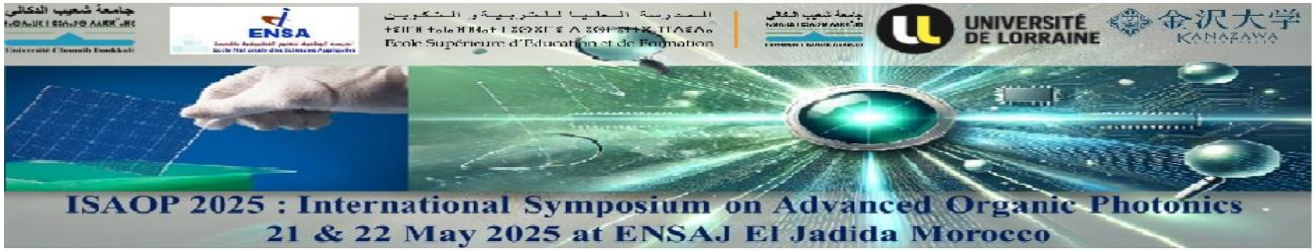
[Short CV] Prof. Hitoshi Kasai received Ph.D. from Tohoku University in 1996, has been a full professor at the same institute since 2016. During his Ph.D., he majored in the creation of organic nanocrystals with the main focus was on their electronics and photonics applications. Not long after, he realized the extreme potential of the technique in the creation of nanocrystals composed of pure anticancer drug molecules. The obtained nano-prodrugs showed greatly enhanced delivery efficacy while reducing the side effects which were usually caused by drug carrier materials in the conventional methods. With the great dedication for the last decade, his laboratory has become one of the first pioneers in the field and gradually strengthened the possibility of the carrier-free DDS. Until date, he has co-authored more than 300 publications including original papers, reviewing articles, book chapters and patents.



Sintering and Coalescence of homo and hetero-Nanoparticles (Ag and Au) and Their Deposition on Ag Substrate (0 0 1) : A Molecular Dynamic Study

Ali SOUHAILI*, Khalid SBIAAI

LS2ME Laboratory, Polydisciplinary faculty of Khouribga, Sultan Moulay Slimane University of Beni Mellal, B.P. 145, 25000 Khouribga, Morocco

* *Corresponding author. E-mail: alisouhailil@gmail.com*

In the present study, we conducted molecular dynamics simulations to investigate the atomic-scale evolution during the solid-state sintering of two identical nanoparticles of Ag and Au (homo-spheres) and two different nanoparticles, Ag-Au (hetero-spheres), along with their deposition on an Ag (001) substrate at temperatures ranging from 400 to 800 K, utilizing the embedded atom method (EAM). Various analyses, x-z plane projection, including radial distribution function, spreading index, and collapsing index, mean square displacement (MSD), were performed to gain deeper insights into the sintering and diffusion processes. Our simulation results reveal a significant temperature dependency in both coalescence and deposition. As the temperature increases, the deposition rate shows a simultaneous rise. Moreover, the sintering and deposition of hetero nanoparticles demonstrate significance at lower temperatures compared to the melting threshold. The degree of coalescence and deposition is strongly temperature-dependent, particularly at high temperatures, where the deposition rate is notably higher. The central objective of this work is to study ways of controlling the assembly of fundamental nanoparticles as an essential building block.

Keywords*:* Molecular dynamics simulation ; Embedded atom method ; Ag nanoparticles ; Au nanoparticles ; Hetero-nanoparticles ; Coalescence ; Sintering

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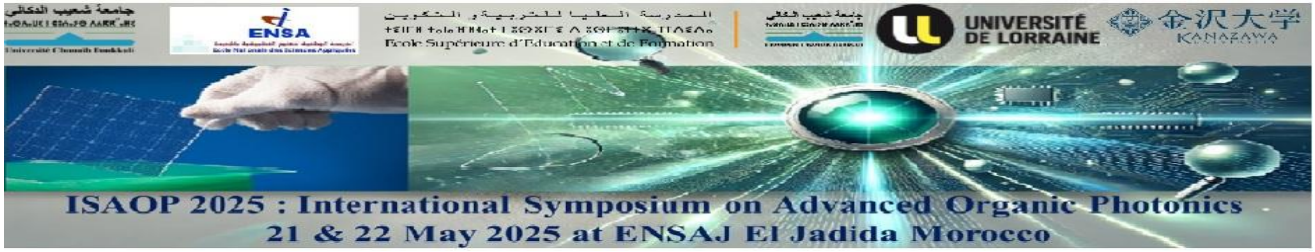
Photonics for Energy



Capacity-Based State of Health Estimation for Lithium-Ion Batteries under Aging Conditions

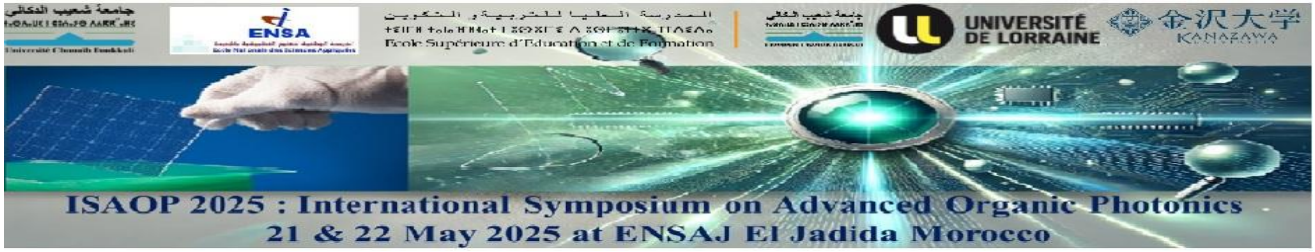
EL KAKE Abdelhadi, LAADISSI El mehdi *

LabSIPE, National School of Applied Sciences, Chouaib Doukkali university, El Jadida, Morocco

* *Corresponding author: elkake.abdelhadi@ucd.ac.ma*

The accurate estimation of the State of Health (SOH) is essential for the safe and reliable operation of lithium-ion batteries, especially in electric vehicles and energy storage systems. This study presents a data-driven framework for SOH estimation based on capacity degradation over aging cycles. By collecting and analyzing real-world aging datasets, the model predicts the remaining usable capacity of the battery as a function of aging indicators such as cycle count, charge-discharge history, and temperature exposure. The proposed approach aims to develop a robust capacity prediction model, which serves as the basis for SOH calculation. Various fitting techniques and machine learning models are evaluated to capture nonlinear degradation trends. This capacity-based method provides a physically meaningful SOH metric, reflecting the battery's ability to store and deliver energy. The methodology is validated using experimental datasets, demonstrating high accuracy and suitability for real-time battery management systems. This work contributes to enhancing battery diagnostics and life prediction, with potential applications in electric mobility and stationary energy systems.

Keywords: Soh estimation Lithium-ion batteries Aging effect Battery performance degradation



Comparative Stability Analysis of TiO_2 and Al_2O_3 Nanofluids Using UV-Vis Spectroscopy Over Extended Storage

Khadija CHAKAR*, Ahmed JASIM, Mahmoud EL MOUDEN, Abdelowahed HAJJAJI1 and Muthanna H. AL-DAHHAN
Laboratory of Engineering Sciences for Energy (LabSIPE). University Research Center (CUR) in Renewable
Energies & Intelligent Systems for Energy "EnR&SIE". National School of Applied Sciences, Chouaib Doukkali University, El Jadida 24000, Morocco.
Multiphase Flows and Reactors Engineering and Education Laboratoty (mFReel), Chemical and Biochemical
Engineering Department, Missouri University of Science and Technology, Rolla, MO, 65409, United States. Department of Nuclear Engineering and Radiation Sciences, Missouri University of Science and Technology, Rolla, MO, 65409, United States.
Technology Development Cell (TechCell), Mohamed VI Polytechnic University (UM6P), Hay Moulay Rachid 43150, Ben Guerir, Morocco.

** Corresponding author: kcct9@umsystem.edu* / chakar.khadija@gmail.com

This study investigates the long-term colloidal stability of nanofluids prepared with TiO_2 and Al_2O_3 nanoparticles using water as the base fluid. Nanofluids were synthesized without the use of surfactants and stored in sealed glass vials under ambient conditions. UV-Visible absorbance measurements were conducted at three-time intervals: immediately after preparation (day 0), after 12 days, and after 3 months. Results revealed a significant decrease in absorbance between day 0 and day 12, indicating initial sedimentation of unstable agglomerates. Interestingly, an increase in absorbance was observed at day 90 in some samples, particularly with Al_2O_3 nanofluids, suggesting natural re-dispersion or a stabilization mechanism over time. Microscopic visual observation showed the formation of filament-like structures reminiscent of micelles, despite the absence of surfactants. This behavior may be attributed to spontaneous nanoparticle self-organization, potentially driven by electrostatic or steric interactions. Comparative analysis between TiO_2 and Al_2O_3 nanofluids showed that while both experienced early sedimentation, Al_2O_3 exhibited a stronger tendency toward long-term stabilization, as reflected by higher absorbance recovery and more visible filamentous structures. These findings suggest that Al_2O_3 nanofluids may offer improved long-term stability under static storage conditions, and that natural re-dispersion phenomena could play a significant role in colloidal recovery without external agitation or additives.

Keywords: Nanofluids, stabilization, UV-Visible absorbance, nanoparticle, base fluid, surfactants.
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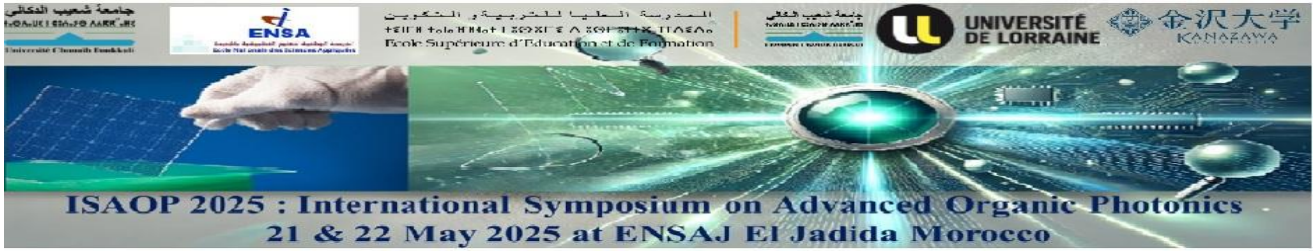

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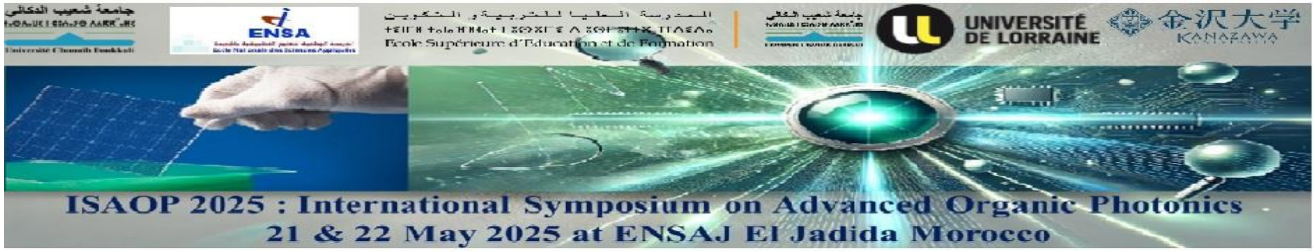

Development and Modeling of Low-Cost Tandem Perovskite/Silicon Solar Cells

Rim Bellarbia, Hassina DERBAL HABAK, Ahmed BENKHALED, Mohammed GUESSASMA, Khaoula FERCHICHI, Mohammed EL GANAOUI, Hicham LABRIM and Aouatif SAAD
Laboratoire des Technologie Innovantes -LTI- équipe MIM -Université de Picardie Jules Verne, France
IUT de l'Oise, Université de Picardie Jules Verne, France 13 Allée de la faïencerie, 60100 Creil, France.
UDSMM - Unité de Dynamique et Structure des Matériaux Moléculaires - Université du Littoral Côté d'Opale, France
LERMAB, Université de Lorraine
ASELab, Advanced Systems Engineering Laboratory, National School of Applied Sciences, Ibn Tofail University, Kenitra, 14000, Morocco

**Corresponding author:* hassina.derbal@u-picardie.fr

For more than half a century, research has been conducted on the development of photovoltaic solar cells based on Schottky diode, organic, hybrid, tandem, and even perovskite cells… in order to find alternatives to fossil fuels. In this optic and in the context of low-carbon energy production, this research focuses on the optimization of a perovskite solar cell. A SCARP simulation is performed and validated by experiments.

Introduction and Objectives: The increasing demand for electricity, the instability of oil prices, and the ongoing climate change crisis necessitate a transition towards renewable energy sources. Current solutions, despite their maturity, face efficiency limitations. To address these challenges, our project aims to develop and model tandem perovskite/silicon solar cells to enhance their efficiency and economic viability. Specifically, we aim to identify perovskite materials that meet predefined criteria for efficiency and stability, develop effective and economical synthesis methods, master all fabrication and testing stages of tandem perovskite/silicon photovoltaic cells, identify and overcome technological barriers, and create and test a prototype cell to validate our research and development efforts

Methodology: We utilized SCAPS (Solar Cell Capacitance Simulator) for modeling, testing various types of perovskites and adjusting parameters such as temperature, thickness, and bandgap to optimize performance. SCAPS simulations guided the physical experiments by predicting the most promising material configurations

Molecular Structure of $FASnI_3$: The molecular structure of $FASnI_3$ (Formamidinium tin triiodide) is characterized by the following composition: FA ($CH(NH_2)_2$) is the organic cation, Sn is the metal cation, and I_3 is the anion.

Influence of Temperature on $FASnI_3$ Performance*: The performance of $FASnI_3$ perovskite was analyzed at different temperatures (300K, 400K, and 500K);*

The data indicates that with increasing temperature, the open-circuit voltage (Voc) decreases significantly, directly impacting the overall efficiency (η). The fill factor (FF) also drops, further reducing efficiency. The short-circuit current density (Jsc) remains relatively stable, suggesting that the carrier collection is less affected by temperature changes.

Conclusion

$FASnI_3$ demonstrates promising potential for use in tandem perovskite/silicon solar cells due to its lead-free composition and reasonable efficiency. Despite the challenges posed by temperature variations, $FASnI_3$ remains a viable and environmentally friendly alternative to lead-based perovskites. Future research will focus on optimizing these parameters to enhance overall cell efficiency, reinforcing $FASnI_3$'s position as a sustainable solution in the development of high-performance tandem solar cells.

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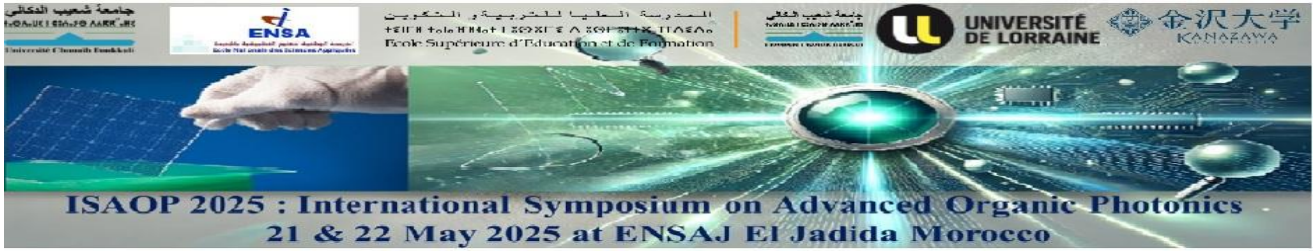
Keywords: Perovskite, Tandem Solar Cells, SCAPS, Efficiency, Environmental Impact, Temperature Influence.



Development of a Stable Ternary Metal Oxide Nanofluid for Heat Transfer Enhancement in Photovoltaic/Thermal Collectors

Khadija CHAKAR*, Ahmed JASIM, Mahmoud EL MOUDEN, Abdelowahed HAJJAJI1 and Muthanna H. AL-DAHHAN

Laboratory of Engineering Sciences for Energy (LabSIPE). University Research Center (CUR) in Renewable

Energies & Intelligent Systems for Energy "EnR&SIE". National School of Applied Sciences, Chouaib Doukkali University, El Jadida 24000, Morocco.

Multiphase Flows and Reactors Engineering and Education Laboratoty (mFReel), Chemical and Biochemical

Engineering Department, Missouri University of Science and Technology, Rolla, MO, 65409, United States.

Department of Nuclear Engineering and Radiation Sciences, Missouri University of Science and Technology, Rolla, MO, 65409, United States.

Technology Development Cell (TechCell), Mohamed VI Polytechnic University (UM6P), Hay Moulay Rachid 43150, Ben Guerir, Morocco.

*Corresponding author: kcct9@umsystem.edu / chakar.khadija@gmail.com

This study investigates the preparation, stability, and heat transfer performance of a novel ternary hybrid nanofluid composed of Fe_2O_3, Al_2O_3, and TiO_2 nanoparticles dispersed in distilled water. The nanofluid is developed as an efficient cooling medium for photovoltaic/thermal (PVT) systems, with the aim of enhancing heat dissipation through improved heat transfer coefficient (HTC). The nanofluid was synthesized using a two-step method without surfactants and homogenized via ultrasonication. Stability was evaluated using UV-Visible spectroscopy, pH measurements, and electrical conductivity, revealing good dispersion behavior and reduced agglomeration due to synergistic effects between the nanoparticles. Experimental evaluation of the heat transfer coefficient was conducted at different volume concentrations (0.1%, 0.3%, and 0.5%) and working temperatures. The ternary hybrid nanofluid exhibited a marked enhancement in HTC compared to mono and binary nanofluids, while maintaining acceptable viscosity levels for effective flow in thermal systems. The results confirm that the Fe_2O_3–Al_2O_3–TiO_2/water nanofluid is a promising candidate for advanced PVT cooling applications, combining strong thermal performance with reliable colloidal stability.

Keywords: Nanofluids, heat transfer, UV-Visible spectroscopy, nanoparticle, distilled water, photovoltaic/therma systems.

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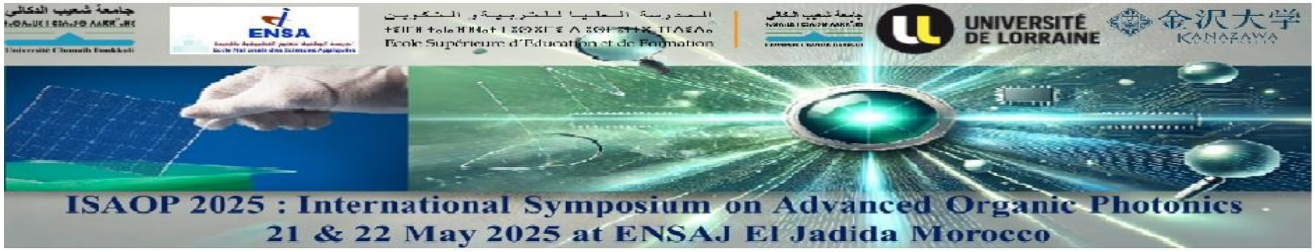
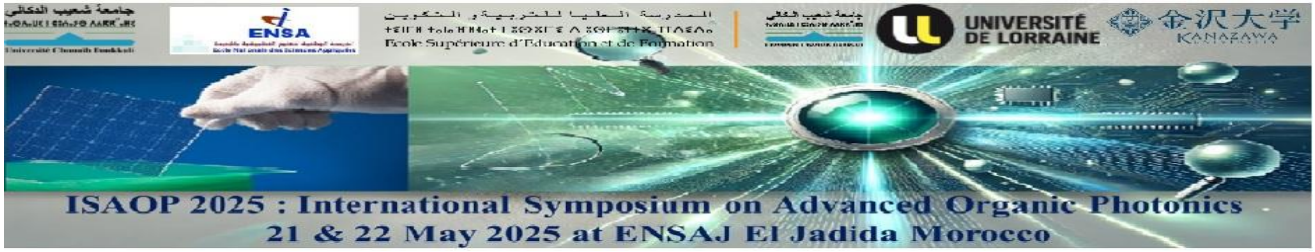


Energy Recovery from Industrial Wastewater Sludge: Challenges Processes, and Sustainable Perspectives

A. HALHALY, L. EL JOUMRI, N. LABJAR*, H. LAOUANE, H. NASRELLAH, H. LABJAR, S. El HAJJAJI
Laboratory of Spectroscopy, Molecular Modeling, Materials, Nanomaterials, Water and Environment, (LS3MN2E-CERNE2D), ENSAM, Mohammed V University in Rabat, Morocco.
Laboratory of Spectroscopy, Molecular Modeling, Materials, Nanomaterials, Water and Environment, (LS3MN2E-CERNE2D), Departmen of Chemistry, Faculty of Sciences, Mohammed V University in Rabat, Morocco.
Higher School of Educating and Training, Chouaib Doukkali University of El Jadida, Morocco.
Laboratory of Membranes, Materials and Environment, Faculty of Sciences and Technologies of Mohammedia, Hassan II University of Casablanca, Morocco.
**Corresponding author:* najoua.labjar@ensam.um5.ac.ma

The management of industrial sludge resulting from wastewater treatment represents a major challenge, both environmentally and economically. These residues, often rich in organic matter but also in potentially toxic compounds, pose complex issues in terms of treatment and disposal. In the context of energy transition and circular economy, the energy recovery of such sludge appears to be a promising pathway. This presentation aims to explore the main available technologies such as anaerobic digestion, incineration, pyrolysis, and gasification. Each process will be analyzed according to its operating principles, implementation conditions, as well as its advantages and disadvantages when applied to industrial sludge. Particular attention will be given to environmental aspects, through a reflection on their integration within a Life Cycle Assessment (LCA) approach. The objective is to provide a global overview of the technical and sustainability-related challenges linked to the energy recovery of these by-products, while identifying current obstacles and optimization levers. Finally, potential strategies will be proposed for integrated management, combining energy recovery, environmental impact reduction, and resource recovery in a sustainability perspective.



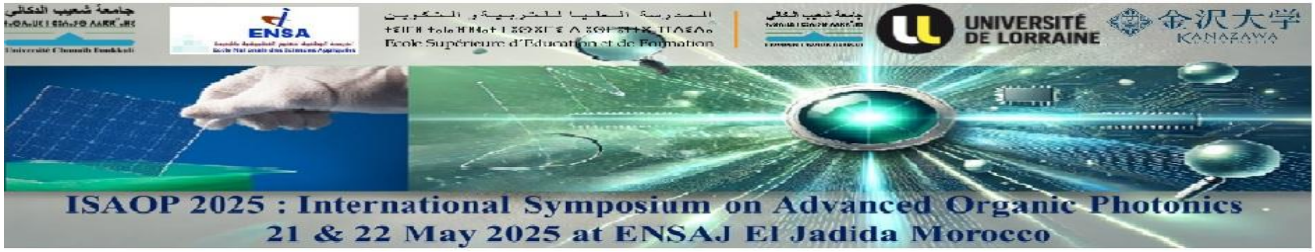
Exploring the potential of 2D Dirac ZrB_2C_2 monolayer as promising anode material for Li-ion and sodium-ion batteries: DFT and AIMD investigation

Ayou ETRINI, Said OUKAHOU, Abdelali.ELOMRANI, Khalid SBIAAI, Abdellatif HASNAOUI

Sultan Moulay Slimane University of Beni Mellal, Polydisciplinary Faculty of Khouribga, LS2ME

**Corresponding author: ayoubetrini@gmail.com*

The design and development of anode materials with high storage capacity, superior stability, ow diffusion barriers, excellent cycle performance, and cost-effectiveness remain critical challenges for advancing the battery industry. In this regard, we explored the 2D material ZrB_2C_2 , which exhibits Dirac cone states, as a potential anode for Li-ion and Na-ion batteries through ab-initio calculations. The results highlight that this material is energetically, thermally, and dynamically stable. By examining the adsorption energy of alkali atoms on the monolayer surface, we identified the most stable sites for lithium and sodium ion accommodation. Moreover, alkali metal ions demonstrated high diffusivity on the ZrB_2C_2 monolayer, with low migration energy barriers of 0.59 and 0.32 eV for Li and Na respectively. Additionally, ZrB_2C_2monolayer demonstrates high ionic and electronic conductivity, and excellent structural stability during the Li/Na loading process with a very small change of 0.85% and 1.91% in the cell parameters, respectively. Moreover, the ZrB_2C_2 monolayer exhibits optimal voltage and high specific capacities of 1028.02 m.A.hg^{-1} for Li storage and 489.53 $m\ A\ hg^{-1}$ for Na storage. These remarkable properties demonstrate that the 2D ZrB_2C_2 holds great potential as an anode material for lithium/ sodium-ion batteries.

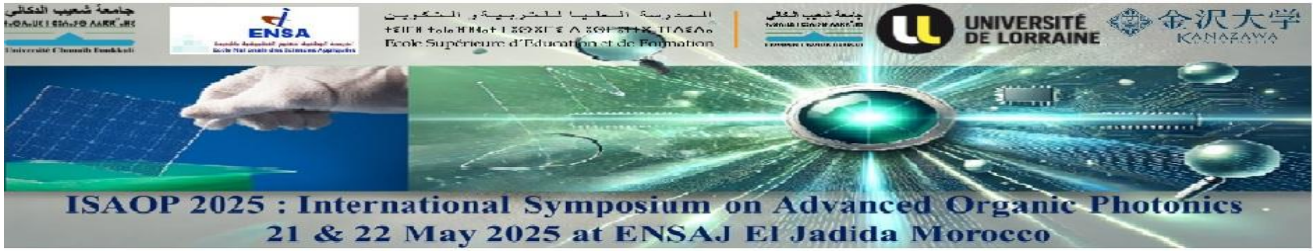


Harnessing Intelligence for Solar Forecasting: ML vs DL Approaches in PV Output Prediction

Oussama KHOUILI*, Mohamed HANINE and Mohamed LOUZAZNI
LTI Laboratory, National School of Applied Sciences, Chouaib Doukkali University, El Jadida 24000, Morocco.
Science Engineer Laboratory for Energy, National School of Applied Sciences, Chouaib Doukkali University of El Jadida, Morocco.

Accurate prediction of photovoltaic (PV) power output is essential for optimizing solar energy integration and grid stability. In this study, we conduct a comparative analysis of traditional machine learning (ML) models and advanced deep learning (DL) architecture for short-term PV output prediction. A comprehensive dataset comprising historical weather and irradiance data was used to train and evaluate various models, including Linear Regression,Decision Trees, and Support Vector Regression on the ML side, and Multilayer Perceptrons (MLP), Long Short-Term Memory (LSTM) networks, and Convolutional Neural Networks (CNN) among DL approaches. The models were assessed using standard performance metrics such as Mean Squared Error (MSE), Root Mean Squared Error (RMSE), Mean Absolute Percentage Error (MAPE), and R-squared (R^2). Our results highlight the strengths and limitations of each paradigm, showing that while DL models generally outperform ML models in capturing nonlinear patterns and temporal dependencies, they require more computational resources and longer training times. This paper offers practical insights into selecting appropriate modeling strategies based on data characteristics, prediction horizons, and operational constraints in PV systems.

Keywords: Photovoltaic Output Prediction, Solar Energy Forecasting, Machine Learning, Deep Learning, Time Series Analysis



High-efficiency Pb Recovery from Perovskite Solar Cells via Ion Exchange Resin

Ruka Yazawa, Md. Shahiduzzaman, Masahiro Nakano, Makoto Karakawa, Jean Michel Nunzi, Hiroshi Hasegawa, Tetsuya Taima*
Graduate School of Natural Science and Technology, Kanazawa University,
Nanomaterials Research Institute, Kanazawa University,
Graduate School of Frontier Science Initiative, Kanazawa University,
Kakuma-machi, Kanazawa 920-1192, Japan
Department of Physics, Engineering Physics and Astronomy, Queens University, Kingston, ON K7L 3N6, Canada
**E-mail : shahiduzzaman@se.kanazawa-u.ac.jp ; taima@se.kanazawa-u.ac.jp*

Organic-inorganic hybrid perovskite solar cells (PSCs) are remarkable for next-generation low-cost photovoltaic technology. They have demonstrated power conversion efficiency (PCE) over 26.5 % for single-junction solar cells[1]. Lead (Pb) is used in the perovskite layer, and its leakage during PSC disposal poses environmental and health risks. As PSCs are thin-film solar cells on plastic substrates, recovery procedures from silicon solar cell technology are not applicable. Recent studies report on recovering substrates and metals [2,3], particularly Pb from PSCs. However, investigations into complete Pb recovery from organic solvents remain limited. This study aims to achieve 100% Pb recovery from PSCs by decomposing devices in solvents and using cation exchange resins. PSCs were decomposed by immersion in solvents such as chlorobenzene, ethanol, and dimethylformamide (DMF). Gold electrodes detached during chlorobenzene immersion with ultrasonic cleaning. After solvent removal, residual materials were dissolved and treated with nitric acid for analysis. Inductively coupled plasma atomic emission spectroscopy (ICP-AES) quantified Pb and other elements. To ensure complete Pb recovery, weakly acidic cation exchange resins modified with carboxyl groups were added to chlorobenzene and DMF solutions. ICP-AES results showed 100% Pb recovery from chlorobenzene and 99.57% from DMF. These findings demonstrate an effective technique for recovering Pb from PSCs. Optimizing solvents and Pb recovery at high concentrations could enhance efficiency.

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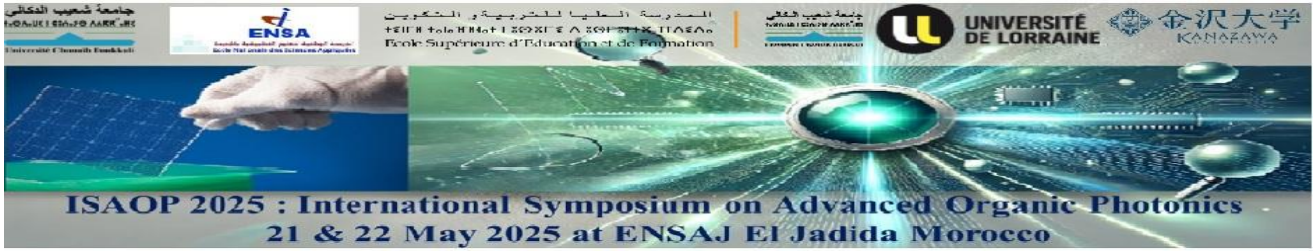

Highly Stable Perovskite Solar Cells via Controlled Intercalation of Cesium Halides into the $MAPbI_3$ Framework

O(D3) Y. Feng, M. Shahiduzzaman*, M. Nakano, M. Karakawa, J. Nunzi1, T. Taima* (1. Kanazawa Univ., 2. Queen's Univ.)
**Corresponding author: shahiduzzaman@se.kanazawa-u.ac.jp, taima@se.kanazawa-u.ac.jp*

【Introduction】 Perovskite solar cells (PSCs) have achieved power conversion efficiencies of up to 26.1%, yet their limited stability remains a major obstacle to commercialization. In contrast, silicon-based photovoltaics last over 25 years, whereas perovskites typically degrade within a year. Enhancing stability through material composition and structural modifications is crucial for practical applications. Methylammonium lead iodide ($MAPbI_3$) is widely used in PSCs due to its tunable bandgap and high absorption coefficient but degrades under light and heat. Stability improvements include substituting the A-site cation (MA^+) with Cs^+ or Rb^+ and replacing the X-site halide (I^-) with Cl^- or Br^-. Halogen doping enhances PSC stability by reducing lattice spacing, improving grain sizes, and slowing degradation. Cl^- and Br^- doping also improves conductivity, suppresses recombination, and enhances long-term stability **[1], [2]**. According to the previous research, our team successfully intercalated CsI into $MAPbI_3$, achieving 18.43% efficiency with over 80% retention after eight months **[3]**. In this study, we introduced vacuum-deposited CsX (CsCl, CsBr, CsI) thin layers for precise intercalation, enhancing perovskite morphology, grain size, and thermal stability. Experimental results show that CsX-intercalated PSCs maintain high efficiency under prolonged exposure to heat, humidity, and light, demonstrating the potential of CsX intercalation for stable and efficient PSCs. **【Method】** The cleaned FTO substrates underwent 20 minutes of plasma treatment. Compact TiO_2 /anatase TiO_2 was then synthesized as the electron transport layer via spin-coating. For double-layer intercalation, a 5 nm CsX layer was first evaporated onto anatase TiO_2, followed by spin-coating a $MAPbI_3$ film and annealing at 140 °C for 10 minutes. Another 5 nm CsX layer was then deposited onto the perovskite film, followed by a second annealing at 140 °C for 30 minutes. Finally, Spiro-OMeTAD was spin-coated, and a 100 nm Au electrode was deposited to complete device fabrication **【Results and Discussion】** As shown in Fig. (a), CsX intercalation improved perovskite morphology, increasing grain size from 250 nm to 600 nm. PSCs with CsX-intercalated films exhibited enhanced stability, retaining over 90% efficiency after 120 minutes of 1 sun illumination (Fig. b) and 80% after 3000 hours at 50%-60% humidity (Fig. c). These findings highlight CsX intercalation as an effective strategy for PSCs. In summary, Cl and Br doping, along with Cs^+ incorporation, enhance perovskite crystal structure and charge transport, reduce defects, optimize the band structure, and improve photoelectric efficiency. Additionally, they enhance moisture and thermal stability, extend PSC lifespan, and support commercialization. **【Conclusions】** The incorporation of vacuum-deposited CsX layers facilitated precise intercalation within $MAPbI_3$ films, leading to enhanced morphological properties and improved stability. This method significantly enhanced the thermal, light, and moisture resistance of

PSCs, providing a promising strategy for the development of more stable and efficient photovoltaic devices.

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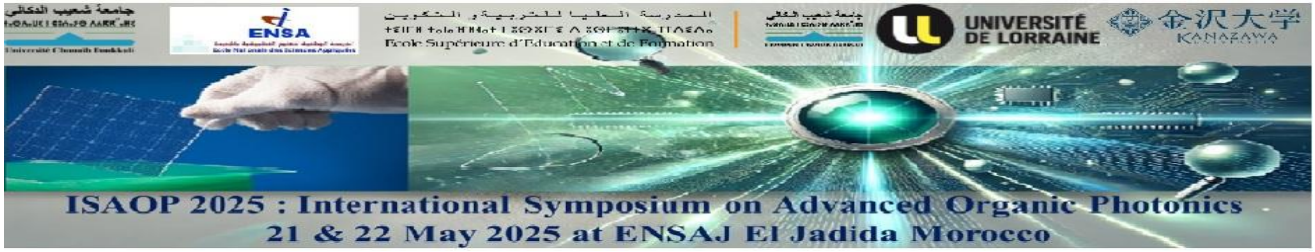
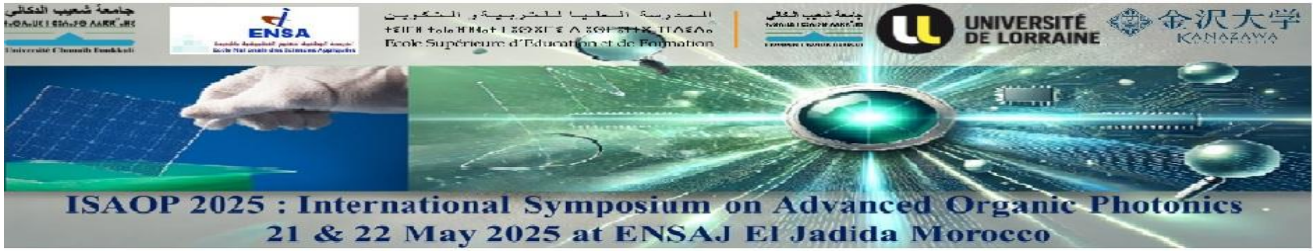


Hybrid Energy Systems: Management Approaches and Critical Analysis

Youssef EL MRINI, Jamal ZEROUAOUI, Badia ETTAKI
Materials and Subatomic Physics Laboratory University of sciences, kenitra,Morocco
Materials and Subatomic Physics Laboratory University of sciences, kenitra,Morocco
School of Information Science Rabat, Rabat, Morocco
*Corresponding author: yousssef.elmrini@uit.ac.ma

Combining solar, wind, diesel, and storage units offer a resilient and sustainable solution to the growing energy demands of remote and urban areas. Yet, managing such diverse sources poses significant challenges due to variability, intermittency, and the complicated interaction between generation and consumption. This paper presents a critical overview of hybrid energy system (HES) management approaches, starting with rule-based strategies to advanced optimization and machine learning techniques. Traditional methods, while simple and intuitive, often lack adaptability and scalability. Conversely, model predictive control (MPC), metaheuristic algorithms, and reinforcement learning frameworks demonstrate remarkable potential for dynamic decision-making and real-time optimization. We analyze the strengths, limitations, and application contexts of each method, highlighting emerging trends towards autonomous, self-learning energy management systems. Summarizing recent advancements, this work could be a base study to guide researchers and practitioners towards optimal design, and more efficient hybrid systems adapted to future energy perspectives.

Keywords: Hybrid Energy Systems (HES), Energy Management, Optimization Algorithms, Model Predictive Control (MPC), Machine Learning, Renewable Energy Integration, Microgrids, Sustainable Energy.



Impact of PbI_2 and A-site Solution Annealing on Perovskite Solar Cell Performance via Vacuum-Assisted Spin Coating

Peng Liu, Md. Shahiduzzaman*, Yue Feng, Neng Hani Handayani, Takeshi Gotanda, Jean Miche Nunzi and Tetsuya Taima*
Graduate School of Frontier Science Initiative, Kanazawa University, Kakuma, Kanazawa 920-1292, Japan
Nanomaterials Research Institute, Kanazawa University, Kakuma, Kanazawa 920-1192, Japan
Graduate School of Natural Science and Technology, Kanazawa University, Kakuma, Kanazawa 920-1192, Japan
Toshiba Energy Systems & Solutions Corporation, Kawasaki, Kanagawa 212-8585, Japan
Corporate Research & Development Centre, Toshiba Corporation, Kawasaki, Kanagawa 230 0024, Japan
Department of Physics, Engineering Physics and Astronomy, Queens University, Kingston K7L 3N6, Ontario, Canada

**Corresponding author:* *shahiduzzaman@se.kanazawa-u.ac.jp, taima@se.kanazawa-u.ac.jp*

【**Introduction**】The quality of the perovskite layer is crucial for fabricating highly efficient and stabl perovskite solar cells (PSCs). Among two-step methods, the evaporation-assisted spin coating technique is an effective method for achieving high-quality perovskite layers [1]. However, a deeper understanding of the interaction between the PbI2 film and A-site solution is essential for optimizing the perovskite layer formation. This study investigates the impact of different annealing durations on the formation of MAPbI3 ($CH_3NH_3PbI_3$) perovskite layers from vacuum-deposited PbI2 films and A-site solutions. PSCs utilizing non-annealed PbI2 films showed significantly improved open-circuit voltage and fill factor, resulting in higher device performance. Additionally, heating the A-site solution enhances ion activity, promoting more effective MAI penetration and full conversion with PbI2. 【**Materials and Method**】A self-assembled monolayer (SAM, 2PACz) was deposited on an ITO glass substrate as the hole transport layer following Al-Ashouri et al [2]. A 100 nm PbI_2 film was then deposited via vacuum evaporation (0.4 Å/s, 3×10^{-6} Pa) and annealed at 250 °C for varying durations (0 s to 30 min). Methylammonium iodide (MAI, 0.063 M in IPA) preheated to 70 °C was spin-coated onto the PbI_2 film (0 rpm for 5 s, then 3000 rpm for 30 s) and annealed at 100 °C for 10 min. A passivation layer of 2-Phenylethylammonium iodide (PEAI, 1.2 mg/mL in IPA) was applied via spin-coating (3000 rpm, 30 s). The electron transport layer consisted of sequentially evaporated 25 nm C_{60} (0.4 Å/s) and 5 nm BCP (0.3 Å/s), with BCP also serving as a buffer layer. A 120 nm Ag (0.5 Å/s) was deposited via vacuum evaporation. 【**Results and Discussion**】Figure 1(a) and (b) show XRD patterns of $MAPbI_3$ layers formed on PbI_2 films annealed for different durations, comparing heated and unheated MAI solutions. All samples exhibit characteristic perovskite peaks, Longer PbI_2 annealing increases grain size, reducing perovskite crystallinity and enhancing the PbI_2 (001) peak, indicating more unreacted PbI_2 . A highly crystallized PbI_2 layer hinders MAI intercalation, restricting perovskite growth. Unheated MAI results in stronger PbI_2 (001) peaks due to slower ion diffusion, while heating

enhances reactivity, improving perovskite quality. Figure 1(c) shows the J–V curves, where unannealed PbI_2 devices achieve the highest PCE (11.59%) with Jsc = 17.79 mA/cm², Voc = 0.97 V, and FF = 0.67. Prolonged annealing (>10 min) reduces current density due to PbI_2 grain growth and film fracture, leading to poor charge transport. Figure 1(d) presents PCE box plots, showing a decline from ~10% (0 s) to <3% (30 min), attributed to hindered MAI infiltration and increased recombination losses.

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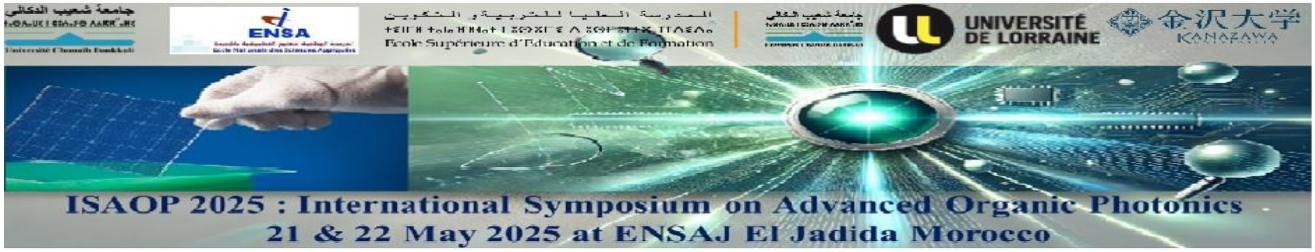
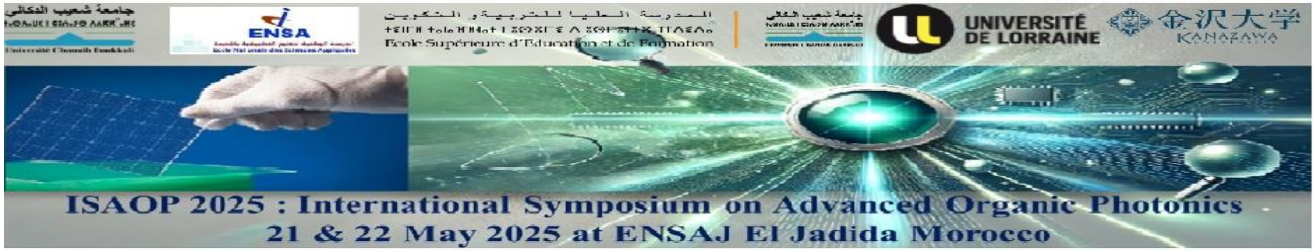


Numerical Investigation of highly efficient and new low cost absorber material Ag2GeS3 using SCAPS 1D

Assia CHOUCHNA*, Kaoutar ELGOUMIRI , Abdelaziz LABRAG , Mohammed KHENFOUCH, Halima CHARKAOUI , BGHOUR Mustapha
Laboratory of Materials, Electrical Systems, Energy and Environment (LM3SE), Materials and Energy Engineering team, Faculty of Applied Sciences, Ait Melloul, Ibn Zohr University, Morocco – Morocco
UNISA-UNESCO Africa Chair in Nanosciences-Nanotechnology, College of Graduate Studies,University of South Africa, Muckleneuk ridge, Pretoria, PO Box 392 – South Africa
Laboratory of Physics of Condensed Matter and Nano-Materials for Renewable Energies, Ibn Zohr University, Agadir, Morocco. – Morocco

**Corresponding author: assia.chouchna.04@edu.uiz.ac.ma*

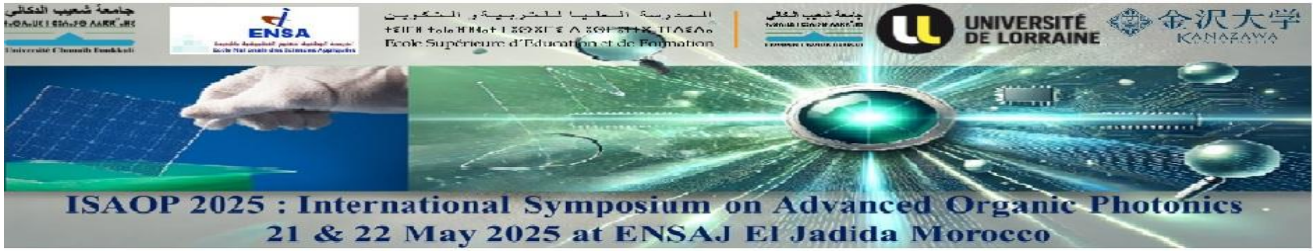


Recyclable Emulsion Liquid Membranes for Nickel Recovery from Synthesized Phosphoric Acid: Performance, Stability, and Reusability

Yousef HAFEZI, Nouhalia FILALI, Muthanna AL-DAHHAN*
Multiphase flow and Reactor Engineering, Applications and Education Laboratory (mFReael), Linda and Bipin
Doshi Department of Chemical and Biochemical Engineering, Missouri University of Science and Technology, Rolla, MO 65409, USA
Applied Chemistry and Engineering Research Center of Excellence (ACER CoE), Mohammed VI Polytechnic University (UM6P), Lot 660, Hay Moulay Rachid 43150, Ben Guerir, Morocco
Department of Mining and Nuclear Engineering, Missouri University of Science and Technology, Rolla 65409, MO, United States
**Corresponding author:* aldahhanm@mst.edu.

The removal of heavy metals from acidic waste streams remains an important challenge in the chemical process industry. In this work, emulsion liquid membranes (ELMs) were investigated for the recovery of Nickel ions from synthesized phosphoric acid under strongly acidic conditions. Two carrier agents−Alamine-336 and D2EHPA−were evaluated in combination with Soltrol 220 and kerosene as diluents. Operational parameters such as carrier concentration, solvent type, and emulsion-to-feed phase ratios were optimized based on preliminary trials and literature recommendations. Alamine-336 demonstrated superior extraction efficiency and membrane robustness compared to D2EHPA. A membrane leakage method based on pH monitoring was used to evaluate emulsion stability and assess performance over multiple extraction cycles. Nickel recovery efficiency remained high across repeated tests, with minimal loss in emulsion integrity, confirming the potential of the system for recyclable operation. These findings support the use of Alamine-336-based ELMs as a promising platform for sustainable heavy metal recovery from industrial acidic solutions.

Keywords: Emulsion Liquid Membrane, Carrier, Heavy Metal Removal, Phosphoric Acid, Nickel



Roll-to-Roll Compatible Ionic Liquid-Assisted Perovskite Film Fabrication in Ambient Air for Highly Stable Solar Cells

Yugo Nakahara, Md. Shahiduzzaman* Ryo Nishiyama, Masahiro Nakano, Makoto Karakawa, Shiro Ikuhara3, Kenji Omote, Kozo Kotani, Jean Michel Nunzi, Kohshin Takahashi, Tetsuya Taima*

Graduate School of Natural Science and Technology, Kanazawa University, Kakuma, Kanazawa 920-1192 Japan

Nanomaterials Research Institute, Kanazawa University, Kakuma, Kanazawa 920-1192, Japan

Reiko Co. Ltd.

Graduate School of Frontier Science Initiative, Kanazawa University, Kakuma, Kanazawa

920-1192, Japan

Design Solar Co. Ltd.

Department of Physics, Engineering Physics and Astronomy, Queens University, Kingston,

ON K7L 3N6, Canada

**Corresponding author: shahiduzzaman@se.kanazawa-u.ac.jp; taima@se.kanazawa-u.ac.jp*

Organic-inorganic hybrid halide Perovskite solar cells (PSCs) has received increasing attention due to their light weight, flexibility and solution-based processing. On the other hand, PSCs have low atmospheric stability and it restrict the fabrication environment to an inert atmosphere, making them difficult to produce at low cost. Previous studies showed that the addition of ionic liquid (IL) significantly improves the hydrophobicity of perovskite layer and prevent the decomposition during thin-film fabrication in ambient air [1, 2]. While the fabrication of perovskite layers under ambient conditions has been actively studied, IL-aided PSC fabrication without a glovebox remains largely unexplored.In this study, we mixed 1-hexyl-3-methylimidazolium chloride in cesium-formamidinium-methylammonium (termed as CsFAMA) perovskite as IL and we obtained large crystal domains in ambient conditions (40% humidity) using the bar-coating technique. It is a preparatory stage to future roll-to-roll processing, thereafter improving the device stability. In addition, IL molecules in the perovskite solution protect the perovskite from interacting with water and realized fabrication at ambient condition. The reference IL-aided-perovskite films fabricated by spin-coating decreased 20% of their initial efficiency after 1000h, while the IL-aided perovskite films deposited by the bar-coating technique kept over 90% of their initial efficiency after 1200 h storage in dark at ambient under a relative humidity in the 40-50% range(Fig.a) This is because the spin-coating method produces crystals as small as a few hundred nm, whereas the bar-coating method produces crystals as large as several tens of μm (Fig.b, c). Moreover, the IL-assisted CsFAMA film shows the superior hydrophobicity of the IL-aided CsFAMA perovskite with contact angle of 78.6°, despite pristine CsFAMA perovskite layer demonstrated lower hydrophobicity with

water contact angle of 68.8°. Improve hydrophobicity of the IL aided- perovskite film indicates water-registant, which with larger crystal domains improves the stability under ambient air conditions of the resulting devices.

Acknowledgement: This work was supported by WISE Program of Kanazawa University b MEXT

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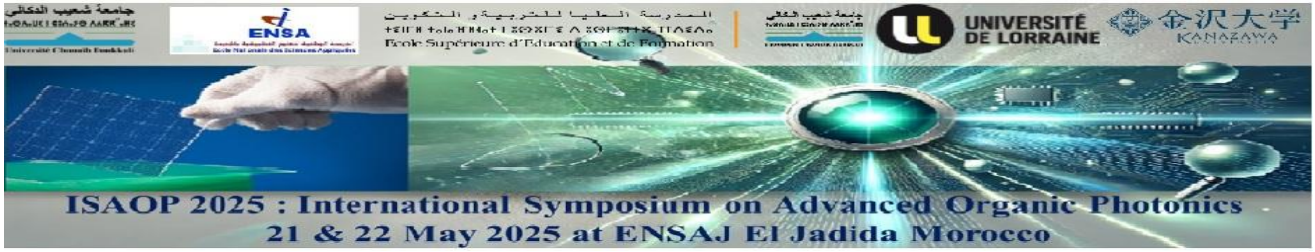

Simulation and characterization perovskite solar cell based on MASnI3 using SCAPS-1D

Hamza AFAK∗, Moloud DARDOURI, Abdellatif HASNAOUI, and Khalid SBIAAI

1LS2ME Laboratory, Sultan Moulay Slimane University of Beni Mellal, Polydisciplinary Faculty of Khouribga – Morocco

**Corresponding author: hzwest123@gmail.com / k.sbiaai@usms.ma*

The solar cell is the backbone of modern renewable energy technologies, offering a clean and sustainable alternative to traditional power sources. Perovskite solar cells, particularly those based on materials like methylammonium tin iodide MASnI3, are renowned for their high efficiency and low production costs. This study presents a comprehensive simulation and characterization of perovskite solar cells (PSC) based on MASnI3, using SCAPS-1D software, with a focus on the NIP device configuration as the optimal structure1. We studied the ideal materials of each layer2¯3; including the back contact, electron transport layer (ETL) and hole transport layer (HTL), and their contribution to achieving higher efficiencies. Our research identified an ideal structure consisting of FTO-ZnO-MASnI3-Cu2O-Pt. Furthermore, we examined the device's electrical and optical properties by varying key parameter such as thickness, gap, doping concentration, interface defects, etc..., along with the effect of temperature on these factors. The results show an optimization potential with an efficiency reaching up to 31,55% under ideal simulated conditions. Additionally, electron-hole recombination was not identified as a significant factor in our simulation. Our findings indicate that MASnI3 based solar cells not only demonstrate impressive performance metrics but also provide insights into design improvements for increased stability and efficiency in renewable energy applications.

Keywords: MASnI3 absorber, Perovskite solar cell, SCAPS 1D simulation, electron transport layer,

hole transport layer

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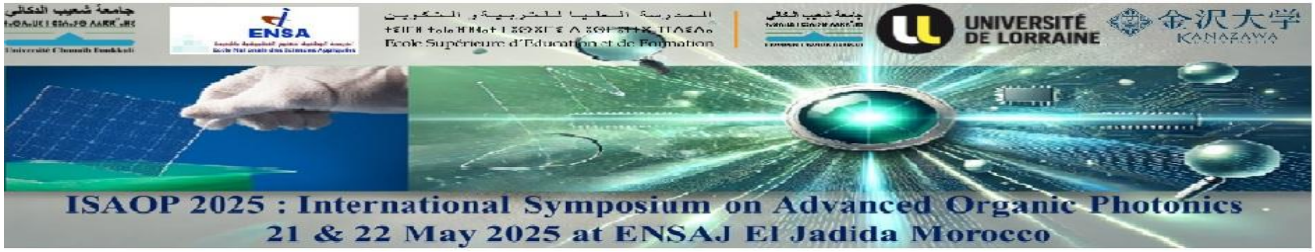


Sustainable Energy Storage Materials and Circular Economy

Bouchra BELAHRACH, Najoua LABJAR * and Souad EL HAJJAJI

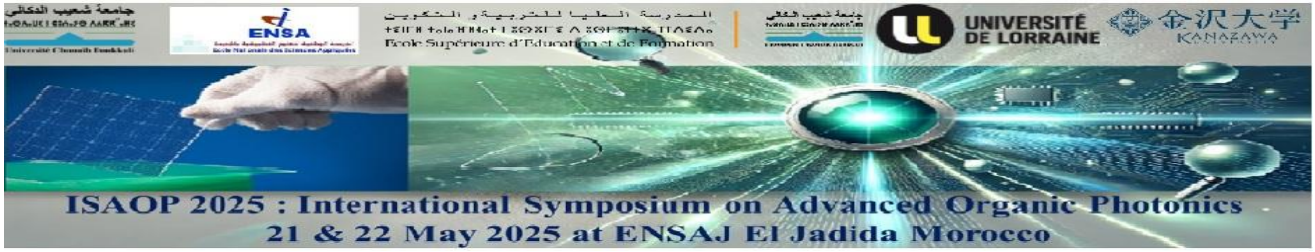
Laboratory of Molecular Spectroscopy Modelling, Materials, Nanomaterials, Water and Environment, CERNE2D, ENSAM, Mohammed V University in Rabat, Morocco ;

Laboratory of Molecular Spectroscopy Modelling, Materials, Nanomaterials, Water and Environment, CERNE2D, Faculty of Science, Mohammed V University in Rabat, Morocco ;

*Corresponding author: najoua.labjar@ensam.um5.ac.ma

The increasing energy usage and environmental concerns have led to a surge in research on sustainable energy storage materials. Currently, as lithium-ion batteries dominate the market, inquiries over the sustainability of these technologies are beginning to arise. Consequently, scientists are seeking alternatives by utilizing more abundant, eco-friendly elements such as salt, potassium, or zinc. Additional storage techniques under investigation include supercapacitors, enabling rapid charging and extended lifespan; flywheels that transform energy into mechanical rotation; and thermal storage utilizing phase-change materials. The circular economy plays a crucial role in this field. The sustainability of storage systems is evaluated through life cycle evaluation. They are formulating techniques for the reutilization and recycling of batteries to mitigate such problems. This study concentrates on the development of innovative materials and systems that enhance resource efficiency within a life cycle framework, facilitating a more sustainable approach to energy storage.

Keywords: Energy storage, life cycle assessment, circular economy, sustainable materials, renewable energy



Toward Efficient and Sustainable Lead-Free Perovskite Solar Cells: Thickness Optimization of $CH_3 NH_3 SnI_3$ Absorber Layer

M.Farajy, N. EL Ghyati,A.Mortadi,A.EL Mellouky,R.EL Moznine,M.EL Mouden

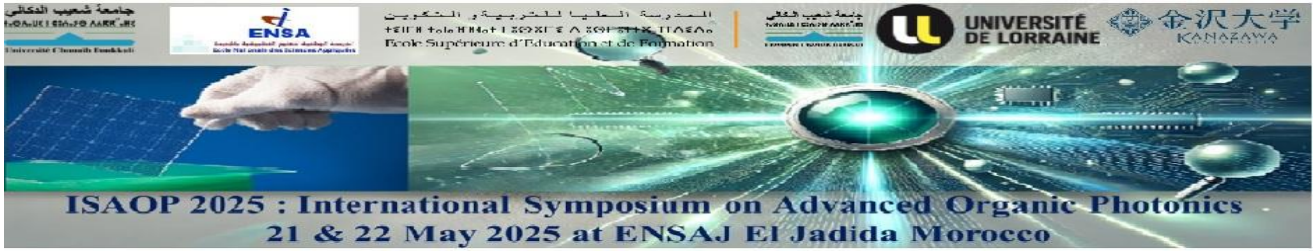
Laboratory of Engineering Sciences for Energy (LabSIPE). University Research Center (CUR) in Renewable Energies & Intelligent Systems for Energy "EnR&SIE". National School of Applied Sciences, ChouaibDoukkali University, El Jadida – Morocco

Laboratory Physics of Condensed Matter (LPMC). University Research Center (CUR) in Renewable Energies & Intelligent Systems for Energy "EnR&SIE". Faculty of Sciences, ChouaibDoukkaliUniversity, El-Jadida, Morocco

** Corresponding author: Farajy.mohammed@ucd.ac.ma –mohammedfarajy@gmail.com*

This study examines the impact of the absorber layer thickness of $CH_3 NH_3 SnI_3$ on the performance of a perovskite solar cell with the structure ZnO/$CH_3 NH_3 SnI_3$ /NiOx/Au. Using SCAPS-1D software and electrochemical impedance spectroscopy, key photovoltaic parameters (Voc, Jsc, FF, η) were analyzed for absorber thicknesses ranging from 100 to 1200 nm. Our analysis shows that a thickness of **900 nm** is optimal for achieving the best efficiency, with the cell exhibiting a **Voc of 1.2041 V**, **Jsc of 34.68 mA/cm²**, and **FF of 86.42%**, resulting in an efficiency of **36.01%**. Impedance analysis, conducted over a wide frequency range from **10^{-3} Hz to 10^{9} Hz**, highlights the influence of thickness on recombination resistance and junction capacitance. These findings underscore the importance of precise optimization in the development of efficient and sustainable lead-free perovskite solar cells.

Keywords: Perovskite solar cell, NiOx, $CH_3NH_3SnI_3$, ZnO, Layer thickness optimization, SCAPS-1D, impedance spectroscopy dielectric.



Treatment of colored effluents by adsorption on Ca10(PO4)1.5(VO4)4.5(OH)2: the case of Methylene Blue, Carmine Indigo and RR14 Red

Fatima Zahra CHAJRI, Meryem BENSEMLALI, Asmaa SANAD, Meryeme JOUDI, Abdelatif AARFANE, Mohamed MONKADE, Mina BAKASSE, Hamid NASRELLAH

Laboratory of Organic Bioorganic Chemistry and Environment, Faculty of Sciences, University Chouaib Doukkali, El Jadida, Morocco.

Higher School of Education and Training, University Chouaib Doukkali, El Jadida, Morocco.

Physics of Condensed Matter Laboratory, Physics Department, Faculty of Science, Chouaib Doukkali University, El Jadida, Morocco

*Corresponding author: chajri.f@ucd.ac.ma

Water purification has become a global priority because of the scarcity of resources and the intensification of pollution linked to urbanisation and industrialisation [1,2]. Among the major pollutants are industrial dyes, mainly from the textile, food and printing industries. Azo dyes, which are widely used (around 700,000 tonnes produced per year, 70% of which in the textile industry), are of particular concern because of their persistence in the environment [3,4]. It is therefore crucial to develop effective and economical methods for eliminating them. Several textile wastewater treatment techniques have been studied, such as coagulation, membrane separation, photo- and electro-degradation. Of these, adsorption stands out for its simplicity, low cost and effectiveness in eliminating contaminants [5]. For this study, we carried out tests on three dyes: reactive anionic type RR141 and cationic type BM. We examined key factors such as dye concentration, pH, adsorbent mass and time. To analyse these factors in depth, we used central composite design (CCD) to enhance Ca10(PO4)1.5(VO4)4.5(OH)2 as an effective adsorbent for dye removal. In addition, to measure the correlation between dye concentration and the amount adsorbed, our experiments also involved a thorough examination of the adsorption isotherms and an assessment of the thermodynamics of the adsorption process.

Keywords: Adsorption, Isothermes, Thermodynamics, Ca10(PO4)1.5(VO4)4.5(OH)2, Dyes.

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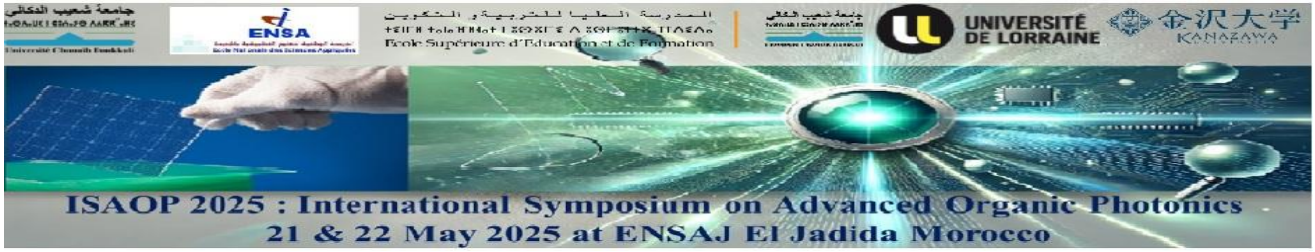

Vacuum-Deposited RbI for Large-Grained, High-Crystallinity, and Stable Perovskite Solar Cells

(D2) N. H. Handayani, Md. Shahiduzzaman*, Y. Feng, Y. Higashi, M. Nishimoto, M. Nakano, M. Karakawa, J. M. Nunzi, T. Taima*

Kanazawa University 1, Iwatani Industry Co., Ltd.2

**Corresponding author: shahiduzzaman@se.kanazawa-u.ac.jp, taima@se.kanazawa-u.ac.jp*

【Introduction】 Hybrid organic-inorganic metal halide perovskite solar cells (PSCs) exhibit high efficiency ; however, their stability limitations hinder their large-scale implementation. A widely used perovskite material in PSCs, MAPbI3 (CH3NH3PbI3), shows excellent charge mobility, tunable bandgap, and suitability for low-temperature processing. However, MAPbI3 is prone to degradation in the presence of water molecules, leading to the formation of PbI2 and CH3NH3I. This instability is mostly attributed to the reactivity of the organic A-site cation, MA+ (CH3NH3 +), to form hydrogen bonds with H2O molecules, causing the 3D perovskite (CH3NH3PbI3) to degrade into 2D sheets separated by water (CH3NH3PbI3·H2O) and isolated PbI6 4- octahedral [1]. To enhance stability, the unstable organic A-site of MAPbI3 is partially incorporated by more stable inorganic A-site materials, such as RbI (rubidium iodide). In contrast to MA+, Rb+ are unable to form hydrogen bonds with water molecules, reducing their sensitivity to water-induced degradation. However, the limited solubility of RbI presents challenges in controlling its composition within the perovskite film, particularly when using the solution method. To address this limitation, our lab previously developed a CsI intercalation technique combining vacuum deposition and solution methods, allowing precise control of inorganic Cs composition. This technology significantly improved grain size and crystallinity, resulting in highly stable perovskite solar cells (PSCs). Given the smaller ionic radius of Rb+ (1.61 Å) compared to Cs+ (1.74 Å), it offers a higher incorporation probability, thereby further enhancing film quality and stability. In this work, we first introduced a thin RbI film utilizing the vacuum deposition method on both sides of the solution-deposited MAPbI3 interfaces with the electron transport layer (ETL) and hole transport layer (HTL) (denoted as ETL/RbI-MAPbI3-RbI/HTL) and investigated its effects on the properties of the perovskite film and the stability of PSCs. **【Method】** TiO2 compact layer and anatase TiO2 nanoparticles were spin-coated onto FTO-patterned glass. Perovskite films were prepared by vacuum-depositing 10 nm RbI on the TiO2, followed by spin-coating 1.5 M MAPbI3 with chlorobenzene as anti-solvent and annealing at 100 ℃ for 10 min. Another 10 nm RbI was deposited on top of MAPbI3 and annealed at 140 ℃ for 30 min. Spiro-OMeTAD was spin-coated on the perovskite, followed by 100 nm Au deposition using vacuum deposition. **【Results and Discussion】** Surface morphology of pristine MAPbI3 and ETL/RbI-MAPbI3-RbI/HTL films are shown in **Fig. 1a-b**. The results reveal that the incorporation of RbI into MAPbI3 resulted in denser films with larger grain sizes. The *J-V* curves for PSCs utilizing MAPbI3 and ETL/RbI-MAPbI3-RbI/HTL films are presented in **Fig. 1c**. The PSCs with the

ETL/RbI-MAPbI3-RbI/HTL film demonstrated improved performance (reverse scan: 17.50%) compared to those with pristine MAPbI3 (reverse scan: 14.81%). The increase in *Voc* and FF values is due to improved grain size and crystalline, reducing trap density and recombination at grain boundaries. For moisture stability investigation, unencapsulated PSCs were stored in the dark under ambient air with 40-55% relative humidity. After more than 2300 hours, the power conversion efficiency (PCE) of PSCs with ETL/RbI-MAPbI3-RbI/HTL remained over 95% of the initial value, whereas the reference device decreased to 60%, as shown in **Fig. 1d.** The hydrogen bonds formed between the MA functional group and water molecules altered the structure of MAPbI3, resulting in the formation of PbI2 and MAI. In contrast, Rb-incorporated MAPbI3 exhibits enhanced hydrophobicity, attributed to reduced hydrogen bonding within the perovskite structure due to the presence of Rb. Therefore, this work presents new strategies for the development of highly stable PSCs through the precise incorporation of RbI into MAPbI3 films, offering potential applications in other perovskite-based devices. **【Conclusions】** PSCs with ETL/RbI-MAPbI3-RbI/HTL as the perovskite film with a large grain size were successfully fabricated, achieving a PCE of 17.50%. The device demonstrated enhanced stability, retaining over 95% of its initial PCE after more than 2,300 hours in dark conditions with 40-55% RH in ambient air (non-encapsulated).

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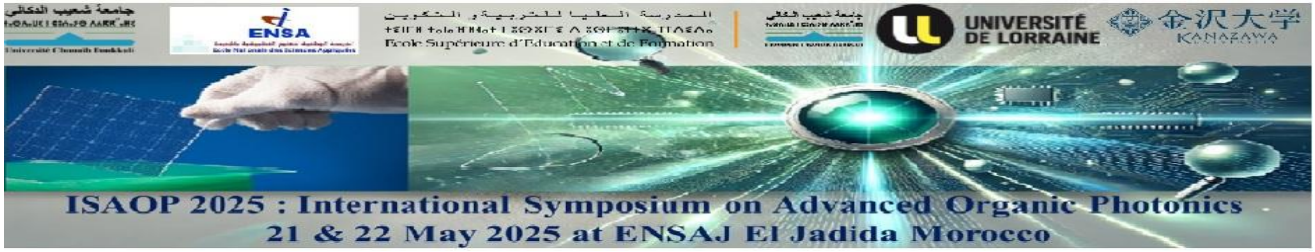
Smart Materials



A Comprehensive Overview of Advanced Methods for designing Composite Hydrogen Storage Vessels

Safia JBILOU*, Youssef BENSMAIL, Abdelkader BOULZEHAR, Mahmoud El MOUDEN, Dennoun. SAIFAOUI

Laboratory for Renewable Energy and Dynamic Systems, FSAC – UH2C, Morocco

Industrial and Surface Engineering Laboratory, FST, USMSBM, Morocco

Laboratory of engineering sciences for energy, ENSA El Jadida, Morocco

**Corresponding author: safiajbilou@gmail.com*

This review paper provides a comprehensive analysis of the analytical and numerical approaches employed in the design of hydrogen storage vessels. The importance of hydrogen storage vessels in various applications is outlined, emphasizing the need for reliable and efficient design methods. The review encompasses an in-depth examination of both analytical and numerical techniques, including pressure analysis, burst pressure prediction, fatigue life assessment, and numerical simulation methods such as finite element analysis and computational fluid dynamics. Furthermore, the paper discusses failure analysis, safety considerations, and optimization strategies for enhancing the performance of hydrogen storage vessel designs. By consolidating and analyzing the latest research in this field, the review aims to contribute to the advancement of hydrogen storage vessel design and facilitate the development of safe and effective hydrogen storage solutions.

Keywords: hydrogen storage; numerical modeling; analytical approaches; optimization; failure analysis

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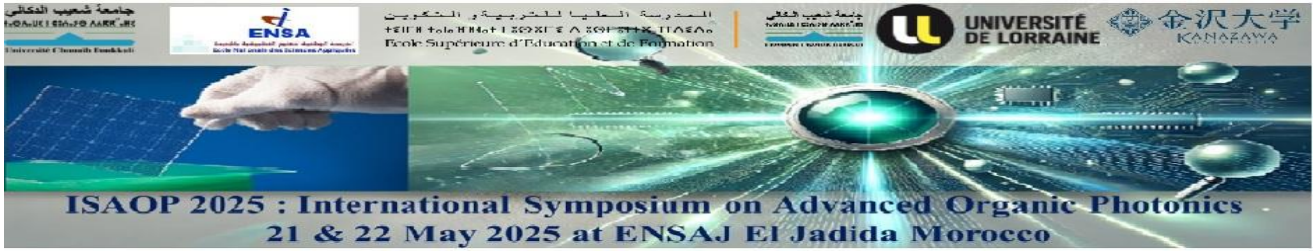


Advancements in Corrosion Protection: Exploring Innovative Coatings, Self-Healing Materials, and Surface Preparation Techniques: a review

Ichraq BOUHOUCHE, Houda LABJAR, Najoua LABJAR*, Hamid NASRELLAH , Ayoub CHERRAT, Ghita Amine BENABDALLAH, Souad EL HAJJAJI

Laboratory of Molecular Spectroscopy Modelling, Materials, Nanomaterials, Water and Environment, CERNE2D, ENSAM, Mohammed V University in Rabat, Morocco;

Laboratory of Membranes, Materiels and Environnement, Faculty of Sciences and Technologies of Mohammedia, Hassan II University of Casablanca, Morocco;

Higher School of Education and Training, Chouaib Doukkali University, El Jadida, Morocco;

Forensic Institute of Gendarmerie Royale, Rabat, Morocco;

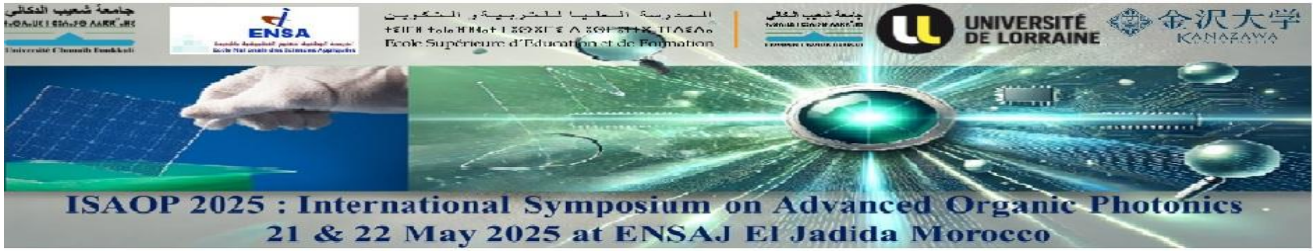
Laboratory Modelling, Materials, Nanomaterials of Molecular Spectroscopy, Water and Environment, CERNE2D, Faculty of Sciences, Mohammed V University in Rabat, Morocco;

(*) Corresponding author: najoua.labjar@ensam.um5.ac.ma

Corrosion presents a constant challenge throughout many industries. It compels them to continue their research and to push forward more protection strategies. This overview looks at the recent developments those many industries have made in surface treatments and coatings. What do these industries now recommend for minimizing appearance issues and serious structural degradation of materials? The first section highlights improvements in surface treatments, focusing on passivation, electroplating, and conversion coatings, each contributing to forming protective barriers that resist corrosion. Robust substrate layers are produced by electroplating and passivation. Conversion coatings such as chromate and phosphate layers add a chemical shield to the substrate surface. The review then explores innovative coating materials and methods, particularly the rise of thin-film technologies. Among the materials under consideration for use in hostile environments are metallic, ceramic, and polymer-based coatings novel constructions that are nanotechnology-enhanced to boost chemical stability and hardness in some cases, really impressive hardness. The coatings we're working with are tailored for next-generation components that must endure extreme temperatures, corrosive environments, and abrasive wear The techniques for preparing surfaces are also discussed here, and their truly critical role in making coatings perform their best is emphasized. Roughening methods are used, as well as primer applications, and the maintenance of the surface before coating it is discussed. These adjuncts to durability are thoroughly evaluated and are made much of in this volume by the authors. Tools used for quality evaluation like scanning electron microscopy and X-ray diffraction also take center stage here. In conclusion, the review examines present obstacles, including the demand for coatings that are not only cost-effective but also environmentally friendly. It offers an overview of the need and opportunity for coatings with multifunctional features and discusses the emerging research on self-healing as a coating property. Most

importantly, the review carries forward the notion that coatings are and will continue to be the principal first line of defense against corrosion.

Keywords: *corrosion protection, thin-film coatings, self-healing materials, surface preparation, nanotechnology, sustainable materials*



Ambient Energy Harvesting Technologies for Railway Applications

Ihssane ZOUINE, Fouad BELHORA * and Houssam AMIRY *

Ihssane ZOUINE (LABSIPE).

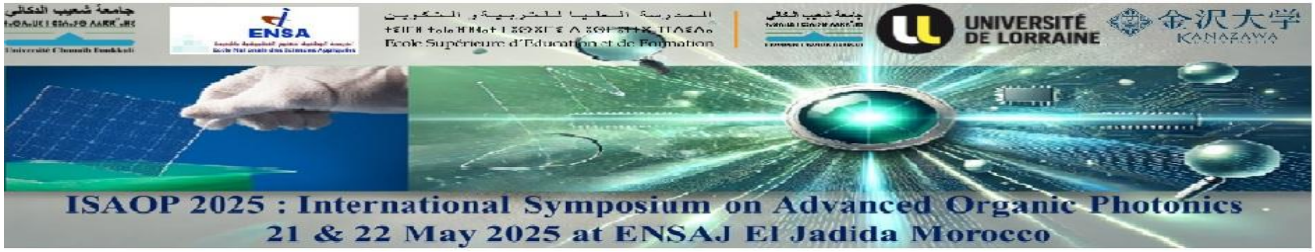
Fouad BELHORA (LABSIPE).

Houssam AMIRY (LABSIPE).

** Corresponding author: zouine.ihssane@ucd.ac.ma*

This communication focuses on ambient energy harvesting technologies applied to the railway sector. Explored sources include acoustic, thermal, magnetic, solar, wind, and vibrational energy. Particular attention is given to vibrational energy, which is especially relevant due to the constant vibrations caused by the track and bogies.

Keywords: Energy Harvesting, Railway vehicles, Energy Recovery, transportation, Vibrational energy.



Cellulose Acetate-Stabilized Cu2O Nanoparticles for Enhanced Catalytic Reduction of Organic Pollutants

El houceine BENHADRIA, Lahoucine BAHSIS, El-Houssaine ABLOUH, Najoua LABJAR, Souad EL HAJJAJI

LS3MN2E, CERNE2D, ENSAM, Mohammed V University in Rabat, Morocco

Université Cadi Ayyad, 4162 Safi, Morocco

Materials Science, Energy and Nanoengineering Department (MSN), Mohammed VI Polytechnic University

(UM6P), Lot 660 – Hay Moulay Rachid, Benguerir 43150, Morocco

LS3MN2E, CERNE2D, faculty of sciences, Mohammed V University in Rabat, Morocco

** Corresponding author: benhadria.smc@gmail.com*

This study examines the potential of catalytic reduction for the removal of specific pollutants in aqueous solutions using copper(I) oxide nanoparticles supported on cellulose acetate as a biosupport. The Cu2O NPs were deposited onto cellulose acetate (CA) under ambient conditions in the presence of hydrazine, which served as the reducing agent. The resulting catalyst was subjected to comprehensive characterization employing a range of techniques, including XRD, FTIR, SEM, EDS, BET, XPS, and TEM analyses. The Cu2O NPCA was evaluated as a catalyst for the catalytic reduction of organic pollutants (p-nitrophenol (PNP) and methylene blue (MB)) in a simple and binary system in the presence of NaBH4.The results of the catalytic tests in PNP and MB solutions demonstrate that the elimination efficiency is influenced by a multitude of factors, including the catalyst dose and the concentration of the pollutant. The Cu2O NPs-CA catalyst demonstrated remarkable catalytic efficacy for the reduction of PNP and MB pollutants, exhibiting maximum apparent rate (k) 0.5100 −1 0.2378 −1 v . T 2O NP-CA catalyst was evaluated on a mixture of PNP/MB pollutants, and the results demonstrated that it exhibited the highest catalytic activity for reducing and degrading these organic pollutants in aqueous solutions, which is a promising outcome. Furthermore, the prepared catalyst exhibited excellent catalytic performance and the ability to be recycled multiple times without significantly losing activity, which could be advantageous for large-scale production and practical usage in water treatment.

Keywords: Nanocatalysts · Cellulose acetate · Organic pollutants · Reducing agent · Copper(I) oxides

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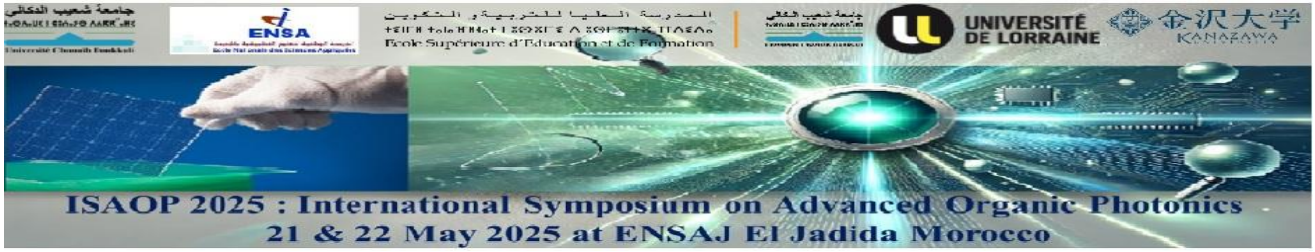

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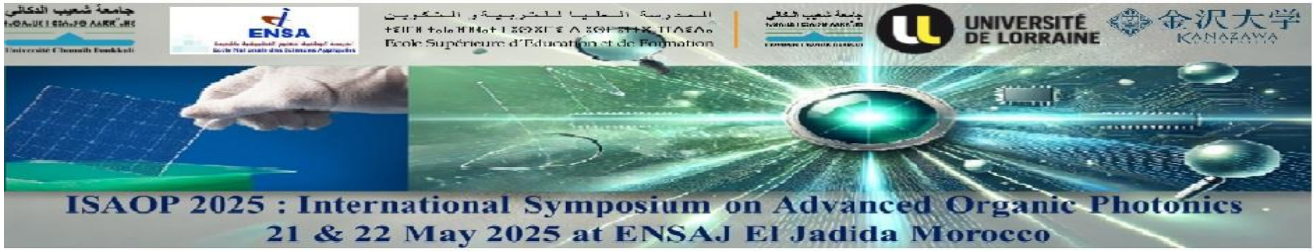


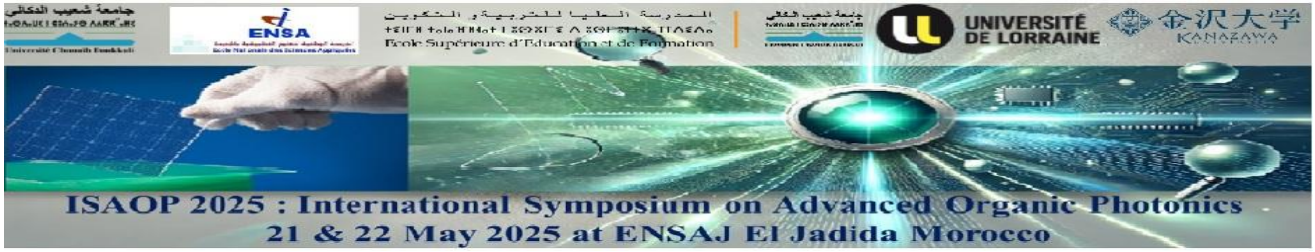
Chemometric advances in COD analysis: Overcoming turbidity interference with a Hybrid PLS-ANN approach

Meryem NINI*, Mohamed NOHAIR

Laboratory of Physical Chemistry and Biotechnology of Biomolecules and Materials, Faculty of Sciences and Techniques, Hassan II University of Casablanca, P.A. 146, Mohammedia, Morocco

In the current context of environmental protection, the accuracy of water quality analyses is crucial, especially chemical oxygen demand (COD) analyses. COD is a key indicator of organic pollutants in water, and is often compromised by turbidity interference at UV wavelengths. Faced with this turbidity challenge, this innovative study proposes an integrated approach, using in situ UV sensors and advanced Chemometric techniques, exploiting the synergy between PLS (Partial Least Square) and ANN (Artificial Neural Network). The research is divided into three main sections: (i) assessment of turbidity interference, (ii) development of a turbidity prediction model and (iii) elaboration of the COD compensation and prediction model. Turbidity significantly alters the UV-Visible absorbance spectrum of COD. By analyzing mixed solutions of COD and turbidity, we quantified this interference and established a turbidity prediction model using spectral areas between 303.5 and 700 nm. Interval PLS identified the most informative spectral regions for COD concentration, highlighting the 200–250 nm interval. To address turbidity interference, we developed a hybrid model combining PLS and ANN regression, and turbidity measurements are incorporated as an explanatory term in the model. This hybrid approach relies on in situ UV sensors to directly capture UV absorbance data in the field and applies robust chemometric models to accurately distinguish the UV absorbance contributions of organic compounds and turbidity. The method not only compensates for the interfering effect of turbidity, but also allows turbidity information to be used to refine COD predictions. Model performance, evaluated using R2, RMSE, and MAE, showed a significant increase in R2 to 0.9972, and decreases in RMSE to 0.94 and MAE to 0.64, demonstrating the method's effectiveness in correcting turbidity-induced deviations and improving COD prediction accuracy. The results of the evaluation on real data show high performance metrics, with recovery percentages close to 100 % and low RMSE and MAE values, indicating the model's robust ability to predict COD in the presence of suspended particles.

Keywords: Chemometric, COD, Turbidity compensation, In-situ UV sensors, Partial Least Squares, Artificial Neural Networks



Comparative study of magnetic properties in V-doped CdX (X = S, Se and Te) compounds: First-Principles Investigation.

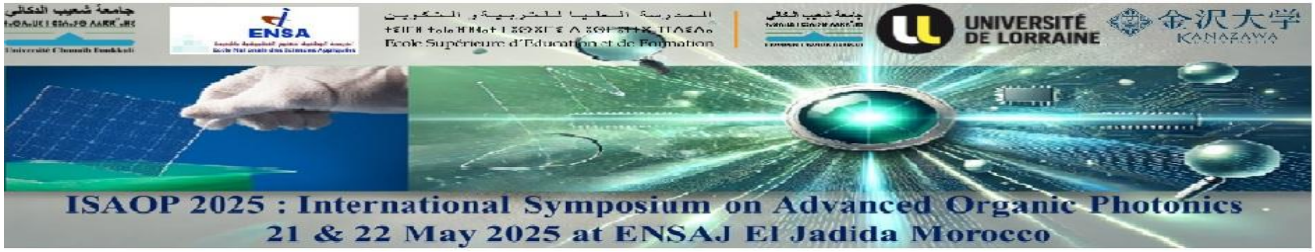
Mohamed BAIBOUD* and Abdelaziz LABRAG

Laboratory of Materials, Electrical Systems, Energy and Environment (LM3SE),

** Corresponding author: deug.fsa@gmail.com*

the electronic structure and magnetic properties in zinc blende phase of Cd1−xVxX (X = S, Se, Te) with (x = 0.125) DMSs have been performed by GGA approximations. The investigation was done by using full potential-linearized augmented plane wave (PBE) method within DFT as implemented in the Castep code. the density of states shows the hybridization between the p (S, Se, Te) and 3d (V) states that creates the antibonding states in the gap, which stabilizes the ferromagnetic ground state associated with the double exchange mechanism. The electronic properties exhibit half-metallic behavior for CdVTe and CdVS and semiconductor behavior in both spins for CdVSe at the same concentations x= 12,5 %. Furthermore, the total magnetic moment of Cd1-xVxX (X = S, Se, Te) compounds are mainly due to the V site with very small contribution of Cd and X = S, Se and Te. These compounds are robust ferromagnets containing diversified gap character in their electronic structures with spin polarization of 100 % , they are predicted as potential candidates for spin injection applications in spintronic devices. opening a new route for experimentalists to confirm our predictions.

Keywords: Magnetic semiconductor, DMS, Cd1-xVxX, First-Principal calculation.



Edge-Dependent Electronic and Optical Properties of Graphene Nanoribbons: A First-Principles Study of Zigzag and Armchair Configurations

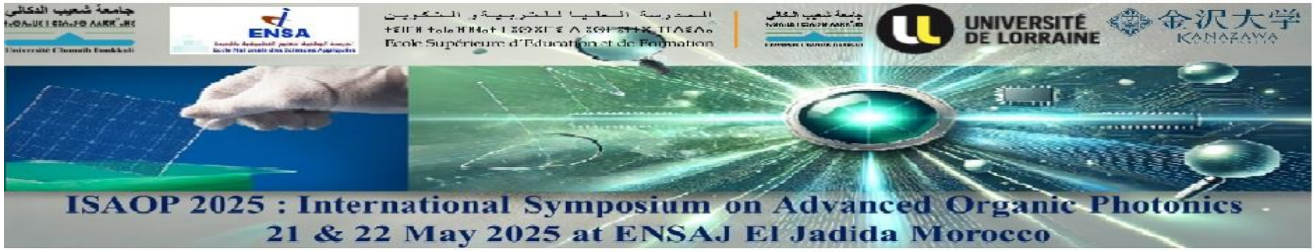
M. Mardy, M. Bghour, M.Benaadad, F.El aissaoui., H.El Ouaddi, and A.Labrg

Laboratory of Physics of Condensed Matter and Nano-Materials for Renewable Energies, Ibn Zohr University, Agadir, Morocco.

Laboratory of Materials, Electrical Systems, Energy and Environment, Ibn Zohr University, Agadir, Morocco.

**Corresponding author: mustapha.mardyy@gmail.com*

In our study, we investigate the influence of edge variation on the electronic and optical properties of graphene nanoribbons with both zigzag and armchair edge configurations. Graphene structures with varying widths characterized by 8, 11, 14, 17, 20, 23, and 26 edges were modeled for both edge types. Using first-principles calculations, we computed the band structures, density of states (DOS), and optical properties of each configuration. The results reveal distinct trends in band gap evolution and optical response as a function of ribbon width, highlighting the critical role of edge geometry in tuning the physical properties of graphene. A comparative analysis between zigzag and armchair nanoribbons demonstrates significant differences in their electronic behavior, which can be harnessed for targeted applications in nanoelectronics and optoelectronics.



From Waste to Energy: Electrocatalytic Electrodes Based on Hydrochar and Nanocellulose for Hydrogen Production in Alkaline medium

Zineb HAMMI, Soraya LAKHLOUFI, Najoua LABJAR*,Houda LABJAR, Hamid NASRELLAH, Ayoub CHERRAT, Amine HALHALY, El Mostapha LOTFI, Abdelouahed DAHROUCH, Souad EL HAJJAJI

LS3MN2E, CERNE2D, ENSAM, Mohammed V University in Rabat, Morocco;

L2ME, Faculty of Sciences and Technologies of Mohammedia, Hassan II University of Casablanca, Morocco,

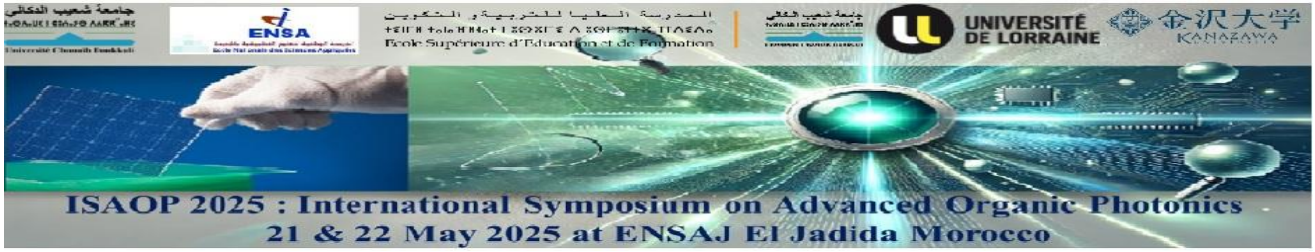
ESEF, University Chouaib Doukkali of El Jadida, Morocco;

LS3MN2E, CERNE2D, Faculty of Science, Mohammed V University in Rabat, Morocco;

Forensic Institute of Gendarmerie Royale, Rabat, Morocco;

**Corresponding author: najoua.labjar@ensam.um5.ac.ma*

One of the most promising and environmentally friendly methods for producing green hydrogen is water electrolysis. Nonetheless, electrode performance and electrolyzer efficiency are closely interconnected, and both have a major influence on energy losses and charge transfer kinetics during electrochemical processes. In this research, date pit biomass (Phoenix dactylifera Linnaeus) was converted into activated hydrochar and nanocellulose, which were subsequently used to fabricate modified electrodes. Through thorough electrochemical characterisation, the hydrogen evolution reaction (HER) activity of these bio-based materials was examined. Compared to unmodified graphite electrodes, electrodes modified with nanocellulose and activated hydrochar exhibited significantly reduced overpotentials. Furthermore, these improved electrodes enabled higher hydrogen production in alkaline electrolysis. This study highlights the promise of biomass valorisation technologies for generating efficient, low-cost, and sustainable electrode materials for green hydrogen production.



Electrodeposition of Hydroxyapatite and β-TCP Coatings: Influence of Deposition Modes

Mouhsine KOUCHTABI*, Said LAASRI, Hamid NASRELLAH, Awatef GUIDARA, and Hassib TOUNSI

Laboratory of Engineering Sciences for Energy (LabSIPE), National School of Applied Sciences, Chouaib Doukkali University, El Jadida, Morocco.

Laboratory of Engineering Sciences for Energy (LabSIPE), National School of Applied Sciences, Chouaib Doukkali University, El Jadida, Morocco.

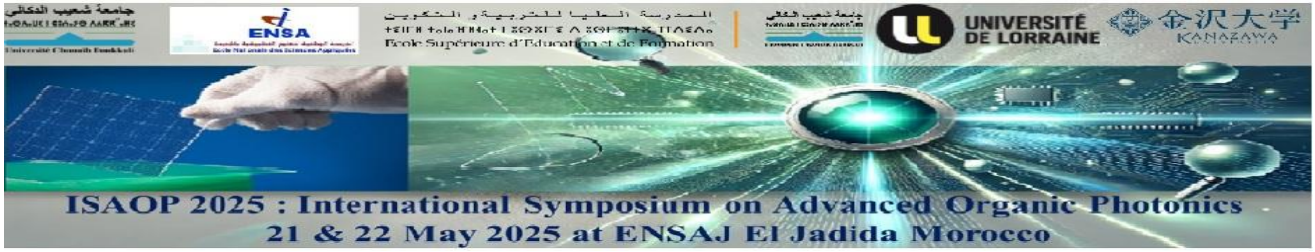
Laboratory of Organic, Bio-Organic, and Environmental Chemistry, Chouaib Doukkali University, El Jadida, Morocco.

Laboratory of Advanced Materials, National School of Engineering, Sfax, Tunisia.

**Corresponding author: kouchtabimouhsine95@gmail.com*

The electrodeposition of calcium phosphate (CaP) coatings, particularly hydroxyapatite (HAP) and β-tricalcium phosphate (β-TCP), on 316L stainless steel substrates enhances orthopedic implants. This study investigates the effects of four deposition modes pulsed current, constant current, potentiostatic, and galvanostatic on the structural, morphological, and physicochemical properties of the coatings. Key parameters such as current density, electrolyte composition, temperature, pH, and potential are optimized for improved biofunctionality. The study explores the incorporation of magnesium, strontium, and zinc to enhance bioactivity, mechanical properties, and adhesion strength. Characterization includes X-ray diffraction (XRD), scanning electron microscopy (SEM), and Fourier-transform infrared spectroscopy (FTIR). Mechanical performance is evaluated via nanoindentation, scratch testing, and electrochemical impedance spectroscopy (EIS). In vitro tests validate the biomedical potential of the coatings. The results show that optimizing deposition parameters and chemical modifications leads to CaP coatings with superior structural stability, enhanced biointegration, and controlled biodegradability, improving th longevity and performance of orthopedic implants.

Keywords: Electrodeposition, Hydroxyapatite, β-Tricalcium Phosphate, Bioactivity, Orthopedic implants.



Energy Harvesting with diverse micro piezoelectric setups

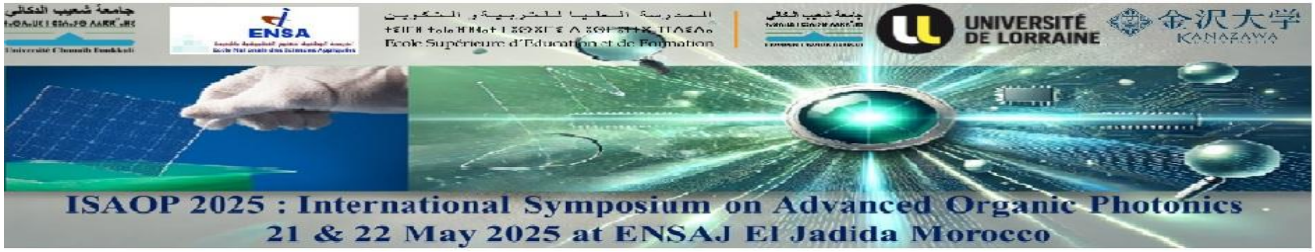
Nada CHERKAOUI JAOUAD *, Fouad BELHORA, Amine ALAOUI-BELGHITI, Imane SALHI, Abdelouahed HAJJAJI

Chouaib Doukkali University of El Jadida, Natl Sch Appl Sci, LabSIPE, El Jadida, Morocco

**Corresponding author: cherkaoui.jaouad.nada@gmail.com*

In recent years, extensive research has been conducted regarding the topic of energy autonomy with a specific focus on sensor supply. Embedded sensors have gained in precision, reliability, and robustness while miniaturizing, but they are still limited by the lifespan of their power supply system. A promising alternative is to recover ambient mechanical energy in order to ensure portable energy self-sufficiency. Harvesting vibrational energy aims to create centimeter sized electric micro-generators enabling the provision of power electronic systems through the absorption of ambient energy in the surrounding environment. A promising application is therefore the supply of autonomous communicating sensors. The advancement of these self-sustaining networks addresses an increasing demand for measuring, analyzing, and controlling changes in our natural environment, the structural integrity of civil or military constructions, and the health status of the human body. Currently, these sensors rely on batteries which require regular maintenance and raise environmental concerns, especially in terms of recycling. If it becomes feasible to substitute these batteries with micro-generators, the adoption of such sensors will become widespread, facilitating the development of more efficient mechatronic systems. This work focuses on vibration control and energy harvesting using embedded piezoelectric elements. First, different forms of piezoelectrical materials are being elaborated. Subsequently, a comparison of the energy harvested from all the elaborate materials has been conducted. Finally, an application of energy harvesting using the most efficient material will be explored.

Keywords: Energy Harvesting, Piezoelectric Materials, Microgenerators, Ceramic.



Energy harvesting through different piezoelectric sensors

Nada CHERKAOUI JAOUAD *, Fouad BELHORA, Amine ALAOUI-BELGHITI, Imane SALHI, Abdelouahed HAJJAJI

Chouaib Doukkali University of El Jadida, Natl Sch Appl Sci, LabSIPE, El Jadida, Morocco

**Corresponding author: cherkaoui.jaouad.nada@gmail.com*

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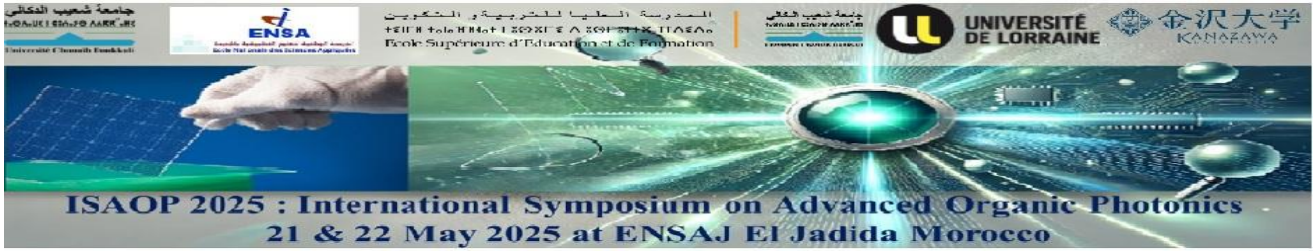
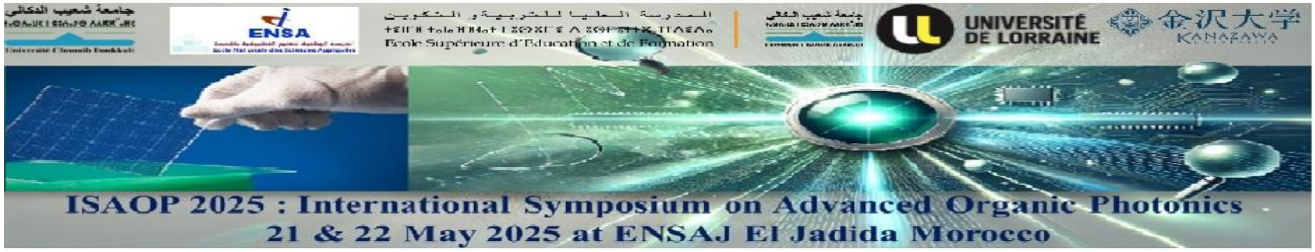


Graphene-Enhanced One-Dimensional Photonic Crystal Biosensors for Ultra-Sensitive Detection of Acetone Concentrations in Wastewater

Abdelkarim EL MOUNCHARIH*, Abdelaziz TCHENKA, Rabi TAKASSA, Fatima ELFATOUAKI, Imad SALYM, Omar FARKAD, Sanaa HASSINE, El Alami IBNOUELGHAZI, Driss ABOUELAOUALIM
LaMEE, Department of Physics, Faculty of Sciences Semlalia, Cadi Ayyad University, P.O. Box 2390, 40000 Marrakech, Morocco
** Corresponding author: a.elmouncharih@gmail.com*

Wastewater containing high concentrations of organic materials poses significant risks to human health. Realizing the significance of precisely detecting acetone concentrations in wastewater by monitoring refractive index (RI) changes, the present work addresses the design and analysis of biosensor performances based on the defective 1D ternary photonic crystal (TPC). The proposed TPC is designed using alternating layers of Si, Nb_2O_5 , and SiO_2, with a central defect layer infiltrated by water mixtures. The well-established transfer matrix method (TMM) is manipulated to study the transmission spectrum of the structure. This work is built upon the strong correlation between the defect mode characteristics and the RI of water mixtures at varying concentrations. Numerous geometrical parameters such as the number of periods, the defect layer thickness, and the angle of incidence are meticulously optimized to realize high sensitivity. Additionally, the impact of graphene insertion on the sensing performance is thoroughly investigated. It is perceived that at an incident angle of 80°, 3 periods, and the defect layer thickness of 2216 nm, the proposed structure bestows a maximum sensitivity of 3344.22 nm/RIU. Finally, the developed biosensor demonstrates the ability to predict organic material concentrations in wastewater with high precision, offering a promising tool for environmental monitoring and ensuring water quality standards.

Keywords: Graphene, Photonic Crystal, Biosensor, wastewater monitoring, Refractive index, Transfer Matrix Method.



Investigation of a new P2-Na0,67Ni0,25Co0,17Mn0,58O2 cathode for sodium-ion batteries: Structural characterization and combined electrochemical and chemical deintercalation studies

Younes CHAALI*, Nouhayla MANSORI, Jihad EL MAKAOUI, Mohammed DAHBI, Abdelwahed CHARI2, Abdessalam BOUDDOUCH, Driss ZAKARIA
Laboratory of Physical Chemistry of Materials (LPCM), Department of Chemistry, Faculty of Sciences, Chouaib Doukkali University, El Jadida, Morocco.
Department of Materials Science Energy and Nanoengineering (MSN), Mohammed VI Polytechnic University, Ben Guerir, Morocco.
* *Corresponding author: chaali.y@ucd.ac.ma*

Given global energy demands and the growing need for sustainable energy sources, energy storage has become crucial, especially in supporting the growth of renewable but often intermittent energy sources. Sodium-ion batteries (NIBs) have garnered renewed attention as a viable option for large-scale energy storage applications, presenting a sustainable alternative to lithium-ion batteries (LIBs) due to the abundant availability and cost effectiveness of sodium. In the pursuit of enhanced performance in NIBs, a variety of cathode materials are under development to achieve high energy density, improved cycling stability, and excellent rate capability. Among these, two-dimensional triangular lattice (2DTL) materials exhibit significant potential. These materials facilitate shortened pathways for sodium ion transport and provide expanded surface areas for ion absorption, making them particularly suitable for high-power applications. Herein, we present a novel cathode material, P2-Na0,67Ni0,25Co0,17Mn0,58O2, synthesized via a combustion method. Comprehensive structural characterization through X-ray diffraction (XRD), confirming the stability of the P2 phase, alongside notable interlayer spacing [1]. Electrochemical tests of this cathode material have demonstrated remarkable stability, both structurally and in terms of cycling performance, underscoring its potential for extended applications in energy storage. Further investigations into chemical deintercalation, supported by XRD and Raman spectroscopy, have elucidated the structural evolutions occurring within the P2 phase during cycling. These analyses revealed phase transitions within the P2 structure, providing valuable insights into the internal mechanisms governing sodium intercalation and deintercalation. In summary, this work highlights P2-Na0,67Ni0,25Co0,17Mn0,58O2 as a promising cathode for NIBs, with performance attributes that are conducive to efficient and sustainable energy storage solutions.

Reference :

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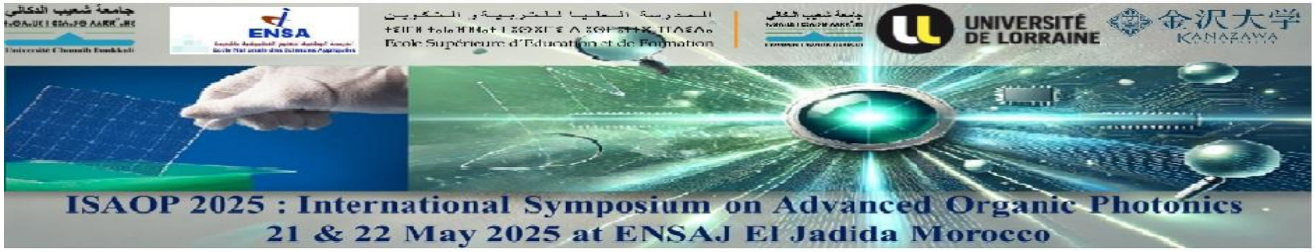
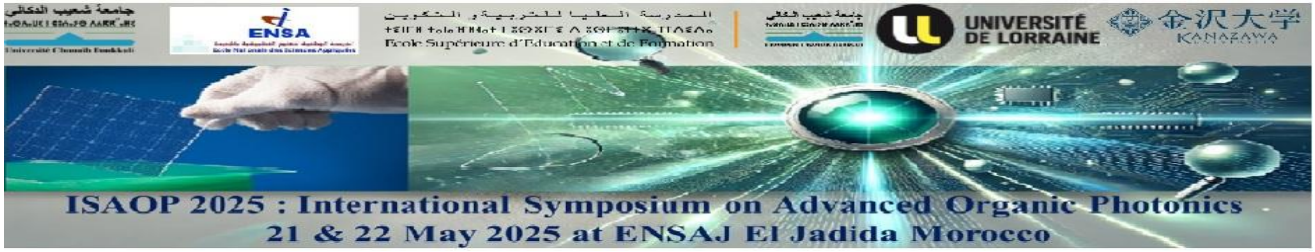


Magnetocaloric Effect of Ba0.8Sr0.2FeO3 Barium-Strontium Ferrites

M. SALAMA,*
LPMC Laboratory, Theoretical Physics Group, Faculty of Sciences, Chouaïb Doukkali University.
* *Corresponding author:* salama.m@ucd.ac.ma

The magnetic properties, magnetocaloric effect and hysteresis behavior of the Barium-Strontium ferrites Ba0.8Sr0.2FeO3 have been studied using the mean-field approximation. The influence of an external magnetic field and temperature on magnetization, magnetic susceptibility, magnetic entropy change and hysteresis behavior was analyzed in detail. The results show that magnetization decreases progressively with increasing temperature until it becomes zero at the critical temperature Tc = 60 K, while the application of an external magnetic field increases the critical temperature Tc by strengthening the alignment of magnetic moments. The variation in magnetic entropy -ΔSm reveals a characteristic peak at Tc, indicating a strong magnetocaloric effect. Furthermore, the relative cooling power RCP increases linearly with the external magnetic field strength. Under a magnetic field of h = 5 T, the maximum values obtained for the variation in magnetic entropy ΔSm and for the relative cooling power RCP are 4.9 J.kg−1.K−1 and 176 J.kg−1 respectively.



Mechanical characterization of the binary CoCr metallic glass using molecular dynamics simulations

Mohammed GOUNZAR, Abdelhadi KOTRI, and Youssef BELKASSMI

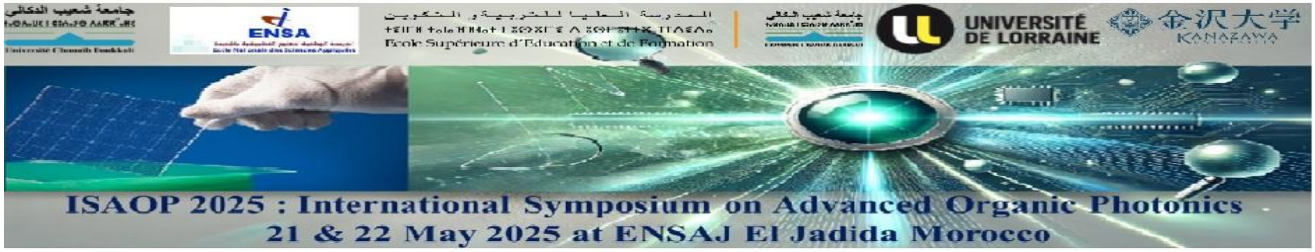
Lab.PETI, Université Ibn Zohr, FPO, Ouarzazate, Maroc.

Equipe Sciences et Technologies (ESTE), ESEF, Université Chouaib Doukkali, El-Jadida, Maroc.

** Corresponding author: mohammed.gounzari@edu.uiz.ac.ma*

In this study, we examined the influence of the cooling rate on the mechanical properties and the glass formation of binary CoCr metallic glasses. We have performed molecular dynamics simulations to investigate the formation, structural, and mechanical properties of the binary CoCr glass. The effect of atomic fraction of each component on the structural and mechanical properties of CoCr metallic glasses is investigated. We studied three compositions; one of them was close to the eutectic point. The findings show that the composition close to the eutectic point had a high glass-forming ability compared to the other compositions investigated. Mechanical properties are found to be not very affected by the cooling rates; the values of the calculated Young's modulus of binary Co0.75Cr0.25 glass are equal to 261 GPa, 273 GPa, 274 GPa, 275 GPa, and 273 GPa for cooling rates equal to 1011 K/s, 1012 K/s, 1013 K/s, 1014 K/s, and 1015 K/s, respectively.

Keywords: Binary CoCr alloy, Molecular dynamics simulations, Metallic glasses, Binary glasses, Structural properties, Mechanical properties.



Optical properties of water under the action of the electromagnetic field in the infrared spectrum

Redouane MGHAIOUINI*, Bouchra BA MOHAMMED, Rachid EL BOUAYADI, EL GHAOUTI Chahid, Abderrahmane ELMLOUKY, Said LAASRI, Mohamed MONKADE,Hicham LABRIM

Advanced Systems Engineering Laboratory, National School of Applied Sciences, Ibn Tofaîl University, Kenitra, Morocco.

Materials, Membranes and Nanotechnology Laboratory, BP: 11201 Zitoune, university of my9 ismail, Faculty of Sciences Meknes, Morocco.

Laboratory of Condensed Matter Physics, University Chouaib Doukkali of El Jadida, 24000, Morocco

Laboratory of Engineering Science for energy (labSIPE) ENSA, Chouaib Doukkali University, El- Jadida,Morocco.

** Corresponding author: redouane.mghaiouini@uit.ac.ma*

The current paper outlines the optical properties of magnetized water compared to other types of water: distilled water and tap water. Tap water was exposed to a weak electromagnetic field (40 nT) for 20 min of circulation at two rates: 0.18 and 0.6 m s−1. The effect of the electromagnetic field on changes in the optical properties of magnetized water (MW) compared to distilled water (DW) and tap water (TW) was analyzed by FTIR spectroscopy to gain insight into the atomic and molecular structure of the water molecule. The absorbance and transmission of magnetized water in the IR spectrum are different from

those of TW and DW, especially in the wavelengths: 3310 cm−1 and 600 cm−1. The width of the OH band of different types of water increases with the intensity of electromagnetic induction and its peak shifts weakly towards low wave numbers. Both phenomena are attributed to the effect of the electromagnetic field on the increase of intermolecular bonds between water molecules which strengthens their structure.

Keywords: Optical properties, IR spectrum, absorbance, electromagnetic field

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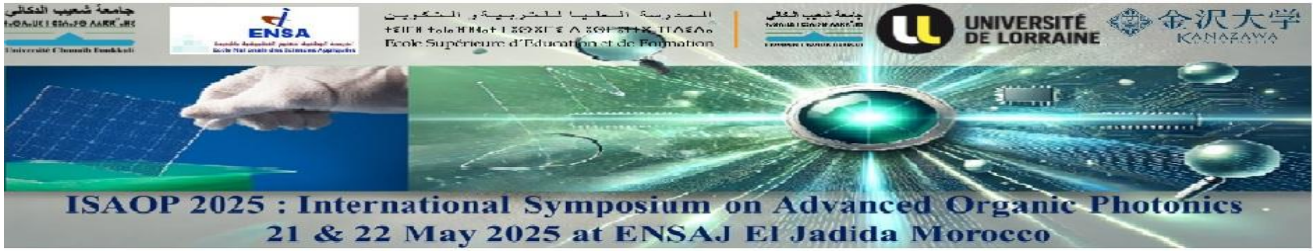


Optoelectronic Properties and Multiscale Numerical Optimization of $CuIn_{1-x}Ga_xSe_2$ Chalcopyrite Thin-Film Photovoltaics: Bridginz DFT+U Insights and SCAPS-1D Device Performance

Bryk MUSTAPHA[1], Dardouri MOLOUDI[1 2], Hasnaoui ABDELLATIF[1] and Sbiaii KHALID[1]*

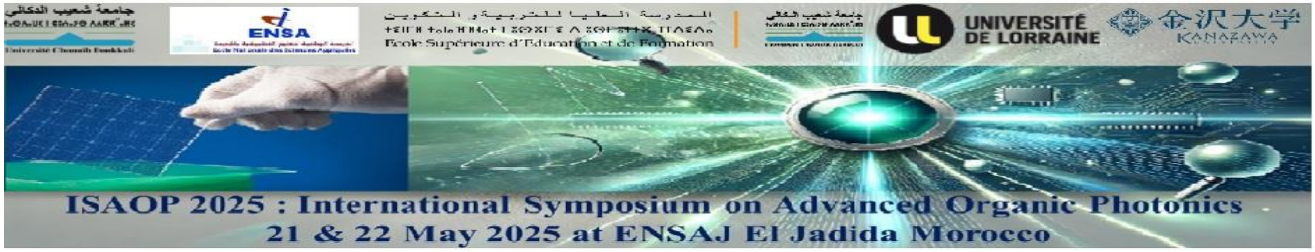
[1] Laboratory of Materials Science, Mathematics, and Environment (LS2ME), Polydisciplinary Faculty of Khouribga, Sultan Moulay Slimane University, 23000 Beni Mellal, Morocco

[2] Laboratory of Condensed Matter Physics (LCMP), Faculty of Science, Chouaib Doukkali University, 24000 El Jadida, Morocco

* Corresponding author: mustaphabryk@gmail.com (e-bryk.m@ucd.ma), ksbiaai@gmail.com

Copper indium gallium selenide ($CuIn_{1-x}Ga_xSe_2$, or CIGS), a chalcopyrite-structured semiconductor, has emerged as a leading material for next-generation thin-film photovoltaics. This study integrates ab initio simulations, device modelling, and impedance spectroscopy to unravel the interplay between gallium composition, optoelectronic properties, and solar cell performance. Density functional theory (DFT+U) calculations reveal a tunable bandgap (1.0–1.7 eV) governed by Vegard's law, driven by Cu-d and Se-p orbital hybridisation, while maintaining structural stability across all Ga/In ratios. These insights guide SCAPS-1D simulations of a glass/Mo/CIGS/CdS/ZnO photovoltaic cell, identifying an optimal gallium content of x = 0.3, which balances light absorption (1.15 eV bandgap) and charge extraction, yielding a simulated efficiency of 22.1%. Higher Ga concentrations reduce infrared response and exacerbate interfacial recombination, while impedance spectroscopy exposes defect-mediated losses linked to CdS/CIGS interfaces. Critical design rules emerge: (1) a 2.0 µm absorber thickness minimises resistive losses, and (2) defect densities below 10^{16} cm^{-3} are essential for stable operation. Beyond efficiency optimisation, this work advocates replacing toxic CdS buffer layers with eco-friendly alternatives, advancing sustainable thin-film technologies.

Keywords: Optoelectronic properties; CIGS solar cells; chalcopyrite structures; DFT simulations; bandga engineering; defect physics.



Predictive Maintenance in Industrial Systems: A Machine Learning Approach for Failure Prediction in Photonic and Smart Material-Based Environments

Soumaya ZAROUAL*, Rahhal ERRATTAHI, Chouaib ENNAWAOUI

Laboratory of Engineering Sciences for Energy, National School of Applied Sciences, University of Chouaib Doukkali, El Jadida – Morocco

Laboratory of Information Technologies, National School of Applied Sciences, University of Chouaib Doukkali, El Jadida - Morocco

** Corresponding author: zaroual.soumaya@ucd.ac.ma*

The industrial sector faces growing challenges with unplanned equipment failures, leading to significant financial and operational losses. Traditional preventive maintenance methods—such as scheduled inspections and part replacements—do not always accurately reflect the real-time health status of equipment and are often either too conservative or insufficient to avert critical breakdowns. This study aims to develop a machine learning-based predictive maintenance approach, focusing on accurately forecasting potential equipment failures and enabling timely interventions, thus optimizing uptime and minimizing unnecessary maintenance costs. Our approach leverages a combination of historical and real-time sensor data collected from industrial machinery, focusing on parameters such as temperature, vibration, pressure, and usage cycles. By using a diverse dataset covering a range of operational conditions, we trained and validated several machine learning models, including Random Forest (RF), Support Vector Machines (SVM), and Neural Networks (NN), each evaluated for accuracy, interpretability, and speed of deployment. The Synthetic Minority Over-Sampling Technique (SMOTE) was applied to address the class imbalance often observed in predictive maintenance datasets, where failure events are relatively rare compared to normal operation. Our analysis identified that models such as Random Forest and Neural Networks, when combined with real-time monitoring and advanced feature engineering techniques, provided high predictive accuracy for imminent equipment failures. By prioritizing features indicative of wear and tear, such as vibration frequency and usage duration, these models can flag early warning signs of potential failure, allowing for preventive actions well before a critical failure occurs. This predictive framework serves as a strategic tool for industries seeking to transition from reactive to proactive maintenance practices, significantly reducing unscheduled downtime and optimizing resource allocation. The implications of this study are profound for industries seeking to embrace Industry 4.0 principles by integrating artificial intelligence and machine learning into their operational strategies. Implementing such predictive maintenance models offers substantial improvements in operational efficiency, cost effectiveness, and equipment longevity. Furthermore, this research contributes to the development of scalable, automated maintenance systems capable of adapting to various industrial contexts, from manufacturing to energy production.

Keywords: Predictive Maintenance, Machine Learning, Industrial Systems, Downtime Reduction, Predictive Analytics.

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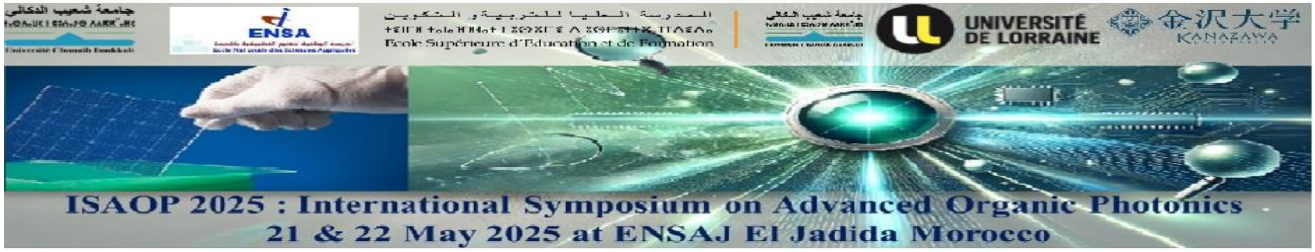


Selection of Gasification technology to maximize hydrogen-rich syngas from biomass using Multi-Criteria Decision-Making Methods

Housna IDRISSI; Najoua LABJAR; Souad EL HAJJAJI; Toufik BOUSHAKI

LS3MN2E, ENSAM, Mohammed V University in Rabat

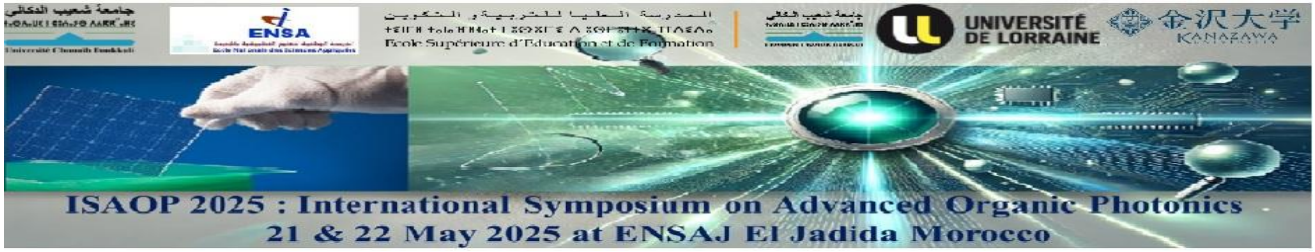
LS3MN2E, Faculty of Sciences, Mohammed V University in Rabat

ICARE-CNRS, University of Orleans, France

* *Corresponding author*: housna.idrissi@um5r.ac.ma

Gasification of solid waste is an efficient and renewable energy recovery method, offering a promising alternative to traditional waste disposal. This process converts biomass and organic waste into syngas, which can be used for electricity and heat production. However, choosing the most suitable gasification technology requires balancing energy efficiency, syngas quality, cost, and environmental impact. This study aims to identify the most suitable gasifier by evaluating four types of gasifiers: fixed bed, fluidized bed, entrained flow, and thermal plasma. Using the Fuzzy TOPSIS (FTOPSIS) method, the technologies are compared according to multiple technical, economic, and environmental criteria. Data from the scientific literature are analyzed, and the importance of each criterion is assessed using two objective weighting methods: ENTROPY and CRITIC. These methods provide consistent results, confirming the robustness of the evaluation. Among the four technologies, the fluidized bed gasifier emerges as the most efficient solution. It offers the best energy efficiency, better management of different fuel compositions, and optimal syngas conversion. A sensitivity analysis confirms its reliability for large-scale applications. This makes the fluidized bed gasifier the recommended choice for maximizing hydrogen yield and ensuring efficient use of resources in waste to energy systems.

Keywords: Gasification technology; Hydrogen production; MCDM method; Syngas



Self-Assembly of Perovskite Nanocrystals and Transfer Printing via Controlled Surface Wettability

Kaoru TAMADA*, Yuto KAJINO, Yuko AIDA, Yusuke ARIMA

Institute for Materials Chemistry and Engineering (IMCE), Kyushu University

* *Corresponding author*: tamada@ms.ifoc.kyushu-u.ac.jp

Lead halide perovskite (LHP) nanocrystals (NCs) have shown great potential in advanced photonics and optoelectronic applications due to their nearly unity photoluminescence (PL) quantum efficiency, narrow emission bandwidth and tunable spectral wavelength. However, LHP NCs are unstable to heat and polar solvents, making it difficult to fabricate spatially uniform ultrathin films over large device areas. In this study, we demonstrated a 2D assembly of various LHP NCs by simple spin-coating on macroscopic surfaces and also multilayered film formation by repeated spin-coating cycles [1]. The key process is careful purification of NCs for assembly (i.e., removing excess ligands), and complete vacuum drying between spin-coating cycles. The optimized methodologies realize strong NC-NC lateral interactions and also vertical stacking and long stability of the self-assembled structures. Another challenge in this study is contact printing of LHP NC films [2]. Traditional lithography techniques are difficult to apply to LHP NC films due to their instability. To solve this problem, a solvent- and heat-free contact printing technique were applied for the transfer and microfabrication of LHP NC self-assembled monolayers. The key process is a precise control of substrate wettability. To realize the multi-step transfer of NC films, it is necessary to increase adhesion forces between the NCs and substrates at each step. On the other hand, fabrication of spatially uniform LHP NC selfassembled monolayers by spin-coating requires some affinity between LHP NCs and the substrates. To meet these two requirements, the initial substrate for spin-coating was modified with a mixture of fluoroalkyl silane and alkyl silane, and the substrate for the final film transfer was modified with hexamethyldisilane. This back-to-basics approach provides a simple and reliable process for the integration of LHP NCs into advanced nano-optoelectronic devices.

Keywords: Perovskite Nanocrystals, self-assembly, monolayer, contact printing, wetting

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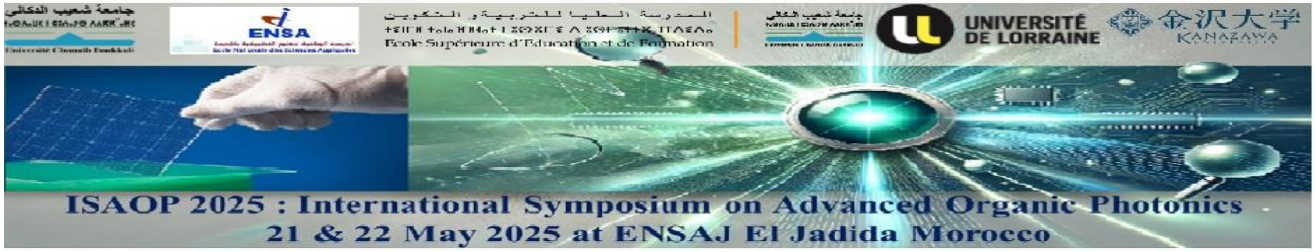

The influence of synthesis methods and experimental conditions on the photocatalytic properties of phosphate-based photocatalysts

Khadija EL FAKIR*, Younes CHAALI, Jihad EL MAKAOUI, Mohammed DAHBI, Ahmed TARA, Driss ZAKARIA and Abdessalam BOUDDOUCH

Laboratory of Physical Chemistry of Materials (LPCM), Department of Chemistry, Faculty of Sciences, Chouaib Doukkali University, El Jadida, Morocco.

Laboratoire MATIM - MATériaux et Ingénierie Mécanique Université de Reims Champagne-Ardenne, Reims, France.

** Corresponding author: Khadijaelfakir250@gmail.com*

Multifunctional materials play a crucial role in the development of advanced technologies thanks to their specific properties suitable for various applications. They are essential in several fields such as energy, environment, electronics, and health. Among them, phosphate based photocatalytic and photoluminescent materials are showing increasing interest for the degradation of pollutants in wastewater, clean energy production, and the development of optoelectronic devices. In this sense, optimizing the preparation conditions of these materials makes it possible to improve their performance, control their structure and their optical properties [1, 2]. In this work, phosphate-based photocatalysts (Mx(PO4)y) with (M = Bi, Mn, Co, Zn) were obtained by several preparation methods. The synthesized samples were calcinated at uniform temperature and were analyzed by X-ray diffraction (XRD), scanning electron microscopy coupled with energy dispersive X-ray analysis (SEM-EDX) and Raman spectroscopy (RS). The photocatalytic activity of the synthesized samples was evaluated by the degradation of anionic and cationic organic dyes in aqueous medium under UV light irradiation. The results showed that the synthesis technique considerably affects morphology, structure and photocatalytic process properties.

Keywords: Mx(PO4)y, photocatalysts, photocatalytic properties and organic dyes.

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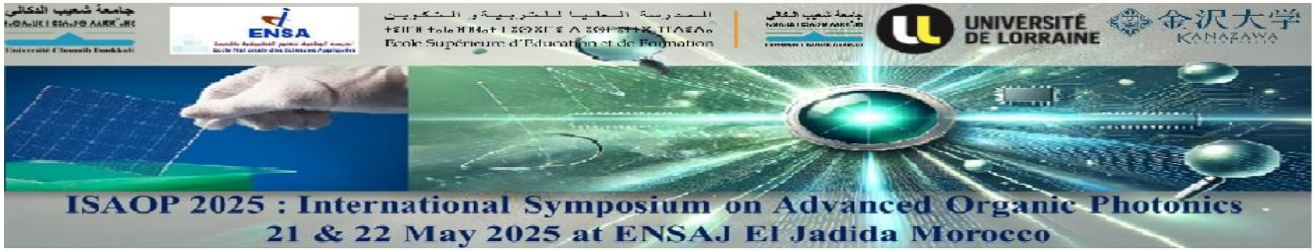


Energy Recovery Technologies in the Rail Sector

Ihssane ZOUINE and Fouad BELHORA *

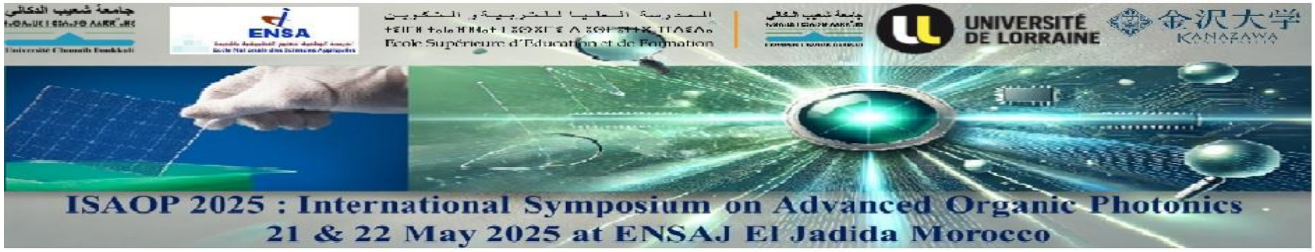
LABSIPE (ZOUINE Ihssane).

LABSIPE (BELHORA Fouad).

** Corresponding author: zouine.ihssane@ucd.ac.ma*

Energy recovery technologies are crucial for modernizing the rail sector. By incorporating systems such as regenerative braking and supercapacitors, trains can convert kinetic energy into reusable electricity, thereby reducing energy consumption and carbon emissions. These innovations not only contribute to more sustainable operations but also result in significant energy cost savings.

Keywords: The Rail Sector, Energy recovery, carbon emissions…



Evaluation of a New Bisbenzoxazole Derivative as Corrosion Inhibitor for Mild Steel in Molar HCl: Experimental and Theoretical Approaches

Mohamed omari[1], Khalid Bouiti[2], Najoua Labjar[2*], Said Jebbari[3,8], Ali Barhoumi[4], Houssaine Ait Sir[3], Souad El Hajjaji[5], Abdelouahed Dahrouch[5], Hamid Nasrellah[6], Mohammed El idrissi[7], Abdessamad Tounsi[1]

[1]Agro-industrial, Environmental and Ecological Processes Team, Faculty of Science and Techniques of Beni Mellal, Sultan Moulay Slimane University, Beni Mellal, Morocco;
[2] Laboratory of Spectroscopy, Molecular Modeling, Materials, Nanomaterials, Water and Environment, CERNE2D, ENSAM, Mohammed V University in Rabat, Rabat, Morocco;
[3]Laboratory of Bio-organic Chemistry, Department of Chemistry, Faculty of Sciences, Chouaib Doukkali University, El Jadida, Morocco;
[4] Molecular Modelling and Spectroscopy Research Team, Faculty of Science, Chouaïb Doukkali University, P.O. Box 20, 24000 El Jadida, Morocco;
[5] Laboratory of Spectroscopy, Molecular Modeling, Materials, Nanomaterials, Water and Environment, CERNE2D, Faculty of Sciences, Mohammed V University in Rabat, Rabat, Morocco;
[6] Laboratory of Organic Bioorganic Chemistry and Environment, University Chouaib Doukkali, Morocco;
[7]Team of Chemical Processes and Applied Materials, Faculty Polydisciplinary Sultan Moulay Slimane University, Beni-Mellal Morocco.
[8]Multi-laboratory LC2A, N °182 Industrial zone, Mohammedia, Morocco
*Corresponding author: najoua.labjar@ensam.um5.ac.ma; *G.S.M: 00212667314722*

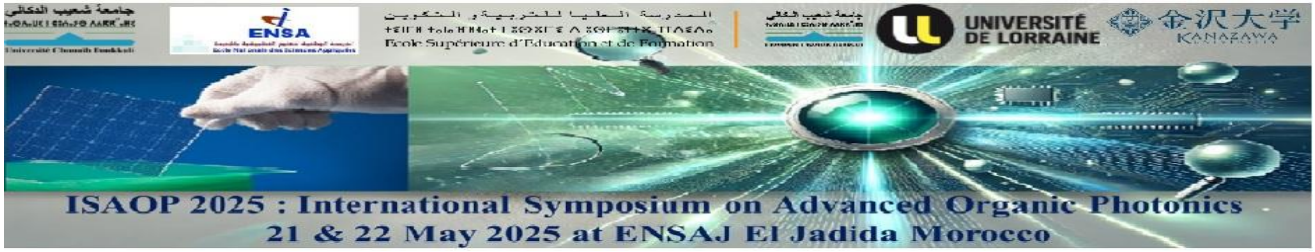
Abstract

This research explores the corrosion inhibition properties of bis-benzoxazole (BBOSZ), a newly synthesized heterocyclic organic compound, on C38 steel immersed in hydrochloric acid solution. The study employs electrochemical impedance spectroscopy (EIS) and potentiodynamic polarization (PDP) to evaluate performance, complemented by spectroscopic characterization.

Electrochemical results show that BBOSZ behaves as a mixed-type inhibitor. The inhibition efficiency obtained from both methods is consistent, reaching a maximum of 96.89% at a concentration of 5.0×10^{-4} mol/L. The adsorption process follows the Langmuir isotherm, with a standard free energy of adsorption ($\Delta G°_{ads}$) of approximately –41.12 kJ/mol. This suggests that BBOSZ adsorbs onto the steel surface through both physical and chemical interactions. Scanning electron microscopy confirms the formation of a protective layer.

To gain deeper insight into the interaction mechanisms, theoretical calculations based on density functional theory (DFT), Monte Carlo (MC), and molecular dynamics (MD) simulations were performed. Theoretical findings align closely with experimental data, confirming that BBOSZ forms a stable adsorbed film that effectively shields the metal surface from corrosion.

Keywords : Benzoxazole-2-thione, BBOSZ, Corrosion inhibition, Hydrochloric acid, C38 steel



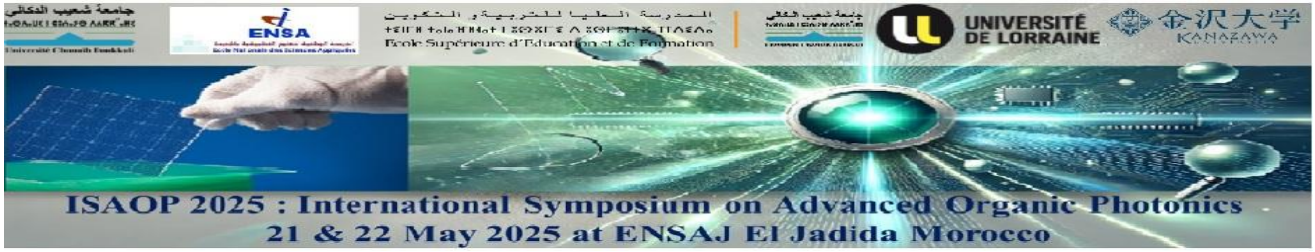
Green synthesis of Ag_2O nanoparticles from fruit seed shells for the removal of organic dyes

Asmae SANAD[1],

[1] Laboratory of Organic Bioorganic Chemistry and Environment, Faculty of Sciences, University Chouaib Doukkali, El Jadida, Morocco.

In response to the growing concern over water pollution caused by industrial dyes, this study investigates the green synthesis of novel Ag_2O nanoparticles derived from fruit shells—an abundant agro-waste material—as an eco-friendly adsorbent. The biosorbent was chemically activated and evaluated for its efficiency in removing methylene blue (MB), under various experimental conditions. To optimize the adsorption process, a Central Composite Design (CCD) was employed to assess the influence of five key factors: solution pH, adsorbent dosage, initial dye concentration, contact time, and temperature. The results revealed significant interactions among these parameters, with pH and adsorbent dose playing particularly crucial roles. Under optimal conditions, the removal efficiency of MB exceeded 97%. This study highlights the potential of fruit shell-based biomaterials as sustainable and eco-friendly alternatives for the treatment of dye-contaminated wastewater.

Keywords: methylene blue; Adsorption; Experiment design; Wastewater treatment.



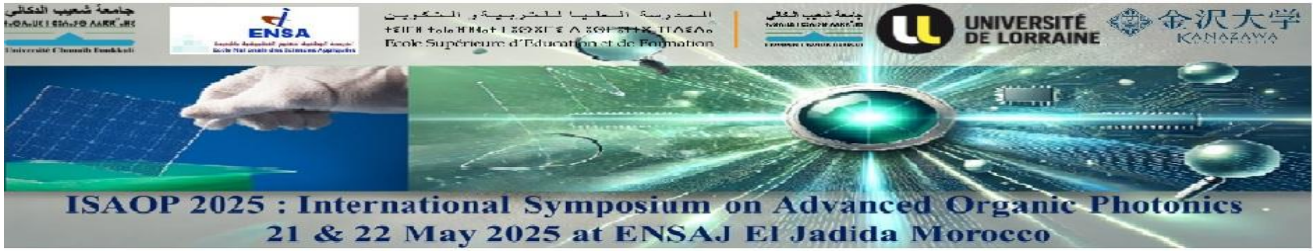
Valorization of phosphogypsum for the synthesis of a MMT-HAP-CTS bio-composite: An efficient adsorbent for arsenic removal

Meryeme Joudi[1,2*], Otman Goudali[2], Mariam Attouch[1], Badreddine Hatimi[1], Asmae Sanad[1], Meryem Bensemlali[1] , Hamid Nasrellah[1,3], Mostapha Siniti[2], Mina Bakasse[1]

1 Laboratory of Organic Bioorganic Chemistry and Environment, Faculty of Sciences, University Chouaib Doukkali, El Jadida, Morocco.
2 Laboratory of Chemistry of Coordination and Analytics, Faculty of Sciences, B.P. 24000, El Jadida, Morocco.
3 Higher School of Education and Training, University Chouaib Doukkali, El Jadida, Morocco
* joudi.m@ucd.ac.ma

Arsenic contamination in water is a major global concern due to its high toxicity, persistence in the environment, and serious health risks, including carcinogenicity. As a result, the development of low-cost, sustainable, and efficient materials for arsenic removal from aqueous media remains a pressing challenge. In this work, a novel bio-inorganic composite film based on Montmorillonite (MMT), Hydroxyapatite (HAP), and Chitosan (CTS) was synthesized and evaluated for its adsorption performance toward arsenic ions. Notably, the hydroxyapatite was derived from industrial phosphogypsum waste, providing an environmentally friendly valorization route for this abundant by-product.
The synthesized MMT-HAP-CTS composite was extensively characterized using Fourier-transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), scanning electron microscopy (SEM), thermogravimetric analysis (TGA), and differential thermal analysis (DTA). The characterization results confirmed the successful integration of the three components, with the formation of a stable, porous, and thermally resistant structure. Batch adsorption experiments demonstrated a high affinity of the composite for arsenic, achieving a maximum adsorption capacity (q_max) of 85.49 mg/g under optimized conditions (initial As concentration: 15 mg/L; adsorbent dosage: 0.2 g/L; pH: 6; temperature: 20 °C).
Thermodynamic analysis indicated that the adsorption process was spontaneous and exothermic, governed by favorable interactions between arsenic species and the active sites of the composite matrix. The synergy between the high surface area of montmorillonite, the ion-exchange and adsorption capacity of HAP, and the film-forming and biocompatible nature of chitosan contributed to the enhanced removal performance. These findings highlight the potential of the MMT-HAP-CTS film as a cost-effective and sustainable adsorbent for the treatment of arsenic-contaminated water, while also promoting the circular use of industrial waste materials.

Keywords:
Arsenic removal; Montmorillonite; Hydroxyapatite; Phosphogypsum; Chitosan; Composite film; Adsorption; Water treatment; Thermodynamic analysis.



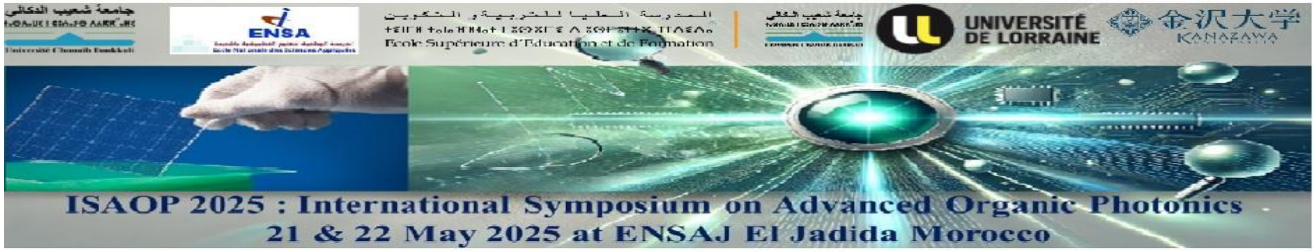
Enhancing Hydrogen Storage in MgH_2: The Role of Mechanical Deformation and Elemental Substitution

Abdelmajid Assila [a,], Ikram Belkoufa [a], Amine Alaoui Belghiti [a], Said laasri [a,**], El-kebir Hlil [b], Abdelowahed Hajjaji [a]*

[a] *Chouaib Doukkali University of El Jadida, National School of Applied Sciences, Energy Science Engineering Lab, El Jadida, Morocco*
[b]*Univ. Grenoble Alpes, CNRS, Grenoble INP, Institut N´eel, 38000, Grenoble, France*
** Corresponding author: assila.a@ucd.ac.ma (A. Assila [a,*]); laasrisaid@yahoo.fr (S.laasri [a,**])*

In this study, we propose a novel approach to enhance the structural, electronic, and thermodynamic properties of magnesium hydride (MgH2) using density functional theory (DFT). Magnesium atoms are partially substituted with 20% aluminum (Mg0.8Al0.2H2), titanium (Mg0.8Ti0.2H2), and vanadium (Mg0.8V0.2H2). The latter compound is further subjected to uniaxial tensile and compressive strains along the Oz axis in the [001] direction. We first calculate the lattice parameters of pure MgH2, followed by those of the substituted hydrides under uniaxial strain, using the generalized gradient approximation (GGA) as formulated by Perdew and Wang (PW91). The volume of substituted hydrides decreases under compression and increases under tension. Pure MgH2 has a volumetric hydrogen capacity of 108 g/L.H2, which increases under tensile strain in Mg0.8M0.2H2 (M = Al, Ti, V), and decreases under compression. Its gravimetric capacity is 7.65%, slightly reduced with substitution, but still above the DOE target of 6%. The formation enthalpy of MgH2 is -71.05 kJ/mol.H2. Under ±3% strain, substituted hydrides show reduced enthalpies, approaching the DOE's optimal value of -40 kJ/mol.H2, with Mg0.8Al0.2H2 reaching -38.19 kJ/mol.H2 under tension. The decomposition temperature of pure MgH2 is 546.53 K. Upon 20% substitution and application of a +3% tensile strain, it decreases to 304.63 K (Mg0.8Al0.2H2), 510.06 K (Mg0.8Ti0.2H2), and 462.97 K (Mg0.8V0.2H2). Under -3% compressive strain, the values drop further to 293.76, 513.52, and 460.90 K, respectively. These temperatures, particularly for Al and V substituted hydrides, fall within or near the PEM fuel cell operating range (289–393 K).

Keywords : hydrogen storage, hydride, MgH2, DFT calculation.



Theoretical Investigation of the Anticorrosion Properties of Benzimidazole Derivatives: A DFT, Molecular Dynamics, and Monte Carlo approach

Imane Bachir[1], Ali Barhoumi[1*], Abdelmalek Matine[1], Mimoun Belhadi[2], Said Jebbari[3], Mohammed Chafi[2], Mohammed Salah[1], Abdellah Zeroual[1]

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

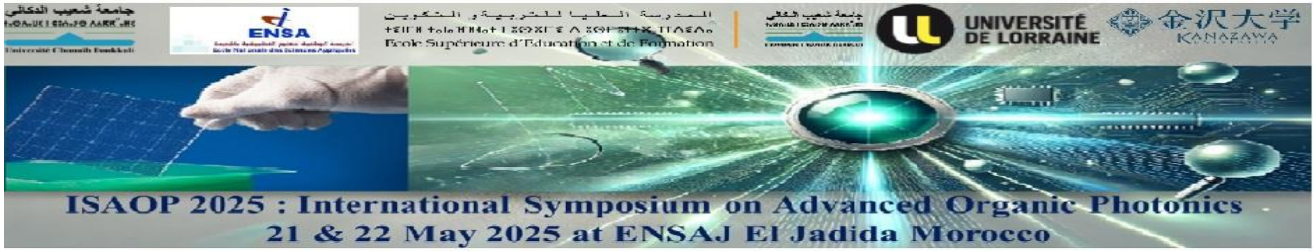
[2] Laboratory of Engineering, Processes and Environment-LIPE-GPIM, Higher School of Technology, University Hassan II of Casablanca, B.P. 8012, El jadida Road, Km7, Casablanca, Morocco

[3] Laboratory of Bio-Organic Chemistry, Department of Chemistry, Faculty of Sciences, Chouaib Doukkali University, El Jadida, Morocco

* Corresponding author: barhoumi2005@yahoo.fr

Organic inhibitors are widely used to protect metal surfaces against corrosion. In this study, we explored, using quantum chemistry calculations, the key factors influencing the efficiency of inhibition processes. The inhibitory properties of organic compounds (6-chloro-1H-benzo[d]imidazole-2-thiol and 6-methyl-1H-benzo[d]imidazole-2-thiol) were evaluated through density functional theory (DFT) calculations using the B3LYP/6-31(d,p) formalism.
The obtained results reveal a strong correlation between the inhibitory efficiency (IE%) of the inhibitors on iron and the quantum reactivity descriptors derived from DFT. Moreover, the interaction between the inhibitory molecules and the Fe (110) metallic surface was studied using molecular dynamics simulations and Monte Carlo (MC) simulations. These analyses highlighted strong interactions between the organic compounds and the iron surface, confirming their excellent inhibitory potential.
In conclusion, the studied inhibitors demonstrate significant efficiency in reducing the metal corrosion rate, suggesting their relevance as promising anticorrosion agents for industrial applications.

Keywords: Corrosion, (DFT), Quantum Descriptors, Monte Carlo Simulation, Molecular Dynamics.



Synthesis and characterization of novel metal complexes-based sulfonamide Schiff base ligand as photosensitizers in dye-sensitized solar cells

Bouchra ES-SOUNNI [1], Amina ABOUZID [1], Ayoub OUADDI [1], Houria RAJI [2], Jean-Claude DARAN [3], Noureddine MAZOIR [1], Ahmed BENHARREF [2], Abdelkrim MOUZDAHIR [1], Rabiaa FDIL [1], Mohamed BAKHOUCH [1]

[1]Bioorganic Chemistry Team, Faculty of Science, Chouaïb Doukkali University, P.O. Box 24, El Jadida 24000, Morocco
[2]Laboratory of Molecular Chemistry, Faculty of Sciences Semlalia, Cadi Ayyad University, P.O. Box 2390, Marrakech 40000, Morocco
[3]Laboratoire de Chimie de Coordination, UPR-CNRS 8241,205, Route de Narbonne, Toulouse Cedex 31077, France

e-mail: bakhouch.m@ucd.ac.ma

Schiff base ligands incorporating sulfonamide frameworks have attracted considerable attention due to their diverse applications in coordination chemistry [1], medicinal chemistry [2,3], and material science [4]. In this work, a novel sulfonamide-based Schiff base ligand was synthesized via the condensation of a sulfonamide bearing a primary amine group with salicylaldehyde. The resulting ligand was subsequently coordinated with divalent transition metal ions, such as Cu(II) and Ni(II), to afford stable mono- and binuclear metal complexes. These complexes were characterized by a range of analytical and spectroscopic techniques including IR, UV-Vis, crystal X-ray diffraction, elemental and thermal analysis. Furthermore, the optoelectronic properties of the synthesized compounds were investigated, revealing promising features for potential applications in electronic and photonic devices. The influence of metal coordination on the electronic behavior of the ligand was also evaluated, providing insights into structure–property relationships.

***Keywords*:** Complex, Schiff base Ligand, spectroscopy, crystal XRD, optoelectronic properties.

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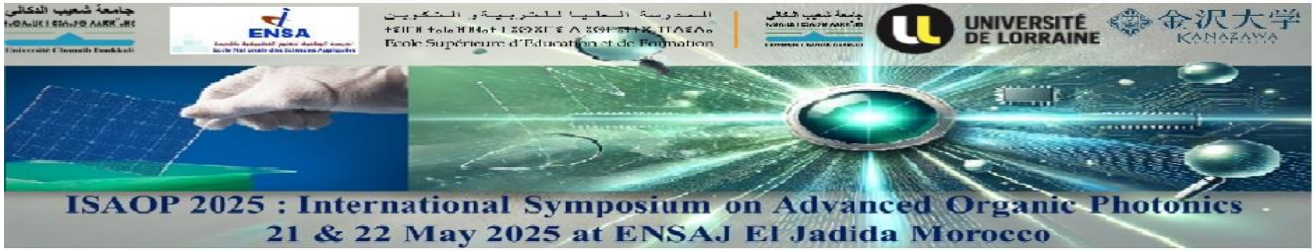


Utilizing Dielectric and Electrical Properties to Investigate Hexavalent Chromium Filtration via an Ultrafiltration Ceramic Membrane

El Ghaouti CHAHID[a,*], Abdelhadi MORTADI[b], El Mokhtar EL HAFIDI[c], Brahim LIZOUL[a], Abdermane. ELMLOUKY[b], R. EL MOZNINE[b], Said LAASRI[c]., Mohamed. Monkade[b].

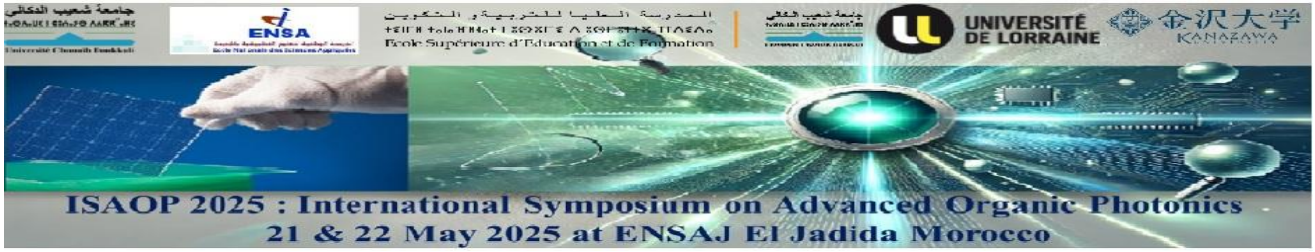
[a]*Polydisciplinary Faculty of Sidi Bennour, Chouaib Doukkali University, El Jadida, Morocco.*
[b]*Laboratory Physics of Condensed Matter (LPMC). Chouaib Doukkali University, El Jadida, Morocco.*
[c]*National School of Applied Sciences, Chouaib Doukkali University, El Jadida, Morocco.*

*Contact : chahidoo@yahoo.fr

In this work, we used impedance spectroscopy to study the monitoring of hexavalent chromium Cr(VI) retention by an ultrafiltration membrane based on $ZnAl_2O^{4-}TiO_2$. The results show that this membrane carries a residual charge that depends strongly on the pH. The effect of concentration on the retention rate of filtered species was investigated. The retention of the ionic species is due to a mechanism based on the electrostatic interactions between the membrane charge and the ions. An alkaline pH is favorable for good retention because the membrane charge becomes less positive, and chromium is in the form of CrO_4^{2-}.

To deepen and complete the study, impedance measurements were conducted in the frequency range from 100 mHz to 100 kHz to monitor treatment. The complex conductivity spectra analysis showed two Cole-Cole relaxation behaviors and an equivalent circuit was developed to extract the main parameters and investigate both relaxation processes further. The results of the electrical parameters deduced from the impedance spectra showed a good correlation with the parameters obtained by the ultrafiltration membrane.

Key words: Membrane, Filtration, Ultrafiltration, relaxation; dielectric dispersion, dielectric permittivity, electrical conductivity.



Electric and dielectric properties of the solid solution $K_xCu_{2-x/2}P_2O_7$ using impedance spectroscopy

Halima. MORTADI[1*], Meryem BENSEMLALI[2],khadija CHOUNI[1],Fatima Zahra BOURAGBA[1],Abdelmonim.ASSEKOURI[1], Elmouloudi SABBAR[1] and Mohammed Bettach[1].

[1]Faculty of Sciences, University Chouaib Doukkali, Chemistry Department, Laboratory of Materials' Physical, Chemicals, El Jadida, Morocco.

[2]Laboratory of Organic Bioorganic and Environmental Chemistry, Chouaib Doukkali University.Morocco

Corresponding author* :halima.mortadi@gmail.com

The pyrophosphate compounds with the general formula $K_xCu_{2-x/2}P_2O_7$, with varying potassium contents (x = 0; 0.05; 0.1; and 0.2), were synthesized via the solid-state route. X-ray diffraction analysis confirmed the formation of the desired phases, all adopting the same crystal structure as the parent compound a-$Cu_2P_2O_7$[1]. This observation indicates that partial potassium doping does not significantly alter the overall crystal structure of the material. Infrared spectroscopy was also used to verify the presence of characteristic P_2O_7 groups, which indicate the structural integrity of the pyrophosphates. The electrical and dielectric properties of these compounds were studied at room temperature using impedance spectroscopy (IS) over a frequency range from 1 Hz to 1 MHz. The obtained impedance spectra were modeled using an equivalent electrical circuit, allowing the extraction of various electrical parameters. The study of the alternating current conductivity (σ_{ac}) revealed a typical behavior following a double power law, indicating the coexistence of multiple charge transport mechanisms. The evolution of this conductivity with potassium content highlighted a significant influence of potassium on conduction properties, suggesting that the introduction of potassium into the crystal lattice significantly affects charge carrier mobility. Finally, the analysis of the dielectric constant and dielectric loss factor as functions of frequency and potassium content provided deeper insight into the present polarization mechanisms and allowed discussion of their dependence on chemical composition.

Keywords: Copper potassium pyrophosphate, ionic conductivity, dielectric properties, impedance spectroscopy.

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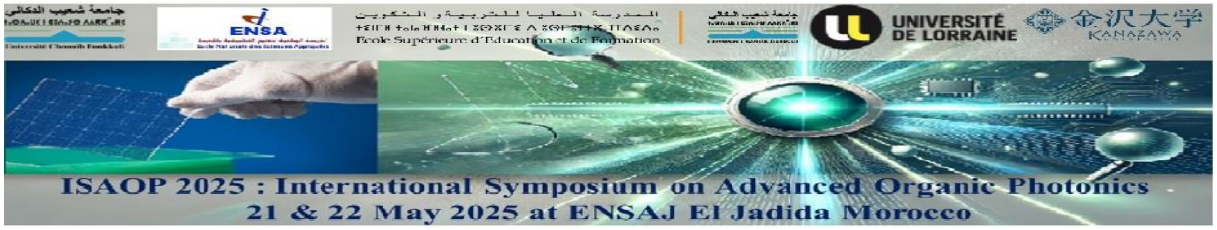

Magnetocaloric Potential of NdPd: A Theoretical Approach for Cryogenic Applications

Labdere OUTMAN*[1] and Salmani EL MEHDI [1]

1 Affiliation (Times New Roman, 10pt).
[1]LaMCScI, Faculty of Science, Mohammed V University, B.P. 1014 Rabat, Morocco
* labdere@gmail.com.

In this study, the fundamental properties and magnetic behavior of the NdPd compound were thoroughly investigated using a combination of ab initio calculations and Monte Carlo simulations. The calculated magnetic moment of the Nd atom (3.11 μ_B) closely matches experimental data. Exchange interactions revealed dominant ferromagnetic coupling, with the first two exchange constants (J_1 = 1.593 meV, J_2 = –0.358 meV) indicating a tendency toward magnetic ordering. Simulations confirmed a ferromagnetic transition at a Curie temperature (T_c) of 16 K. Furthermore, the isothermal magnetic entropy change under a 5 T field exhibited strong agreement with experimental observations, highlighting the promising potential of NdPd as a magnetocaloric material for cryogenic refrigeration below 20 K.

Keywords: NdPd compound, Magnetic properties, Ab initio calculations, Monte Carlo simulations, Exchange interactions, Magnetic entropy change

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