EMCMRE-8

EURO-MEDITERRANEAN CONFERENCE ON MATERIALS AND RENEWABLE ENERGIES - 8

MARRAKECH
MOROCCO

JUNE 29 -
JULY 02, 2026

GRAND MOGADOR
AGDAL HOTEL
5 ★

**Uniting Science,
Innovating Materials,
Powering a
Sustainable Future**

MATERIALS | RENEWABLE ENERGIES | INNOVATION | SUSTAINABILITY

Académie Hassan II des Sciences et Techniques
université PARIS-SACLAY FACULTÉ DES SCIENCES D'ORSAY
ISMO Institut des sciences moléculaires d'Orsay
CNRST
gasup
STARM

كلية العلوم والتقنيات - مراكش
FACULTE DES SCIENCES ET TECHNIQUES - MARRAKECH
MARRAKECH UNIVERSITÉ CADI AYYAD

كلية العلوم السملالية - مراكش
FACULTÉ DES SCIENCES SEMLALIA - MARRAKECH
MARRAKECH UNIVERSITÉ CADI AYYAD

LIÈGE université
GREEnMat

Foreword

On behalf of the organizing committee, we warmly welcome you to Marrakech for the 8th Euro-Mediterranean Conference on Materials and Renewable Energies (EMCMRE-8). The primary aim of this conference is to enhance collaborations among materials scientists and researchers from Europe, the USA, and countries in the southern and eastern Mediterranean regions. The conference will focus on topics such as 2D materials, energy storage, green hydrogen, novel and advanced materials, and advanced characterization.

This year, the conference will highlight significant advancements in nanomaterials and two-dimensional (2D) materials aimed at enhancing processes relevant to renewable energies, particularly in photovoltaics, batteries, and hydrogen production. These subjects align closely with the research priorities of Mediterranean countries.

The event will cover various topics, including energy storage, and materials for renewable energies, with a special emphasis on nanoscience and nanotechnology. The interdisciplinary nature of the conference will bridge the fields of physics, chemistry, biology, and computer science, all contributing to renewable energy advancements. We welcome students, faculty, researchers, and engineers from universities, engineering schools, research institutes, and industry.

The conference will feature oral and poster presentations, along with invited talks. The active participation of graduate students from both sides of the Mediterranean is crucial to the mission of the EMCMRE conference series.

We extend our sincere gratitude to ISMO and Paris-Saclay University, GREEnMat and University of Liège, Hassan II Academy Of Science and Technology, Cadi Ayyad University, Faculty of Sciences Semlalia and Faculty of Sciences and Technology of Marrakech, National Center for Technical and Scientific Research, Groupement d'Assurances du Supérieur (GASUP) and STARM for their financial support. Our heartfelt thanks also go to all other sponsors and the local organizing committee members for their invaluable contributions.

The Steering Committee

Invited speakers

2D Materials

Chair: Dr. Yannick Dappe, C2N-CNRS, France

Invited speakers:

Dr. Laurent Simon, Institut de Science des Matériaux de Mulhouse, France
Prof. Sébastien Lebègue, CNRS – Université de Strasbourg, France
Prof. Laurence Masson, Aix-Marseille University, France
Prof. Yann Girard, Université Paris Cité, France
Prof. Tristan Cren, CNRS - Sorbonne University, France
Prof. Marie Hervé, CNRS - Sorbonne University, France
Dr. Jérôme Lagoute, Université Paris Cité, France
Prof. Chun-Liang Lin, National Yang Ming Chiao Tung University, Taiwan
Dr. Vincent Huc, Paris-Saclay University, France
Prof. Ludovic Tortech, Sorbonne University – CEA de Saclay, France
Dr. Yannick Dappe, C2N-CNRS, France

Energy Storage

Chair: Dr. Abdelfattah Mahmoud, Liège University, Belgium

Invited speakers:

Dr. Damian Cupid, Austrian Institute of Technology, Austria
Dr. Jolanta Światowska, CNRS – PSL University, France
Prof. Ulla Lassi, University of Oulu, Finland
Dr. Mustapha Balarabe Idris, University of South Africa, South Africa
Dr. Abdelfattah Mahmoud, Liège University, Belgium

Green Hydrogen and Novel Materials

Chair: Prof. Omar Mounkachi, UM6P – Mohammed V University, Morocco

Invited speakers:

Prof. Abdelilah Benyoussef, Mohammed V University, Morocco
Dr. Majid El Kassaoui, University Mohammed VI Polytechnic, Morocco
Prof. Omar Mounkachi, UM6P – Mohammed V University, Morocco

Advanced Materials and characterization

Chair: Dr. Hamid Oubaha, Liège University, Belgium

Invited speakers:

Dr. Nouha Gazbour, CEA INES, France

Dr. Hamid Oubaha, Liège University, Belgium

EMCMRE-8 organizing committees

Chairs

Prof. Abdelkader Kara, University of Central Florida, USA

Prof. Hamid Oughaddou, Cergy-Paris University and ISMO-CNRS, France

Co-Chairs

Dr. Yannick Dappe, C2N-CNRS, France

Prof. Mustapha Ait Ali, Cadi Ayyad University, Morocco

Steering Committee

Prof. Mustapha Ait Ali, Cadi Ayyad University, Morocco

Prof. Karima Lasri, University Mohammed VI Polytechnic, Morocco

Prof. Yahya Boughaleb, ENSA Université Chouaib Doukkali, El Jadida, Morocco

Prof. Khalil Amine, Argonne National Laboratory, USA

Prof. Jean-Louis Lemaire, Paris, France

Prof. Abdelkader Kara, University of Central Florida, USA

Prof. Hamid Oughaddou, Cergy-Paris University and ISMO-CNRS, France

Dr. Yannick Dappe, C2N-CNRS, France

Dr. Moulay Tahar Sougrati, CNRS-Montepllier, France

Dr. Abdelfattah Mahmoud, Liège University, Belgium

Prof. Abdou Lachgar, Wake Forest University, USA

Prof. Mustapha Mabrouki, Sultan Moulay Slimane University, Morocco

Prof. Mohamed Monkade, Université Chouaib Doukkali, Morocco

Prof. Omar Mounkachi, UM6P and Mohammed V University, Morocco

Advisory Committee

Prof. Karima Lasri, University Mohammed VI Polytechnic, Morocco

Prof. Omar Mounkachi, UM6P and Mohammed V University, Morocco

Prof. Yahya Boughaleb, ENSA Université Chouaib Doukkali, El Jadida, Morocco

Prof. Mustapha Ait Ali, Cadi Ayyad University, Morocco

Prof. Khalil Amine, Argonne National Laboratory, USA

Prof. Abdelilah Benyoussef, Mohammed V University, Morocco

Prof. Abdelkader Kara, University of Central Florida, USA

Prof. Abdessadek Lachgar, Wake Forest University, USA

Prof. Jean-Louis Lemaire, Paris, France

Prof. Hamid Oughaddou, Cergy-Paris University and ISMO-CNRS, France

Dr. Yannick Dappe, C2N-CNRS, France

Dr. Moulay Tahar Sougrati, CNRS-Montepllier, France

Dr. Abdelfattah Mahmoud, Liège University, Belgium

Prof. Mustapha Mabrouki, Sultan Moulay Slimane University, Morocco

Prof. Mohamed Monkade, Université Chouaib Doukkali, Morocco

Prof. Said Laasri, Université Chouaib Doukkali, Morocco

Honorary committee

Prof. Belaid Bougadir, President of Cadi Ayyad University, Morocco

Prof. El Hassan El Mouden, Dean of the Faculty of Sciences Semlalia, Marrakech, Morocco

Prof. Said Rakrak, Dean of the Faculty of Sciences and Technology, Marrakech, Morocco

Prof. Yahia Boughaleb, ENSA Université Chouaib Doukkali, El Jadida, Morocco

Scientific Committee

Prof. Hicham Benyoucef, University Mohammed VI Polytechnic, Morocco

Prof. Mustapha Ait Ali, Cadi Ayyad University, Morocco

Prof. Karima Lasri, University Mohammed VI Polytechnic, Morocco

Prof. Michael Altman, Hong Kong University of Science and Technology, China

Prof. Khalil Amine, Argonne National Laboratory, USA

Prof. Nour-Eddine Benkhettou, Sidi Bel Abbès University, Algeria

Prof. Abdelilah Benyoussef, Mohammed V University, Morocco

Prof. Abdelilah Kaddouri, Cadi Ayyad University, Morocco

Prof. Abdessadek Lachgar, Wake Forest University, USA

Prof. Jean-Louis Lemaire, Paris, France

Dr. Yannick Dappe, C2N-CNRS, France

Prof. Mohamed Monkade, Université Chouaib Doukkali, Morocco

Prof. Mustapha Mabrouki, Sultan Moulay Slimane University, Morocco

Prof. Abdelmadjid Almaggoussi, Cadi Ayyad University, Morocco

Dr. Abdelfattah Mahmoud, Liège University, Belgium

Dr. Hamid Oubaha, Liège University, Belgium

Prof. Omar Mounkachi, UM6P and Mohammed V University, Morocco

Dr. Moulay Tahar Sougrati, CNRS-Montepllier, France

Prof. Abdelkader Kara, University of Central Florida, USA

Prof. Hamid Oughaddou, Cergy-Paris University and ISMO-CNRS, France

Prof. Nabil Rochdi, Cadi Ayyad University, Morocco

Prof. Yahia Boughaleb, ENSA Université Chouaib Doukkali, El Jadida, Morocco

Prof. Said Laasri, Université Chouaib Doukkali, Morocco

Prof. Said Yagoubi, University of Paris Saclay, France

Local Committee

Prof. Abdelmadjid Almaggoussi, Cadi Ayyad University, Morocco

Prof. Mustapha Ait Ali, Cadi Ayyad University, Morocco

Prof. Nabil Rochdi, Cadi Ayyad University, Morocco

Prof. Abdelkader El Kissani, Cadi Ayyad University, Morocco

Prof. Ayoub Abdelkader Mekkaoui, Cadi Ayyad University, Morocco

Prof. Othmane Zakir, Cadi Ayyad University, Morocco

Prof. Ali Hasnaoui, Cadi Ayyad University, Morocco

Prof. Ismail Hdoufane, Cadi Ayyad University, Morocco

Detailed Program

2D Materials

Energy Storage

Green Hydrogen and Novel Materials

Advanced Materials and Characterization

Poster Highlights

Monday, June 29, 2026	
08:30 – 09:30	**Registration at Faculty of Sciences Semlalia**
09:30 – 10:00	**OPENING CEREMONY**
10:00 – 10:30	**Coffee Break**
Session: Green Hydrogen and Novel Materials **Chair: Prof. Omar Mounkachi**, UM6P – Mohammed V University, Morocco	
10:30 – 11:00	**Prof. Abdelilah Benyoussef**, Mohammed V University, Morocco (Invited) *Theoretical Insights into Hydrogen Energy Applications Using 2D Materials and Metal–Organic Frameworks*
11:00 – 11:15	**Prof. Ayoub Abdelkader Mekkaoui**, Cadi Ayyad University, Morocco *Waste-to-Resource: Reusing an Industrial Mining Waste in Selective Heterogeneous Catalytic Chlorination*
11:15 – 11:45	**Dr. Majid El Kassaoui**, University Mohammed VI Polytechnic, Morocco (Invited) *Towards Sustainable Hydrogen Energy: Engineering MOFs for Efficient Hydrogen Storage*
11:45 – 12:00	**Hamza Eljabbar**, Cadi Ayyad University, Morocco *Biogenic Synthesis of Nanoparticles using Carboxymethyl Cellulose as an Efficient Stabilizer and Matrix*
12:00 – 12:15	**Achraf Razouk**, Mohammed V University, Morocco *Improving Hydrogen Storage in MgH_2 (110) via Transition Metal Oxide Catalysts: Insights into Kinetics and Thermodynamics*
12:15 – 14:00	**LUNCH**

	Session: Energy Storage **Chair: Dr. Abdelfattah Mahmoud**, Liège University, Belgium
14:00 – 14:30	**Dr. Damian Cupid**, Austrian Institute of Technology, Austria (Invited) *STREAMS: Sustainable Technologies for Reducing Europe's bAttery raw MaterialS dependence*
14:30 – 14:45	**Zouhir Mansouri**, University Mohammed VI Polytechnic, Morocco *First-principles-guided design of robust electrode materials for grid-scale zinc-ion batteries*
14:45 – 15:15	**Dr. Jolanta Światowska**, CNRS – PSL University, France (Invited) *Aqueous Metal–Air Batteries: Challenges in Mastering the Electrode–Electrolyte Interface*
15:15 – 15:30	**Nouhaila Laaribi**, Cadi Ayyad University, Morocco *Recycling of End-of-Life reverse osmosis membranes for wastewater treatment*
15:30 – 15:45	**Abdessamad Nidlhaj**, Université Moulay Ismaïl, Morocco *Ni/F Co-Doped $NaFePO_4$ as a Cathode Material for Sodium-Ion Batteries: A First-Principles Study*
16:00 – 16:30	**Coffee Break**
	Session: Poster Highlights **Chair: Prof. Mustapha Ait Ali**, Cadi Ayyad University, Morocco
16:30 – 16:35	**Khadija Seyagh**, Cadi Ayyad University, Morocco *Magnetically Recoverable Nanocomposites: A Sustainable Approach for Photocatalytic Degradation of Organic Dyes in Wastewater Treatment*
16:35 – 16:40	**Mohammed El-Bassri**, Cadi Ayyad University, Morocco *Monoethanolamine (MEA) Concentration Effect on the Physical Properties of Tin Sulfide (SnS) Thin Films*
16:40 – 16:45	**Yassine Bounnaiche**, University Mohammed VI Polytechnic, Morocco *Complexing agents' addition effect on the physical properties of electrodeposited Sb_2S_3*
16:45 – 16:50	**Mouhcine Ourbaa**, Cadi Ayyad University, Morocco *Nitrogen-annealing-induced interfacial diffusion in RF sputtered SnO_2/Cu/SnO_2 multilayers toward improved photocatalytic performance*
16:50 – 16:55	**Noureddine Lebrini**, Cadi Ayyad University, Morocco *Influence of Sn Dopant Concentration on NiS_2 Thin Films Prepared by Spin Coating for Supercapacitor Applications*
16:55 – 17:00	**Aymane Ezerraf**, Cadi Ayyad University, Morocco *Machine Learning and DFT-Assisted Design of Eco-Friendly Organic Corrosion Inhibitors for Mild Steel Protection in Acidic Media*
17:00 – 17:05	**Rachid Haroudi**, Cadi Ayyad University, Morocco *DFT Investigation of the PtS_2/ZrS_2 Heterojunction for Enhanced Photocatalytic Hydrogen Evolution*

17:05 – 17:10	**Adil Mojahid**, Cadi Ayyad University, Morocco *Investigation of the Electronic and Optical Properties of Doped Borophene*
17:10 – 17:15	**Ikram Oughaddou**, Cadi Ayyad University, Morocco *Towards Multiscale Modeling of Lithium-Ion Transport in NMC Cathode Materials Using Deep Learning Potentials*
17:15 – 17:20	**Oualid Mouktaoui**, Cadi Ayyad University, Morocco *Development of New Chelating Agents for Heavy Metal Complexation*
17:20 – 17:25	**Imad Salym**, Cadi Ayyad University, Morocco *Optoelectronic enhancement and exciton control in Si-doped KGeF3 perovskites*
17:25 – 17:30	**Jihane Ziraoui**, Cadi Ayyad University, Morocco *Using Waste Jute Bags as Reinforcement to Enhance Geopolymers: An Eco-Friendly Solution for Sustainable Construction*
17:30 – 17:35	**Brahim Fakrach**, Cadi Ayyad University, Morocco *A Raman Spectroscopy Study of Double-Walled Carbon Nanotubes at Optimal Interlayer Distance*

Tuesday, June 30, 2026

Session: 2D Materials **Chair: Dr. Yannick Dappe**, C2N-CNRS, France	
08:30 – 09:00	**Prof. Laurence Masson**, Aix-Marseille University, France (Invited) *Epitaxial growth and properties of silicene and other 2D allotropes of Si: the case of the Si/Ag interface*
09:00 – 09:15	**Mohammed Benchtia**, Cadi Ayyad University, Morocco *Electronic tunability and anisotropy in 2D P–N allotropes under strain*
09:15 – 09:45	**Prof. Sébastien Lebègue**, CNRS – Université de Strasbourg, France (Invited) *Some recent advances in 2D materials using ab initio calculations*
09:45 – 10:00	**Youssef Chlikhy**, Hassan II University of Casablanca, Morocco *Single Atom decoration for enhanced adsorption and gas sensing performance*
10:00 – 10:30	**Coffee Break and Poster Session**
Session: 2D materials **Chair: Prof. Laurence Masson**, Aix-Marseille University, France	
10:30 – 11:00	**Dr. Laurent Simon**, Institut de Science des Matériaux de Mulhouse, France (Invited) *From 2D to 1D carbon allotrope. Two examples of recent advances: functionalized graphene and carbyne based polymers*
11:00 – 11:30	**Dr. Jérôme Lagoute**, Université Paris Cité, France (Invited) *Electronic interactions in hexagonal phosphorus and Au(111)*
11:30 – 11:45	**Hamza El Garni**, Université Paris-Saclay, France *Reactivity of Black Phosphorene toward Oxygen and Its Passivation: A DFT and MD Study*
11:45 – 12:15	**Prof. Yann Girard**, Université Paris Cité, France (Invited) *Growth of phosphorus on metallic surfaces: steps care*
12:15 – 14:00	**LUNCH**
Session: Energy Storage **Chair: Dr. Jolanta Świątowska**, CNRS – PSL University, France	
14:00 – 14:30	**Dr. Mustapha Balarabe Idris**, University of South Africa, South Africa (Invited) *Mesoporous Graphitic Carbon Nitride: A Promising Electrode Material For Supercapacitor*
14:30 – 14:45	**Prof. Othmane Zakir**, Cadi Ayyad University, Morocco *Siloxene Nanosheets as Promising Anode Materials for Lithium-Ion Batteries: Synthesis and Characterization*

14:45 – 15:15	**Dr. Abdelfattah Mahmoud**, Liège University, Belgium (Invited) *Direct recycling of spent Li-ion batteries: innovative processes for sustainable cathode regeneration*
15:15 – 15:30	**Zineb Miftah**, University Mohammed VI Polytechnic, Morocco *A Continuum Electrochemical Modeling Approach for Investigating Transport and Performance Limitations in Lithium-Ion Batteries*
15:30 – 16:00	**Prof. Ulla Lassi**, University of Oulu, Finland (Invited) *Recovery of lithium from spent LIBs and Bayer cake to improve sustainability of battery value chain*
16:00 – 16:30	**Coffee Break and Poster Session**
Session: Advanced Materials and Characterization **Chair: Dr. Hamid Oubaha**, Liège University, Belgium	
16:30 – 17:00	**Dr. Nouha Gazbour**, CEA INES, France (Invited) *Sustainability Standards: A New Era for Photovoltaic Technologies*
17:00 – 17:15	**Abd Elaziz Rahhou**, Cadi Ayyad University, Morocco *Synthesis, Characterization and Photovoltaic Performance of Schiff Base Metal Complexes as Sensitizers for Dye-Sensitized Solar Cells (DSSCs)*
17:15 – 17:30	**Abdellah Hbab**, Ibnou Zohr University, Morocco *DFT Investigation of the Structural, Electronic, and Optical Properties of Cubic Tantalate Perovskites $ATaO_3$ (A = Cs, K, Na)*

Wednesday, July 01, 2026

	Session: 2D materials **Chair: Dr. Laurent Simon**, Institut de Science des Matériaux de Mulhouse, France
08:30 – 09:00	**Prof. Tristan Cren**, CNRS - Sorbonne University, France (Invited) *Misfit compounds as a platform for engineering doping, charge density waves and topological superconductivity*
09:00 – 09:30	**Prof. Marie Hervé**, CNRS - Sorbonne University, France (Invited) *Higher order topological defects in the moiré lattice of a van der Waals magnetic material*
09:30 – 10:00	**Prof. Ludovic Tortech**, Sorbonne University – CEA de Saclay, France (Invited) *Tuning the thin film interfaces for efficient devices: impact of the geometric organization of the molecules on specific electronic property*
10:00 – 10:30	**Coffee Break and Poster Session**
	Session: 2D materials **Chair: Prof. Marie Hervé**, CNRS - Sorbonne University, France
10:30 – 11:00	**Dr. Yannick Dappe**, C2N-CNRS, France (Invited) *Charge Density Waves propagation in van der Waals heterostructures*
11:00 – 11:30	**Dr. Vincent Huc**, Paris-Saclay University, France (Invited) *Graphene-like 2D carbon nitrides*
11:30 – 11:45	**Mohamed Mamlouk**, C2N-CNRS, France *Intelligent Molecular Switches for Brain-like Devices*
11:45 – 12:15	**Prof. Chun-Liang Lin**, National Yang Ming Chiao Tung University, Taiwan (Invited) *Characterization of Interfaces between Contact Metals and Monolayer 2D Semiconductor*
12:15 – 14:00	**LUNCH**
14:00 – 19:30	***Free Afternoon***
19:30 – 23:00	**BANQUET**

Thursday, July 02, 2026	
Poster Highlights **Chair: Prof. Mustapha Ait Ali**, Cadi Ayyad University, Morocco	
09:00 – 10:00	**Poster Session**
10:00 – 10:30	**Coffee Break**
Advanced Materials and Characterization **Chair: Prof. Nabil Rochdi**, Cadi Ayyad University, Morocco	
10:30 – 11:00	**Dr. Hamid Oubaha**, Liège University, Belgium (Invited) *Waste-to-Value Silicon: Pilot-Scale Upcycling of EoL PV Silicon into Si/C Li-ion batteries Anodes*
11:00 – 11:15	**Khadija Khaldoune**, Cadi Ayyad University, Morocco *Design and Functionalization of Schiff Base-Based Materials for Advanced Applications*
11:15 – 11:30	**Abderrazak Alihiane**, Cadi Ayyad University, Morocco *Interfacial Engineering of the ETL/Perovskite Interface Using a Thiophene-Based Capping Layer for Efficient Perovskite Solar Cells*
11:30 – 11:45	**Sokaina El Ouakili**, Cadi Ayyad University, Morocco *Sol-gel Synthesis and Interface Engineering of CZTS Thin Films Using ZnO/TiO_2 Buffer Layers*
11:45 – 12:15	**AWARDS and CLOSING CEREMONY**
12:15 – 14:00	**LUNCH**

Monday, June 29, 2026

GREEN HYDROGEN AND NOVEL MATERIALS **Invited Speaker**

Theoretical Insights into Hydrogen Energy Applications Using 2D Materials and Metal–Organic Frameworks

Abdelilah Benyoussef

Hassan II Academy of Science and Technology, Rabat, Morocco
LaMCScI, Faculty of Sciences, Mohammed V University, Rabat, Morocco

E-mail: benyous.a@gmail.com

Abstract:
This study presents a detailed first-principles analysis of two-dimensional (2D) and porous materials aimed at hydrogen energy applications, with particular emphasis on hydrogen generation and storage. For the investigated 2D materials, several important physicochemical descriptors are systematically evaluated, including hydrogen adsorption free energies, electronic charge redistribution, band structures, density of states, and reaction pathways involved in the hydrogen evolution reaction (HER). These characteristics provide insight into catalytic efficiency and help identify the active sites responsible for hydrogen adsorption and release.
In addition to 2D systems, porous frameworks—especially metal–organic frameworks (MOFs) such as MOF-5 and IRMOF-10—are studied for their potential in hydrogen storage. Owing to their exceptionally large surface areas, adjustable pore architectures, and chemical tunability, these materials represent attractive candidates for hydrogen physisorption. Key parameters such as hydrogen–framework interaction energies, adsorption behavior, and storage thermodynamics are analyzed to evaluate their storage performance under different operating conditions.
To achieve a more realistic description of material behavior beyond static density functional theory (DFT) calculations, Molecular Dynamics (MD) simulations are employed to examine thermal stability and structural robustness at finite temperatures. Furthermore, Kinetic Monte Carlo (KMC) simulations are used to investigate hydrogen diffusion, adsorption kinetics, and long-timescale dynamic processes.
The work covers several emerging 2D materials, including phosphorene, InP, SiC, BN, and selected two-dimensional carbides, all of which exhibit promising electronic tunability, strong surface activity, and high accessible surface areas. Hybrid architectures and heterostructures integrating 2D materials with MOFs are also explored in order to identify synergistic effects capable of improving both catalytic HER activity and hydrogen storage efficiency.
The comparative investigation demonstrates that modifications in composition, surface chemistry, and structural arrangement strongly affect hydrogen adsorption strength, electronic charge distribution, and catalytic performance. These results provide important guidelines for the rational design and optimization of advanced materials dedicated to hydrogen energy technologies.

Back to the program

Green Hydrogen and Novel Materials

Waste-to-Resource: Reusing an Industrial Mining Waste in Selective Heterogeneous Catalytic Chlorination

Salim Adam Labyad [1], Lahcen Fkhar [2], Abdelfattah Mahmoud [2], **Ayoub Abdelkader Mekkaoui** [3,*], Soufiane El Houssame [1]

[1] Laboratoire des Sciences des Matériaux, Mathématiques et Environnement, Université Sultan Moulay Slimane, Faculté Polydisciplinaire de Khouribga, BP 145, Khouribga 25000, Morocco

[2] GREEnMat, CESAM Research Unit, Chemistry Department, University of Liège, Quartier Agora, 13 Allée du 6 Août, 4000, Liège, Belgium

[3] Cadi Ayyad University, UCA, Faculté des Sciences Semlalia Marrakech, Département de Chimie, Laboratoire de Chimie Moléculaire, Equipe de Chimie de Coordination et de Catalyse, BP 2390, Marrakech 40001, Morocco

E-mail: mekk.ayoub@gmail.com; a.mekkaoui@uca.ac.ma

Abstract:

Waste management is a central advantage of heterogeneous catalysis, as it enables catalyst recovery, reuse and a significant reduction in hazardous byproducts, thereby improving environmental sustainability [1]. In this context, the catalytic chlorination reaction provides an efficient route to synthesize natural allylic chloride derivatives [2], which are important intermediates that serve as building blocks for more complex atomic arrangements [3], supporting cleaner and more sustainable chemical processes.

The present work focuses primarily on the advanced characterization of an iron-rich industrial mining waste by XRD, XRF, FTIR, Raman, ^{57}Fe Mössbauer spectroscopy, SEM-EDX, BET and Zeta-seizer analyses. Thereafter, we have investigated for the first time its application as an efficient magnetically recoverable heterogeneous catalyst in the selective catalytic chlorination of terpenic olefins.

The studied waste material presents a novel alternative to unlock the heterogenization of the chlorination reaction, aligning with waste recycling strategy. This highlights the novelty of applying waste-to-resource approach by reusing an iron-rich industrial mining waste as high magnetically recoverable heterogeneous catalyst for a better circular economy and sustainable chemistry.

References:

[1] C. Vogt, B.M. Weckhuysen. Nature Reviews Chemistry 6, 89 (2022).

[2] S.A. Labyad, A.A. Mekkaoui, M. Laayati, H. Orfi, L. El Firdoussi, S. El Houssame. RSC Adv. 13, 30548 (2023).

[3] A.A. Mekkaoui, M. Laayati, H. Orfi, L. El Firdoussi, S. El Houssame. Journal of Chemistry 2020, 1 (2020).

Back to the program

GREEN HYDROGEN AND NOVEL MATERIALS **Invited Speaker**

Towards Sustainable Hydrogen Energy: Engineering MOFs for Efficient Hydrogen Storage

Majid El Kassaoui

College of computing, Mohammed VI Polytechnic University, Lot 660, Hay Moulay Rachid Ben Guerir, 43150, Morocco

E-mail: psmajid0@gmail.com, Majid.ELKASSAOUI-EXT@um6p.ma

Abstract:
Metal-organic frameworks (MOFs) have emerged as highly promising materials for hydrogen storage due to their exceptionally high surface area, tunable pore structure, and structural versatility. The importance and impact of MOFs were recently recognized by the 2025 Nobel Prize in Chemistry, awarded to Omar M. Yaghi, Susumu Kitagawa, and Richard Robson for the development of metal-organic frameworks. In the context of sustainable energy systems, hydrogen is considered a clean energy carrier; however, its efficient storage remains a key challenge. MOFs offer a unique platform to enhance hydrogen uptake through rational design of metal nodes and organic linkers, enabling optimized adsorption sites and improved binding interactions. This presentation highlights the fundamental principles governing hydrogen adsorption in MOFs, recent advances in material design strategies, and performance enhancement approaches such as pore engineering, functionalization, and structural optimization. Overall, MOFs represent a powerful class of materials for achieving high-capacity and reversible hydrogen storage, contributing to the development of future clean energy technologies. The talk will present our recent developments in designing and optimizing MOFs for efficient hydrogen storage applications, using state-of-the-art theoretical calculations.

Back to the program

GREEN HYDROGEN AND NOVEL MATERIALS

Biogenic Synthesis of Nanoparticles using Carboxymethyl Cellulose as an Efficient Stabilizer and Matrix

Hamza Eljabbar [1,2,*], Salim Adam Labyad [1], Larbi El Firdoussi [2], Ayoub Abdelkader Mekkaoui [2], Soufiane El Houssame [1]

[1] Laboratoire des Sciences des Matériaux, Mathématiques et Environnement, Université Sultan Moulay Slimane, Faculté Polydisciplinaire de Khouribga, BP 145, Khouribga 25000, Morocco

[2] Cadi Ayyad University, UCA, Faculté des Sciences Semlalia Marrakech, Département de Chimie, Laboratoire de Chimie Moléculaire, Equipe de Chimie de Coordination et de Catalyse, BP 2390, Marrakech 40001, Morocco

E-mail: hamza.eljabbar@usms.ac.ma

Abstract:

The development of sustainable nanomaterials has accelerated interest in the biogenic synthesis of nanoparticles, as an eco-friendly alternative to conventional physical and chemical methods [1]. In this context, biopolymers play a crucial role as renewable stabilizers capable of enhancing the dispersity and stability of nanoparticles [2]. Among these, carboxymethyl cellulose (CMC) is widely used owing to their easily functionalization process, cost effectiveness, and availability, which provides a variety of possibilities for the design of advanced materials [3,4].

The present work seeks to investigate a biogenic synthesis development of carboxymethyl cellulose-based nanoparticles, studying effect of different parameters, i.e, pH and concentrations. Advanced characterization technics, such as UV-VIS, XRD, FT-IR, FE-SEM, and Zeta-seizer, were used in this study. Hence, the results showed a high stability and dispersity of the prepared nanocolloids, with average size of 168 nm.

References:

[1] D.S. Chormey, B.T. Zaman, T.B. Kustanto, S.E. Bodur, S. Bodur, Z. Tekin, O. Nejati, S. Bakırdere. Nanoscale 15, 19423 (2023).

[2] S. Haider, T. Kamal, S.B. Khan, M. Omer, A. Haider, F.U. Khan, A.M. Asiri. Applied Surface Science 387, 1154 (2016).

[3] J. Ning, X. Luo, F. Wang, S. Huang, J. Wang, D. Liu, D Liu, D. Chen, J Wei, Y Liu. Sensors 19, 5482 (2019).

[4] A.A. Mekkaoui, H. Orfi, K. Bejtka, M. Laayati, S.A. Labyad, L. El Firdoussi, C. F. Pirri, A. Chiodoni, S. El Houssame. Environmental Science and Pollution Research 30, 81619 (2023).

Back to the program

GREEN HYDROGEN AND NOVEL MATERIALS

Improving Hydrogen Storage in MgH_2 (110) via Transition Metal Oxide Catalysts: Insights into Kinetics and Thermodynamics

A. Razouk [1,*], M. EL Kassaoui [2], M. Boubkri [1], H. Abu-Farsakh [3], M. Bououdina [3], O. Mounkachi [1,2]

[1] Laboratory of Condensed Matter and Interdisciplinary Sciences, Faculty of Sciences, Mohammed V University, 1014 Rabat, Morocco
[2] College of computing, Mohammed VI Polytechnic University, Lot 660, Hay Moulay Rachid Ben Guerir, 43150, Morocco
[3] Department of Mathematics and Sciences, Faculty of Humanities and Sciences, Prince Sultan University, Riyadh, Saudi Arabia

E-mail: achrafrazzouk1997@gmail.com

Abstract:
Hydrogen storage materials play a vital role in the development of sustainable energy systems by enabling efficient energy storage and release. Among them, magnesium hydride (MgH_2) is considered a promising candidate due to its high hydrogen capacity and low cost. However, its practical application is hindered by slow hydrogen desorption kinetics and elevated operating temperatures. In this study, the MgH_2 (110) surface is investigated using density functional theory (DFT) and ab initio molecular dynamics (AIMD) simulations to better understand its hydrogen storage behavior. The impact of incorporating Nb_2O_5 and V_2O_5 clusters on surface stability and hydrogen release is systematically explored. The results show that these catalysts significantly weaken the surface stability, thereby facilitating hydrogen desorption and reducing the required operating temperature. Notably, the V_2O_5-modified MgH_2 system exhibits superior performance, with enhanced hydrogen release kinetics and a reduced desorption temperature of 341.77 K. Furthermore, diffusion analysis reveals a marked decrease in activation energy barriers, with the lowest value of 0.189 eV observed for the V_2O_5-containing system. These findings provide valuable insights into catalyst-assisted hydrogen transport mechanisms and highlight effective strategies for improving Mg-based hydrogen storage materials.

Back to the program

ENERGY STORAGE **Invited Speaker**

STREAMS: Sustainable Technologies for Reducing Europe's bAttery raw MaterialS dependence

Damian M. Cupid

AIT Austrian Institute of Technology GmbH, Giefinggasse 4, 1210, Vienna, Austria

E-mail: damian.cupid@ait.ac.at

Abstract:
STREAMS is a HORIZON Europe project which aims to strengthen the European battery materials supply chain, reduce Europe's dependency on imported raw materials supplies and increase its resilience, competitiveness and strategic autonomy in the global battery manufacturing industry. To achieve this, the STREAMS consortium develops a comprehensive portfolio of flexible and scalable technologies and solutions to sustainably produce battery-grade precursors and their respective cathode and anode active materials from primary sources, secondary sources, and black mass.
In this presentation, the scientific coordinator of STREAMS will show the advancements made in technologies and processes for the recovery of lithium, transition metals, and graphite from secondary sources and lithium-ion black mass. These technologies include selective electrowinning, supported liquid membranes, electrochemical lithium recovery, deep eutectic solvent leaching and direct recycling.
For example, STREAMS has developed atmospheric leaching and solvent extraction processes to recover Li as Li_2CO_3 from the Bayer cake with a 90% recovery rate. In addition, STREAMS has designed a single, saleable process, which allows the Bayer cake to be used as a reagent to purify the leachate originating from lithium-ion battery waste while simultaneously increasing the concentration of Li in the leachate. Regarding the transition metals, solvent extraction techniques have been developed to recover Co, Ni and Mn sulphate salts from pyrite mining tailings, which exhibit the purities required for processing into cathode active materials for lithium-ion batteries. Finally, deep eutectics have been explored as solvents for the efficient recovery of Ni, Co and Mn from lithium-ion black, allowing them to be directly precipitated as mixed hydroxide precursors with defined chemical compositions.
On the anode side, graphite has been recovered, purified and rehabilitated from end-of-life batteries, and its electrochemical performance has been tested in half-cells and full-cells using aqueous electrode processing. Furthermore, STREAMS shows that biochar can be processed into a conductive additive and used in electrode formulations for NMC 811 cathodes.
This project has received funding from the European Union's Horizon Europe research and innovation programme under the Grant Agreement No 101137771. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the European Climate, Infrastructure and Environment Executive Agency (CINEA). Neither the European Union nor the granting authority can be held responsible for them.

Back to the program

ENERGY STORAGE

First-principles-guided design of robust electrode materials for grid-scale zinc-ion batteries

Zouhir Mansouri [1,*], Omar Mounkachi [2]

[1] College of Computing, Mohammed VI Polytechnic University, 43150 Ben Guerir, Morocco
[2] Laboratoire de Matière Condensée et Sciences Interdisciplinaires (LaMCScI), B.P. 1014, Faculty of Science, Mohammed V University, Rabat, Morocco

E-mail: zouhirmansouri.2016@gmail.com

Abstract:
"Silent" zinc-based batteries are emerging as a compelling non-Li option for electrification and, in particular, large-scale and long-duration energy storage. Zinc has powered battery innovation since the early 1800s, from Volta's early cells onward, offering more than two centuries of technological history, compared with roughly three decades of commercial Li-ion deployment (since 1991). Owing to zinc's low cost, intrinsic safety, and broad availability, multiple Zn chemistries are being actively advanced toward grid-relevant applications, with growing industrial engagement. Despite this momentum, extending cycle life and round-trip energy efficiency remains the central challenge: aqueous systems are constrained by the narrow stability window of water (1.23 V), while practical cells must suppress zinc-anode dendrites, corrosion and hydrogen evolution, optimize electrolyte chemistry (including water activity and salt chemistry), and mitigate structural degradation/dissolution in V- and MnO_2-based cathodes, thus driving intense R&D on battery electrodes. In this presentation, I will shed light on how computational prediction can accelerate the discovery and screening of stable, high-performance Zn-battery materials, illustrated through representative examples with a focus on robust polyanionic compounds.

Back to the program

ENERGY STORAGE **Invited Speaker**

Aqueous Metal–Air Batteries: Challenges in Mastering the Electrode–Electrolyte Interface

G. Lin, Ya. Zhou, Yu. Z, S. Zanna, A. Seyux, **J. Światowska***

PSL Research University, Institut de Recherche de Chimie Paris, CNRS – Chimie ParisTech, Paris, France

E-mail: jolanta.swiatowska@chimieparistech.psl.eu

Abstract:

Metal–air batteries, including Li–, Zn–, Al–, and Mg–air systems, are promising candidates for next-generation energy storage due to their high theoretical energy densities and the abundance of their constituent materials. Among them, Mg–air batteries stand out with a high specific capacity (2200 mAh g^{-1}), a theoretical discharge voltage of 3.1 V, and the natural abundance and low environmental impact of magnesium. However, their practical deployment remains limited by the high reactivity of Mg, which leads to significant self-corrosion and parasitic hydrogen evolution [1]. This issue is particularly critical in chloride-containing electrolytes, where the formation of insoluble corrosion products such as $Mg(OH)_2$ and MgO reduces anodic efficiency and lowers the discharge voltage.

A key challenge in improving Mg–air battery performance is therefore to control corrosion processes at the electrode–electrolyte interface. Two main strategies can be considered: modification of the negative electrode and optimization of the electrolyte.

For the electrode, alloying magnesium with selected elements is an effective strategy to tune corrosion behavior. Calcium is particularly attractive due to its abundance, low toxicity, and more negative standard electrode potential compared to Mg. We have ininvestigated the influence of Ca content in Mg–Ca alloys used as anodes in 0.6 M NaCl solution and demonstrated that at low Ca content (Mg–0.2Ca), a dense and relatively homogeneous oxide/hydroxide layer forms, improving corrosion resistance and electrochemical stability [2]. In contrast, higher Ca content (Mg–2Ca) promotes the formation of secondary phases, leading to micro-galvanic coupling, localized corrosion, and reduced performance. These effects directly impact battery behavior, with Mg–0.2Ca delivering a significantly higher energy density (1529 Wh/kg) than Mg–2Ca (889 Wh/kg).

The second strategy focuses on electrolyte modification. Adjusting the salt or solvent, or introducing corrosion-inhibiting additives, provides efficient and cost-effective solutions. For example, replacing NaCl with KNO_3 [3], $NaNO_3$, or CH_3COONa improves corrosion resistance. Additives such as sodium 5-sulfosalicylate enhance surface dissolution kinetics while limiting redeposition of discharge products. Similarly, acetic acid combined with $NaNO_3$ promotes the formation of a homogeneous bilayer that suppresses Mg self-corrosion and prolongs cell life [4]. Other approaches include hybrid electrolytes (e.g., water/ethanol mixtures) [5] and strong Mg^{2+} complexing agents [6], which further enhance anodic activity.

Overall, this work demonstrates that both electrode and electrolyte composition are critical to balancing corrosion resistance and electrochemical activity in Mg-based systems. It also highlights the strong link between interfacial chemistry and battery performance, providing guidelines for the design of high-performance aqueous Mg–air batteries.

References:

[1] Y. Zhou, X. Lu, G. Lin, F. Wang, J. Światowska. Corros. Sci. 253, 113016 (2025).
[2] G. Lin, Y. Zhou, X. Chen, C. Chen, W. He, S. Zanna, A. Seyeux, J. Światowska. Electrochim. Acta 553, 148278 (2026).
[3] G. Lin, Y. Zhou, S. Zanna, A. Seyeux, P. Marcus, J. Światowska. J. Magnesium and Alloys 12, 3646 (2024).
[4] Y. Zhou, F. Sun, G. Lin, S. Zanna, A. Seyeux, P. Marcus, J. Światowska. J. Magnesium and Alloys, 12, 825 (2024).
[5] Y. Zhou, J.-T. Li, S. Zanna, A. Seyeux, P. Marcus, J. Światowska. Appl. Surf. Sci. 614, 156070 (2023).
[6] Y. Zhou, X. Lu, A. Seyeux, J. Światowska, F. Wang. Corros. Sci. 240, 112512 (2024).

Back to the program

ENERGY STORAGE

Recycling of End-of-Life reverse osmosis membranes for wastewater treatment

Nouhaila Laaribi [1,*], Abdallah Nayad [2], Yahya Agzenai Ben Salem [2], Mustapha Ait Ali [1]

[1] Molecular Chemistry Laboratory, Unit of Coordination Chemistry and Catalysis, Faculty of Science Semlalia, Cadi Ayyad University, Marrakesh, Morocco
[2] High Throughput Multidisciplinary Research Laboratory (HTMR), College of Chemical Sciences and Engineering (CCSE), Mohammed VI Polytechnic University (UM6P)

E-mail: nouhaila.laaribi@gmail.com

Abstract:
The global water crisis has driven scientists and researchers to explore innovative and efficient solutions for the treatment of natural water and wastewater. Among these technologies, reverse osmosis (RO) remains the most widely used method for desalination due to its operational simplicity and relatively low energy consumption. However, membrane fouling and chemical degradation significantly limit membrane lifespan. As a result, it is estimated that more than 840,000 end-of-life (EoL) RO membrane modules are discarded worldwide each year, most of which end up in landfills. To address this issue, various management approaches have been proposed to extend the life cycle of RO membranes, including reuse and recycling techniques. The most common practice involves converting spent RO membranes into lower-grade filtration membranes by oxidizing the outer polyamide layer using sodium hypochlorite (NaOCl). While effective, high concentrations of NaOCl can damage the underlying polysulfone support layer, thereby weakening the membrane's mechanical integrity. An alternative and promising strategy to enhance the reusability of recovered EoL membranes is surface modification through polymer coating. Within the framework of the circular economy, this study investigates the durability and performance stability of recovered thin-film composite (TFC) RO membranes coated with biodegradable polymers. Chitosan (CS), a hydrophilic and biocompatible biopolymer, possesses excellent film-forming properties but limited mechanical strength. Therefore, CS was blended with biodegradable poly(vinyl alcohol) (PVA). The resulting blend exhibits synergistic effects arising from the complementary properties of the two materials, combining improved mechanical performance with maintained biocompatibility and functionality.

Back to the program

ENERGY STORAGE

Ni/F Co-Doped $NaFePO_4$ as a Cathode Material for Sodium-Ion Batteries: A First-Principles Study

Abdessamad Nidlhaj*, Brahim Fakrach

LEM2A Laboratory, Université Moulay Ismaïl, Meknès, Morocco

E-mail: ab.nidlhaj@edu.umi.ac.ma

Abstract:
In this work, Density Functional Theory (DFT) within the GGA+U framework is used to investigate NaFePO4 as a cathode material for sodium-ion batteries. Analysis is done on how the structural, electrical, and electrochemical characteristics are affected by co-doping of Ni and F. The optimized structures show that after co-doping, the olivine framework stays stable. According to electronic structure calculations, substitutions of Ni and F greatly alter the electronic characteristics, improving conductivity by reducing the band gap. The Nudged Elastic Band (NEB) method is used to study Na diffusion and calculate the activation energy barrier, while the average intercalation voltage is used to assess the electrochemical performance.
According to the findings, $NaFePO_4$ is a viable option for sodium-ion battery applications since Ni/F co-doping improves both electronic and ionic transport capabilities.

Back to the program

POSTER HIGHLIGHTS **Poster 01**

Magnetically Recoverable Nanocomposites: A Sustainable Approach for Photocatalytic Degradation of Organic Dyes in Wastewater Treatment

Khadija Seyagh [1,*], Lahcen Fkhar [2], Nayad Abdallah [1,3], Abdelhadi Louroubi [1], Ali Hasnaoui [1], Mustapha Ait Ali [1], Larbi El Firdoussi [1]

[1] Molecular Chemistry Laboratory, Coordination and Catalysis Team, Cadi Ayyad University, Faculty of Sciences Semlalia (UCA-FSSM), B.P. 2390 – 40000 Marrakech, Morocco
[2] GREENMAT, CESAM, Institute of Chemistry B6, University of Liege, 4000 Liège, Belgium
[3] High Throughput Multidisciplinary Research (HTMR), Mohammed VI Polytechnic University, Benguerir 43150, Morocco

E-mail: k.sayeh.ced@uca.ac.ma

Abstract:
This study reports the synthesis of magnetic $MnCoFe_2O_4$/Siloxene (MCFO/SN) nanocomposites for enhanced water treatment. The materials were characterized using XRD, FT-IR, SEM, and DRS UV-vis spectroscopies. Photocatalytic tests demonstrated that the MCFO/SN sample exhibits superior activity for methylene blue degradation under visible light. Under optimized conditions (25 mg/L dye concentration; 10 mg catalyst dosage), the composite achieved a 97% degradation efficiency. Comparative evaluations across five organic dyes confirmed the catalyst's versatility, reaching removal rates up to 98%. Furthermore, stability and reusability tests proved that the photocatalyst maintains high performance over multiple cycles. The inherent magnetic properties of the spinel ferrite ensure rapid and efficient recovery from the reaction medium, making MCFO/SN a promising candidate for sustainable wastewater remediation.

Back to the program

POSTER HIGHLIGHTS **Poster 02**

Monoethanolamine (MEA) concentration effect on the Physical Properties of Tin Sulfide (SnS) Thin Films

M. El-Bassri [1,*], A. Almaggoussi [1,2], A. Abounadi [1], A. Rajira [1]

[1] IMED-Lab, Faculté des Sciences et Techniques Marrakech, FSTG, Université Cadi Ayyad, Morocco

[2] ACER Mohammed VI Polytechnic University, Lot 660, Hay Moulay Rachid, Ben Guerir, 43150, Morocco

E-mail: m.elbassri.ced@uca.ac.ma

Abstract:

In this study, we investigated the influence of monoethanolamine (MEA) on the physical properties of SnS thin films. The objective is to examine how the addition of MEA to the precursor solution affects the morphology, crystallinity, optical, and electrical properties of the films, aiming to optimize their performance for photovoltaic applications.

The SnS thin films were synthesized using the spin coating technique on glass substrates from a precursor solution containing tin chloride ($SnCl_2$) and Thiourea ($SC(NH_2)_2$). All samples underwent thermal annealing at a constant temperature of 500°C for 2 hours, with different MEA concentrations corresponding to the ratios [Sn:MEA] = [1:0], [1:0.5], [1:1], [1:1.5], [1:2], and [1:3]. The obtained results show that the MEA concentration plays a crucial role in the phase composition and crystallinity of SnS thin films. X-ray diffraction (XRD) analysis reveals that all samples exhibit an orthorhombic structure. The [1:2] ratio sample demonstrates significantly improved crystallinity, with no secondary phases such as SnS_2. Morphological analysis using scanning electron microscopy (SEM) highlights a progressive evolution of the films morphology as the MEA concentration increases. The [1:2] ratio sample stands out with an optimized morphology, characterized by a denser, more homogeneous, and smoother surface. Optical analysis reveals low transmittance for the [1:2] ratio sample. The bandgap energy varies between 1.24 eV and 1.89 eV for all samples. Finally, electrical characterization shows a gradual increase in charge carrier density as the MEA concentration increases. Simultaneously, the resistivity decreases, indicating an enhancement in the electrical conductivity of the films. All samples exhibit n-type conductivity.

Back to the program

POSTER HIGHLIGHTS **Poster 03**

Complexing agents' addition effect on the physical properties of electrodeposited Sb_2S_3

Y. Bounnaiche [1,*], A. Almaggoussi [1,2], Y. Koumya [3], A. Abounadi [1], A. Rajira [1]

[1] IMED-Lab, Faculté des Sciences et Techniques Marrakech, FSTG, Université Cadi Ayyad, Morocco
[2] ACER Mohammed VI Polytechnic University, Lot 660, Hay Moulay Rachid, Ben Guerir, 43150, Morocco
[3] Department of Chemical & Biochemical Sciences-Green Process Engineering (CBS), Mohammed VI Polytechnic University (UM6P), BenGuerir, 43150, Morocco

E-mail: y.bounnaiche.ced@uca.ac.ma

Abstract:
The Stibine Sb_2S_3 is a promising material for photovoltaic applications thanks to its remarkable properties. It has a high absorption coefficient ($\alpha > 10^4$ cm^{-1}) and a bandgap ranging from 1.7 to 2.5 eV. The aim of the present work is the optimization of the experimental conditions for the synthesis of Sb_2S_3 and the study of the effect of the addition of complexing agents on the physical properties of Sb_2S_3. Therefore, Sb_2S_3 was electrodeposited on ITO substrate from a solution containing a mixture of 2.10^{-3} M of Antimony Trichloride ($SbCl_3$) and 10^{-2} M of Sodium Thiosulfate ($Na_2S_2O_3$) and a complexing agent Diethanolamine ($HN(CH_2CH_2OH)_2$, DEA) or Ethylenediamine Tetraacetic Acid ($C_{10}H_{16}N_2O_8$, EDTA) . The XRD analysis showed that the obtained films are polycrystalline and correspond to orthorhombic Sb_2S_3. It is found that annealing changes the preferential growth orientation from (420) to (211) and leads to significative reduction of stress and dislocations. The Raman characterization confirms the obtention of polycrystalline Sb_2S_3 with the presence of other secondary phases. SEM analysis revealed that the addition of complexing agent modifies the morphology of the films and increases the grain size. Analysis of the chemical composition by EDAX shows that the addition of DEA leads to good stoichiometry. The obtained optical transmission values are very low, not exceeding 10%, which underlines the absorbent nature of this material. It was found that the addition of complexing agents shifted the gap towards lower energies. These results highlight the significant influence of complexing agents on the optical properties of the Sb_2S_3 material.

Back to the program

POSTER HIGHLIGHTS **Poster 04**

Nitrogen-annealing-induced interfacial diffusion in RF sputtered $SnO_2/Cu/SnO_2$ multilayers toward improved photocatalytic performance

Mouhcine Ourbaa*, Nourddine Lebrini, Mohssine Baali, Said Elmassi, Abdelkader Outzourhit, Abdelkader Elkissani, Abdelfattah Narjis, Lahcen Nkhaili

Materials, Energy and Environment Laboratory, Faculty of Sciences Semlalia, Cadi Ayyad University, PB 2390, Marrakech, Morocco

E-mail: m.ourbaa.ced@uca.ac.ma

Abstract:

SnO_2-based photocatalysts are attractive for water treatment due to their chemical stability and strong oxidative power; however, their practical performance is often limited by electron-holer recombination and poor recyclability in powder form. To address these challenges, this work proposes an industrially compatible and recyclable photocatalytic strategy based on RF-sputtered $SnO_2/Cu/SnO_2$ multilayer thin films. Controlled nitrogen annealing was used to engineer interfacial diffusion and enhance charge separation and transport. Structural and electrochemical analyses ((XRD, SEM/EDX, UV–Vis, Hall effect, and Mott–Schottky analyses) identified the optimized film annealed at 450 °C, which achieved ≈75% methylene blue degradation under low-power UV-LED irradiation. The introduction of a low and carefully controlled H_2O_2 dosage, acting solely as an auxiliary oxidant, further enhanced the degradation efficiency up to 93% within 3.5 h, by promoting additional radical activation while maintaining the dominant photocatalytic role of the multilayer film. This synergistic behavior highlights the effectiveness of combining interfacial engineering with controlled oxidant assistance, confirming the strong potential of RF-sputtered $SnO_2/Cu/SnO_2$ multilayer thin films as efficient, reusable, and cost-effective photocatalytic platforms for sustainable water purification.

Back to the program

POSTER HIGHLIGHTS **Poster 05**

Influence of Sn Dopant Concentration on NiS_2 Thin Films Prepared by Spin Coating for Supercapacitor Applications

Noureddine Lebrini [1,2,*], Mouhcine Ourbaa [2], Taoufik Erraji [1,2], Lahcen Nkhaili [2], Mustapha Beraich [1,2]

[1] Laboratory of Applied Sciences for Sustainable Development, Higher School of Technology of El Kelaa Des Sraghna, Cadi Ayyad University, Marrakech, Morocco
[2] Laboratory of Materials, Energy and the Environment (LaMEE), Faculty of Science Semlalia. Cadi Ayyad University, P. O. Box 2390, Marrakech, 40000, Morocco

E-mail: n.lebrini.ced@uca.ac.ma

Abstract:
Nickel disulfide (NiS_2) thin films doped with tin (Sn) were successfully prepared using the spin-coating method, followed by annealing at 400 °C under a controlled nitrogen and sulfur atmosphere. This study aims to systematically investigate the effect of Sn doping concentration on the structural, optical, and electrical properties of NiS_2 thin films, with particular emphasis on their potential application in supercapacitors. X-ray diffraction (XRD) analysis confirmed the formation of a cubic crystal structure with a lattice parameter of approximately 0.561 nm, while the appearance of secondary phases was observed at higher Sn concentrations. Scanning electron microscopy (SEM) revealed a uniform and well-defined surface morphology at low doping levels, with noticeable textural changes as the Sn content increased. Optical measurements showed a gradual reduction in the band gap from 2.05 to 1.74 eV with increasing Sn incorporation. Furthermore, electrical characterization indicated a significant improvement in conductivity, especially in films with high crystallinity and minimal secondary phases. These results demonstrate that Sn doping is an effective strategy for tuning the physicochemical properties of NiS_2 thin films, making them promising candidates for high-performance supercapacitor electrodes and advanced energy storage applications.

Back to the program

POSTER HIGHLIGHTS **Poster 06**

Machine Learning and DFT-Assisted Design of Eco-Friendly Organic Corrosion Inhibitors for Mild Steel Protection in Acidic Media

Aymane Ezerraf [1,*], Abd Elaziz Rahhou [1,2], Ali Hasnaoui [1], Rachid Idouhli [3], Mohamed Maatallah [1,*]

[1] Molecular Chemistry Laboratory, Faculty of Sciences Semlalia, Cadi Ayyad University, BP 2390 Bd My Abdellah, 40000 Marrakech, Morocco
[2] IMED-Lab, Faculty of Sciences and Techniques, Cadi Ayyad University, Bd Abdelkrim Al Khattabi, BP 549, 40000, Marrakech, Morocco
[3] Laboratory of Physical-Chemistry of Materials and Environment, Faculty of Sciences Semlalia, Cadi Ayyad University, PO Box 2390, Marrakesh 40000, Morocco

E-mail: a.ezerraf.ced@uca.ac.ma, m.maatallah@uca.ma

Abstract:
The development of efficient and environmentally friendly corrosion inhibitors is essential for protecting metallic materials used in industrial processes operating under acidic conditions. In this work, an integrated computational strategy combining machine learning (ML) and density functional theory (DFT) was employed to design and evaluate novel organic corrosion inhibitors for mild steel in a 1M HCl medium.
A dataset of previously reported organic compounds was used to construct predictive ML models capable of estimating inhibition efficiency (IE%) based on molecular descriptors. Several algorithms were tested, and the artificial neural network (ANN) model was selected as the most performant for screening new candidate molecules with high predicted anticorrosion performance.
To validate the ML predictions and gain molecular - level insight, DFT calculations were carried out on the selected compounds. Global reactivity descriptors derived from frontier molecular orbital (FMO) energies (HOMO and LUMO), molecular electrostatic potential (MEP) maps, Fukui functions, and molecular dynamics (MD) simulations were estimated and analyzed. These complementary approaches allowed rationalization of the inhibitor - surface interaction mechanisms and provided theoretical support for the predicted inhibition efficiencies.
The results revealed that molecules possessing strong electron-donating ability, favorable charge distribution, and strong adsorption affinity toward the steel surface exhibited high predicted inhibition efficiency (IE% > 90%).
The combined ML - DFT approach enabled the rapid identification of promising eco-friendly corrosion inhibitors while significantly reducing experimental cost and time.
This study demonstrates the potential of artificial intelligence-assisted quantum chemical modeling as a powerful tool for the rational design of sustainable materials for corrosion protection in industrial applications.

Back to the program

POSTER HIGHLIGHTS **Poster 07**

DFT Investigation of the PtS_2/ZrS_2 Heterojunction for Enhanced Photocatalytic Hydrogen Evolution

R. Haroudi*, I. Salym, M.Tabarani, Z. Seyagh, A. Mojahid, R.Takassa, A. El mouncharih, O. Farkad, A. El Boujlaidi, D. Abouelaoualim

LaMEE, Department of Physics, Faculty of Sciences Semlalia, Cadi Ayyad University, P.O. Box 2390,40000 Marrakech, Morocco

E-mail: r.haroudi.ced@uca.ac.ma

Abstract:
The search for efficient catalytic materials for hydrogen production via photocatalysis or electrocatalysis is at the forefront of current efforts in the field of green energy. In this context, heterojunctions formed between two transition metal dichalcogenides (TMDs) have attracted increasing attention due to their structural and electronic synergies. In this work, we employed density functional theory (DFT) to investigate the PtS_2/ZrS_2 heterostructure, focusing on its electronic, optical, and catalytic properties for the hydrogen evolution reaction (HER). Our results demonstrate that PtS_2/ZrS_2 heterojunction holds great potential as promising candidates for next generation photocatalysts.

Back to the program

POSTER HIGHLIGHTS **Poster 08**

Investigation of the Electronic and Optical Properties of Doped Borophene

A. Mojahid*, I. Salym, R. Haroudi, M. Tabarani, Z. Sayer, A. El Mouncharih, R. Takassa, O. Farkad, A. El Boujlaidi, D. Abouelaoualim

LaMEE, Department of Physics, Faculty of Sciences Semlalia, Cadi Ayyad University, P.O. Box 2390,40000 Marrakech, Morocco

E-mail: a.mojahid.ced@uca.ac.ma

Abstract:
In this work, we investigate the structural, electronic, and optical properties of doped borophene monolayers using first-principles density functional theory. By GGA-TB-mBJ approximations, we analyzed the effects of doping on this 2D material's fundamental characteristics. Our results demonstrate that controlled incorporation of dopants induces: (i) tunable bandgap opening through state hybridization near the Fermi level, (ii) enhanced anisotropic optical response improvement in visible-range absorption, and (iii) maintained structural stability. These findings provide quantitative design principles for engineering borophene's optoelectronic properties, particularly for applications in green energy.

Back to the program

POSTER HIGHLIGHTS **Poster 09**

Towards Multiscale Modeling of Lithium-Ion Transport in NMC Cathode Materials Using Deep Learning Potentials

Ikram Oughaddou [1,*], Majid El Kassaoui [1], Omar Mounkachi [1,2]

[1] College of computing, Mohammed VI Polytechnic University, Lot 660, Hay Moulay Rachid Ben Guerir, 43150, Morocco

[2] Laboratory of Condensed Matter and Interdisciplinary Sciences, Faculty of Sciences, Mohammed V University, 1014 Rabat, Morocco

E-mail: oughaddou.ikram22@gmail.com

Abstract:

Lithium-ion batteries have become the dominant energy storage technology for portable electronics, electric vehicles, and renewable energy applications. Among the various cathode materials, layered nickel–manganese–cobalt oxides (NMC) are widely used due to their high energy density and excellent electrochemical performance. In particular, NMC622 ($LiNi_{0.6}Mn_{0.2}Co_{0.2}O_2$) offers an attractive balance between capacity, stability, and cost. However, understanding lithium transport mechanisms in these materials remains challenging, as atomistic diffusion processes occur over spatial and temporal scales that are difficult to access through both experimental techniques and conventional computational methods.

In this work, a machine-learning interatomic potential is developed using the Deep Potential Molecular Dynamics (DeePMD) framework for NMC622. The model is trained on datasets generated from *ab initio* molecular dynamics simulations and validated against Density Functional Theory (DFT) reference energies and forces. By combining near-DFT accuracy with substantially lower computational cost, the trained potential enables molecular dynamics simulations on larger systems and longer timescales than those accessible with conventional first-principles approaches.

Back to the program

POSTER HIGHLIGHTS **Poster 10**

Development of New Chelating Agents for Heavy Metal Complexation

Oualid Mouktaoui*, Abdelaziz Rahhou, Ali Hasnaoui, Rachid Idouhli, Larbi El Firdoussi, Mustapha Ait Ali

Molecular chemistry laboratory, Faculty of sciences semlalia, Cadi Ayyad University, BP 2390 Bd My Abdellah, 40000 Marrakech, Morocco

E-mail: o.mouktaoui.ced@uca.ac.ma

Abstract:
Chelating ligands play a central role in modern coordination chemistry due to their ability to form stable, thermodynamically favourable complexes with metal ions through multidentate bonding. Unlike monodentate ligands, chelating agents such as EDTA, DTPA, bipyridine and porphyrins offer increased stability and selectivity of the complexes, which is essential for controlling the reactivity, solubility and redox behaviour of metal ions. This topic highlights the fundamental principles of chelating agent design and their diverse applications in the complexation of transition metals, lanthanides and toxic heavy metals. Furthermore, it explores their emerging role in electrochemistry, where chelated metal complexes are used as redox mediators, electrocatalysts for water splitting and CO_2 reduction, and agents for modifying electrode surfaces. The ability of chelating ligands to adjust the formal reduction potential, limit metal precipitation and prevent passivation makes them indispensable for sensors, batteries and environmental remediation. Current challenges and future opportunities in the design of functional chelators for electrochemical systems are also discussed.

Back to the program

POSTER HIGHLIGHTS **Poster 11**

Optoelectronic enhancement and exciton control in Si-doped KGeF3 perovskites

I. Salym*, R. Haroudi, A. Mojahid , R. Takassa , O. Farkad, Z. Seyagh , M. Tabarani, F. Elfatouaki, A. El Mouncharih, M. EL Aatmani, D. Abouelaoualim, A. El Boujlaidi

LaMEE, Department of Physics, Faculty of Sciences Semlalia, Cadi Ayyad University, Marrakech, Morocco
Laboratory of Materials Science and Process Optimization, Faculty of Sciences Semlalia, Cadi Ayyad University, Marrakech, Morocco

E-mail: I.salym.ced@uca.ac.ma

Abstract:
This work presents a first-principles investigation of the structural, electronic, excitonic, and optical properties of Si-substituted KGeF 3 fluoroperovskites. Structural optimization was performed within density functional theory using the PBEsol functional, while the TB-mBJ potential, with and without spin–orbit coupling (SOC), was employed to obtain a reliable description of the electronic, excitonic, and optical properties. The results- (No. 221) perovskite structure and show that all studied compositions remain stable in the cubic Pm 3m preserve a direct semiconducting character. Silicon incorporation induces a lattice contraction and a progressive reduction of the band gap, mainly due to the gradual replacement of Ge-derived states by Si-derived states near the band edges. More specifically, the valence band is mainly formed by hybridized Ge-4s/Si-3s and F-2p states, whereas the conduction-band edge evolves from predominantly Ge-4p character in KGeF 3 to Si-3p character in KSiF 3 . Spin–orbit coupling further modifies the band dispersion, enhances band splitting, and significantly affects the carrier effective masses and dielectric screening. Within the TB-mBJ+SOC scheme, the band gap decreases from 2.76 eV for KGeF 3 to 1.36 eV for KSiF 3 . At the same time, the electron effective mass decreases from 0.0501 m 0 in KGeF 3 to 0.0195 m 0 in KSiF 3 , while the exciton binding energy is markedly reduced, indicating a transition from strongly bound excitons in Ge-rich compounds to weakly bound and more delocalized excitons in Si-rich phases. The corresponding exciton dissociation temperature decreases from 781 K to 145 K, indicating that Si-rich phases promote free-carrier generation at room temperature. Optical calculations further reveal a redshift of the absorption edge, high absorption coefficients, and enhanced optical conductivity with increasing Si concentration. Overall, the KGeF 3 –KSiF 3 alloy series exhibits remarkable composition-dependent tunability, highlighting its potential as an environmentally friendly platform for advanced optoelectronic applications.

Back to the program

POSTER HIGHLIGHTS **Poster 12**

Using Waste Jute Bags as Reinforcement to Enhance Geopolymers: An Eco-Friendly Solution for Sustainable Construction

Jihane Ziraoui [1,2,*], Hicham Majdoubi [1], Youssef Tamraoui [1], Hassan Chehouani [2], Hicham Mastouri [1]

[1] Mohammed VI Polytechnic University, Benguerir, Morocco
[2] Laboratoire des Procédés pour l'Energie Durable et Environnement (ProcEDE), Cadi Ayyad University, Marrakech, Morocco

E-mail: jihane.ziraoui@ced.uca.ma

Abstract:
This study investigates the enhancement of geopolymer performance through reinforcement with natural jute fibers. The effect of fiber content on compressive and flexural strengths was evaluated by incorporating varying percentages of jute fibers into a phosphate washing sludge (PWS) based geopolymer matrix to form composite materials. Mechanical properties, including compressive and flexural strengths, were characterized, and the microstructure was analyzed using scanning electron microscopy (SEM). The results showed that the control sample (without fiber) achieved a compressive strength of 50 MPa. Adding 0.5 wt.% and 1 wt.% fibers reduced compressive strength by 21% and 32%, respectively, while the addition of 0.75 wt.% fiber resulted in a 17% reduction, maintaining a compressive strength of 40.8 MPa. In contrast, flexural strength increased with the addition of fibers. At 0.5 wt.%, it rose by 2%, reaching 9.6 MPa, and at 0.75 wt.%, it peaked at 12.3 MPa, representing a 30% improvement. However, further fiber addition (1 wt.%) led to a significant decrease in flexural strength to 6.2 MPa. SEM analysis revealed a toughened matrix with fiber-induced crack deflection, enhancing both toughness and ductility. These findings suggest that jute fibers can improve flexural properties without significantly compromising compressive strength, presenting a promising eco-friendly solution for sustainable construction materials.

Back to the program

POSTER HIGHLIGHTS **Poster 13**

A Raman Spectroscopy Study of Double-Walled Carbon Nanotubes at Optimal Interlayer Distance

B. Fakrach [1,*], O. El bouayadi [1,2], S. Elhadfi [1], J. Chenouf [1], S.A.A. Abdelkader [2], Chadli Hassane [1], AH. Rahmani [1], A. Rahmouni [3]

[1] Laboratory of Advanced Materials Study and Applications (LEM2A), Moulay Ismail University FSM-ESTM, BP 11201, Zitoune, Meknes, 50000, Morocco
[2] Laboratory of Solid State Physics, Department of Physics, Faculty of Science Dhar El Mahraz, Sidi Mohamed Ben Abdellah University, Fez, Morocco
[3] School of Applied and Engineering Physics, Mohammed VI Polytechnic University, Ben Guerir, 43150, Morocco

E-mail: b.fakrach@umi.ac.ma

Abstract:
In this work, we investigated the energetic stability and Raman spectra of the one-dimensional van der Waals (1D vdW) systems composed of two coaxially stacked single-walled carbon nanotubes (SWCNTs), commonly referred to as double-walled carbon nanotubes (DWCNTs). Calculations are performed using the spectral moments method coupled to the bond polarizability model.
First, the energetic stability of the DWCNT systems (8,0)@(n,m) was examined using the Lennard–Jones potential. The equilibrium interlayer distance between the inner (8,0) nanotube and the outer (n,m) nanotube was calculated and compared with the experimental results. Then, we present the calculated Raman spectra of the isolated SWCNT(8,0), SWCNT(17,0), and the DWCNT(8,0)@(17,0) at the optimized interlayer distance. We examine the energetic stability and the possible interlayer charge-transfer effects occurring between the inner and outer SWCNTs. The analysis of the frequency shifts of the radial breathing modes (RBMs) and the G-band in the DWCNT(8,0)@(17,0) provides valuable theoretical benchmark data for understanding the nature of interlayer coupling in such 1D vdW systems.

Back to the program

Tuesday, June 30, 2026

2D MATERIALS **Invited Speaker**

Epitaxial growth and properties of silicene and other 2D allotropes of Si: the case of the Si/Ag interface

Laurence Masson [1,*], Thomas Léoni [1], Geoffroy Prévot [2], Romain Bernard [2], Conor Hogan [3], Fabio Ronci [3]

[1] Aix-Marseille Université, CNRS, CINaM, AMUtech, Marseille, France
[2] Sorbonne Université, CNRS, Institut des NanoSciences de Paris, INSP, Paris, France
[3] CNR-Istituto di Struttura della Materia (CNR-ISM), Rome, Italy

E-mail: laurence.masson@univ-amu.fr

Abstract:
With the advent of graphene, tremendous efforts have been made to search for two-dimensional (2D) materials composed of other Group 14 elements, in particular silicon and germanium, due to their valence electronic configuration similar to that of carbon and their widespread use in the semiconductor industry. Silicene, the silicon counterpart of graphene, has been particularly studied, both theoretically and experimentally. Theoretical studies were the first to predict a low-buckled honeycomb structure for free-standing silicene possessing most of the outstanding electronic properties of graphene [1]. From an experimental point of view, as no layered structure analogous to graphite exists for silicon, the synthesis of silicene requires the development of alternative methods to exfoliation. Epitaxial growth of silicon on silver substrates has been widely exploited in attempts to form 2D Si honeycomb structures [2].
In this talk, I will present an overview about the synthesis of silicene on Ag substrates since 2005, year which can be considered as the beginning of the silicene story from an experimental point of view. In the challenging task to form silicene, other 2D allotropes of Si have been found growing on silver substrates and I will also present the studies related to these new 2D Si allotropes. I will show that the grown superstructures are formed through an interplay between the Si adsorbates and the Ag substrates. In the perspective of applications, I will discuss the results concerning the measurements of the electronic band structure of the grown 2D materials, showing that the Si-Ag interaction has to be considered to interpret the experimental band structure. Most of the studies I will present have been conducted in the framework of combined experimental-theoretical works.

References:
[1] S. Cahangirov, M. Topsakal, E. Aktürk, H. Şahin, S. Ciraci. Phys. Rev. Lett. 102, 236804 (2009).
[2] L. Masson, G. Prévot. Nanoscale Adv. 5, 1574 (2023).

Back to the program

2D MATERIALS

Electronic tunability and anisotropy in 2D P–N allotropes under strain

Mohammed Benchtia [1,*], Abdellah Sellam [2], Abderrahim Bakak [2], Driss Lahboub [2], Abdelaziz Koumina [2], Mohamed Lotfi [1], Rodolphe Heyd [3]

[1] Materials, Energy & Environment Laboratory (LaMEE), FSSM, Cadi Ayyad University, Marrakech, Morocco
[2] Interdisciplinary for Research on Bioresources, Energy and Materials Laboratory (LIRBEM), ENS, Cadi Ayyad University, Marrakech, Morocco
[3] Angevin Laboratory of Mechanics, Processes and InnovAtion (LAMPA), ENSAM ParisTech, Angers, France

E-mail: benchtiamohamed@gmail.com

Abstract:
Two-dimensional phosphorus–nitrogen (P–N) allotropes are emerging as promising candidates for advanced nanoelectronic and optoelectronic applications. Using density functional theory, we investigated four monolayers: phosphorene (P_4) and three P–N derivatives (P_2N_2, P_3N, and PN_3). Cohesive energy calculations show that P_2N_2 and PN_3 are more stable than P_4, with phonon spectra confirming their dynamical stability. Electronic analysis reveals diverse bandgap behaviors: a tunable direct bandgap in P_4, stable indirect bandgaps in P_2N_2 and P_3N, and the smallest bandgap among the studied structures in PN_3 . Strain engineering, applied through biaxial and uniaxial deformations from −5% to +5%, further highlights distinctive responses, including indirect-to-direct bandgap transitions in P4, strong anisotropy in PN_3 (bandgap up to 1.163 eV along the *a* axis), and moderate variations in P_2N_2. These results indicate that P–N two-dimenaional allotropes combine thermodynamic stability with tunable and anisotropic electronic properties, positioning them as versatile platforms for strain-engineered devices.

Back to the program

2D MATERIALS **Invited Speaker**

Some recent advances in 2D materials using ab initio calculations

Sébastien Lebègue

LEMTA, CNRS and Université de Lorraine, France

E-mail: sebastien.lebegue@univ-lorraine.fr

Abstract:
In this talk, I will present, through some examples from recent works, how ab initio calculations can provide a better understanding of the physical and chemical properties of different compounds. I will start with our results [1] concerning the electronic structure of systems consisting of different halogen atoms adsorbed on Cu (111) and Cu (110) surfaces: our calculations are compared with ARPES and STS experiments and an excellent agreement between theory and experiment was found. Then results on the screening of zeolites for nuclear applications will be shown, as well as a method to predict the binding energy of molecules in zeolites with improved accuracy [2]. Finally, I will present a methodological development [3,4] that allows for GW/BSE-level calculations with implicit solvation and show applications to 2D materials and photocatalysis.

References:
[1] W.J. Kim, S. Xing, G. Kremer, M. Sicot, B. Kierren, D. Malterre, G. Contini, J. Rault, P. Le Fèvre, F. Bertran, D. Rocca, Y. Fagot-Revurat, S. Lebègue. J. Phys. Chem. C. 123, 26309-26314 (2019).
[2] B. Herzog, A. Gallo, M. Chagas da Silva, A. Irmler, F. Hummel, M. Badawi, T. Bucko, S. Lebègue, A. Grüneis, D. Rocca. NPJ Computational Materials 10, 68 (2024).
[3] S.-J. Kim, S. Lebègue, S. Ringe, H. Kim. J. Phys. Chem. Lett. 13, 7574 (2022).
[4] S. Kim, S. Lebègue, S. Ringe, H. Kim. J. Phys. Chem. Lett. 15, 4575 (2024).

Back to the program

2D MATERIALS

Single Atom decoration for enhanced adsorption and gas sensing performance

Youssef Chlikhy [1,*], Sébastien Lebègue [2], M'hammed Mazroui [1]

[1] Laboratory of Condensed Matter Physics, Faculty of Sciences Ben M'Sick, Hassan II University of Casablanca, Casablanca, Morocco
[2] Lorraine University, CNRS, LEMTA, F-54000 Nancy, France

E-mail: youssef.chlikhy-etu@etu.univh2c.ma

Abstract:
Decorating with single-atom catalysts (SACs) is a promising strategy for enhancing adsorption mechanisms and improving the performance of sensing devices. Here we propose a functionalized Ti_2CO_2 MXene with SACs to enhance its adsorption capabilities for volatile organic compounds (VOC) such as toluene, acetonitrile, formaldehyde, and isopropanol. Incorporation of SACs enabled the chemisorption of the molecules, with single atoms acting as bridges that facilitate charge transfer and promote chemical bond formation. Band structure and density of states analyses further revealed significant changes in the electronic properties of the adsorbed systems. The sensing performance was estimated by performing a work function and band structure analysis. The strong interaction of VOCs with the SA-decorated Ti_2CO_2 was found to cause significant alterations in conductivity, thereby leading to substantial sensing responses. This work provides valuable insights for designing MXene functionalized with SACs, offering improved sensitivity for VOC detection, and demonstrates the potential of SACs in advanced gas sensing applications.

Back to the program

2D MATERIALS **Invited Speaker**

From 2D to 1D carbon allotrope. Two examples of recent advances: functionalized graphene and carbyne based polymers

Laurent Simon

IS2M-Université de Haute-Alsace, CNRS, Institut de Science des Matériaux de Mulhouse UMR 7361,3Bis rue Alfred Werner, 68093 Mulhouse, France

E-mail: laurent.simon@uha.fr

Abstract:
In this talk, I will present two recent systems we are currently investigating. The first is a novel 2D material: graphene functionalized with ordered intercalated Erbium atoms. This system enables us to achieve unprecedentedly high e-doping levels of graphene, surpassing the Lifshitz transition, the highest electron doping ever achieved through intercalation alone [1]. The doped system exhibits a large flat band at the Fermi level. By studying its magnetic properties, we have identified an antiferromagnetic transition. We will discuss the analogy of this system with heavy fermion alloys, where here, localized 4f electrons from Erbium interact with delocalized π-band electrons in the top graphene layer and show how this interaction can be further tuned through additional graphene functionalization [2]. In a second part I will present the recent synthesis with a host-guest polymerization strategy by supramolecular co-crystalization of 1D nanostructure of polymerized from self-organized diiododiacetylene monomer by topochemistry (formation of Poly(Diiododiacetylenes) (PIDA chains) and our attempts to control its transition to the so-called “allusive” carbyne an infinite chain of alternating single and triple C-bonds [3]. We will report four probe conductivity measurements under a SEM and their correlation with quantitative Raman spectroscopy. We also studied the reactivity of the PIDA with gold surface leading to the formation of long Carbyne chains evidenced by STM.

References:
[1] A. Zaarour et al Physical Review Research 5, 013099 (2023).
[2] A. Zaarour et al. (in preparation).
[3] Y. Zubchuk, et al. (submitted).

Back to the program

2D MATERIALS **Invited Speaker**

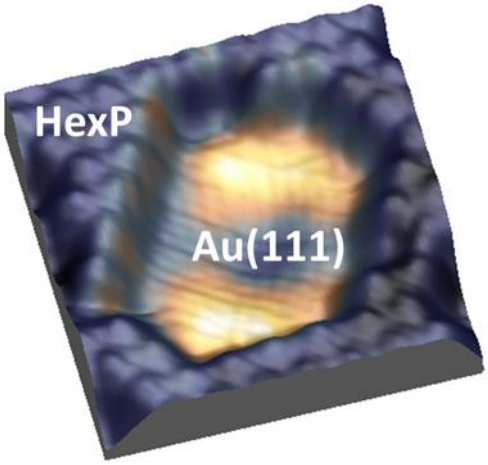
Electronic interactions in hexagonal phosphorus and Au(111)

A. Karn [1], I.E. Michel [2], M. Lezoualc'h[2], C. Chacon [1], Y. Girard [1], A. Smogunov [2], Y.J. Dappe [3], **J. Lagoute** [1,*]

[1] Laboratoire Matériaux et Phénomènes Quantiques, CNRS, Université Paris Cité, France
[2] SPEC, CEA, CNRS, Université Paris-Saclay, CEA Saclay, France
[3] C2N, CNRS, Université Paris-Saclay, France

E-mail: jerome.lagoute@u-paris.fr

Abstract:
Among two-dimensional (2D) materials, phosphorene has attracted special attention due to its monoelemental nature and tunable electronic bandgap. While puckered allotropes such as black phosphorus and blue phosphorene have been extensively studied, we recently reported the growth of a flat, hexagonal phosphorus layer (HexP) on Au(111), where P atoms form a $\sqrt{3} \times \sqrt{3}\, R30°$ overlayer on the gold substrate [1]. Scanning tunneling spectroscopy (STS) combined with and ab-initio calculations revealed an interatomic coupling between the P atoms mediated by the Au(111) substrate. This coupling leads to the formation of unoccupied electronic band involving a partial flat band appearing as a sharp peak in STS. The interplay between P atoms and Au(111) is further revealed by the properties of Au(111) nanopores embedded within the Hexp layer. Using STM/STS and tight-binding modeling, we show that HexP nanostructures induce quantum confinement of the Shockley surface state, with confined states spatially localized within nanopores. The energy and distribution of these states are well reproduced by a tight-binding model revealing how phosphorus decouples surface Au atoms. Beyond the intrinsic properties of phosphorus single layers, hybrid systems combining phosphorus with organic molecules are promising for combining the potential of 2D materials with molecular electronics. This will be exemplified through the interaction of magnetic molecules on HexP. These findings highlight the potential of HexP/Au(111) as a versatile platform for exploring quantum phenomena and engineering interfaces between 2D materials and molecules.



STM image of HexP structure with a nanopore, color coded by the differential conductance map at 45 mV

References:
[1] A. Karn et al. Small 20, 2405924 (2024).

Back to the program

2D MATERIALS

Reactivity of Black Phosphorene toward Oxygen and Its Passivation: A DFT and MD Study

Hamza El Garni [1,2,*], Anass Sibari [3], Youness Kaddar [4], Abdelilah Benyoussef [5], Hamid Oughaddou [1,2,6], Omar Mounkachi [1,4]

[1] Laboratory of Condensed Matter and Interdisciplinary Sciences, Department of Physics, Faculty of Sciences, Mohammed V University in Rabat, 1014 Rabat, Morocco
[2] Université Paris-Saclay, CNRS, Institut des Sciences Moléculaires d'Orsay, 91405 Orsay, France
[3] Complex Systems and Interactions Research Center, Ecole Centrale Casablanca, Bouskoura-Ville Verte, Casablanca, Morocco
[4] College of Computing, Mohammed VI Polytechnic University, Lot 660, Hay Moulay Rachid Ben Guérir, 43150, Morocco
[5] Hassan II Academy of Science and Technology in Rabat, Rabat 10112, Morocco
[6] Département de physique CY Cergy Paris Université Cergy-Pontoise Cedex F-95031, France

E-mail: hamza.el-garni@universite-paris-saclay.fr, hamza.elgarni@um5r.ac.ma

Abstract:
Two-dimensional (2D) materials beyond graphene; particularly semiconducting ones, have attracted significant attention due to their exceptional electronic properties, such as high carrier mobility and tunable band gaps. Among them, black phosphorene stands out for its remarkable physical properties and strong potential for nanoelectronic and optoelectronic applications. However, its high reactivity toward oxygen remains a major limitation to its stability [1].
In this oral presentation, I will focus on the oxidation mechanism of black phosphorene and its passivation, investigated using density functional theory (DFT) and molecular dynamics (MD) [2]. We study the effect of oxygen on black phosphorene from monolayer up to five layers, analyzing both electronic and optical properties. In addition, we explore the use of an organic molecule, NTCDA, as a potential protective layer. Two systems are considered: (I) NTCDA adsorbed on a black phosphorene monolayer, and (II) a combined system involving oxygen, NTCDA, and black phosphorene, in order to evaluate the effectiveness of passivation. Furthermore, we investigate the stability of these systems at 300 K using molecular dynamics simulations.

References:
[1] Z. Mansouri et al. Journal of Power Sources 587, 233719 (2023).
[2] H. El Garni et al. Journal of Applied Physics 139, 064302 (2026).

Back to the program

2D MATERIALS **Invited Speaker**

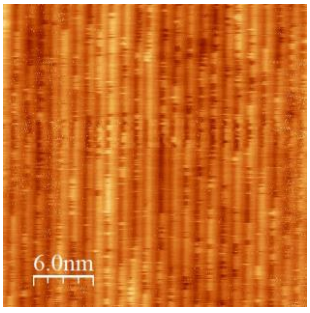
Growth of phosphorus on metallic surfaces: steps care

Yann Girard*, Wissem Ghariani

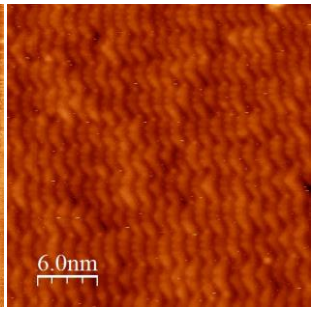
Université Paris Cité, Laboratoire Matériaux et Phénomènes Quantiques/MPQ, 75013 Paris, France

E-mail: yann.girard@u-paris.fr

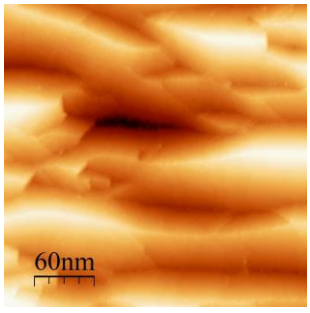
Abstract:
Black phosphorus thin films bridge the gap between graphene and transition metal dichalcogenides due to its high carrier mobility and moderate band gap. Few layers of BP exhibit adjustable electronic band gap with the number of layers (0.3 for bulk to 2 eV for a monolayer), with high interest in optic or electronic engineering. It has been predicted theoretically that a single layer of phosphorus atoms, called phosphorene, present a huge number of possible 2D-allotropes. Each of them has modulable properties according to their atomic structure and size or shape of low-dimensional phosphorene nanostructures. To date, only three allotropes have been experimentally synthesized: black, blue and violet phosphorus. The synthesis of new phosphorus allotropes remains an important challenge in materials science. In this talk, I will introduce a physical approach based on the controlled evaporation of phosphorus onto metallic substrates (Au and Cu). I will show that, in contrast to the widely accepted paradigm — where the substrate dictates the structure of the epilayer through surface stress — the inverse mechanism can dominate: the phosphorus overlayer reshapes the substrate. I will demonstrate that, on Cu, the density and orientation of surface steps play a decisive role, driving faceting phenomena that give rise to self-organized periodic mesostructures and to the emergence of chiral phases.



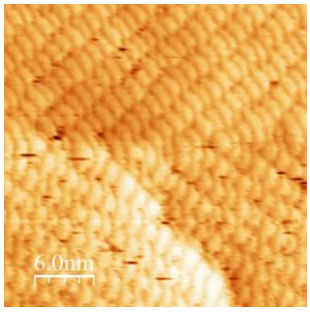
Clean Cu(332)



Phosphorus on Cu(332)



Faceting of Cu(755) induces by phosphorus



Details of faceted P-Cu(755)

Back to the program

ENERGY STORAGE **Invited Speaker**

Mesoporous Graphitic Carbon Nitride: A Promising Electrode Material For Supercapacitor

Mustapha Balarabe Idris*, Bhekie B. Mamba, X. Fuku

Institute for Nanotechnology and Water Sustainability, College of Science, Engineering and Technology, University of South Africa, Florida Science Campus, 1710 South Africa

E-mail: idris.mb@fud.edu.ng, idrisbm@unisa.ac.za

Abstract:
Graphitic carbon nitride (g-C_3N_4), a metal-free polymeric semiconductor with a layered two-dimensional structure, has recently emerged as a promising candidate for next-generation energy storage systems owing to its chemical stability, tunable electronic properties, and earth-abundant composition [1,2]. However, pristine g-C_3N_4 suffers from intrinsic limitations, including low electrical conductivity, limited surface area, and sluggish charge transport, which hinder its electrochemical performance in supercapacitor applications [3].
To address these challenges, mesoporous engineering of g-C_3N_4 has been extensively explored as an effective strategy to enhance ion accessibility, increase the number of active surface sites, and improve charge-storage kinetics [1]. The introduction of hierarchical porosity not only facilitates rapid electrolyte diffusion but also promotes efficient electron transport pathways, thereby significantly improving specific capacitance, rate capability, and cycling stability. Furthermore, synergistic integration with conductive materials, heteroatom doping, and defect engineering has been demonstrated to modulate the electronic structure and optimise electrochemical activity. This presentation provides a comprehensive overview of recent advances in the design and synthesis of mesoporous g-C_3N_4-based electrode materials for high-performance supercapacitors. Particular emphasis is placed on structure–property–performance relationships, including the role of pore architecture, surface chemistry, and heteroatom in enhancing charge storage mechanisms. In addition, electrolyte engineering and emerging strategies will be discussed. Overall, mesoporous g-C_3N_4 represents a versatile and sustainable platform for advanced electrochemical energy storage, offering significant potential for developing high-efficiency, low-cost, and environmentally benign supercapacitor systems.

References:
[1] M.B. Idris, Z. Musa Mohammed, S. Nuhu, H. Aliyu, H. Abba, B.B. Mamba, D. Sappani, F. Xolile. ACS Omega 10, 18184 (2025).
[2] M.B. Idris, S. Devaraj. J. Energy Storage 26, 101032 (2019).
[3] A. Vinu, K. Ariga, T. Mori, T. Nakanishi, S. Hishita, D. Golberg, Y. Bando. Adv. Mater. 17, 1648 (2005).

Back to the program

ENERGY STORAGE

Siloxene Nanosheets as Promising Anode Materials for Lithium-Ion Batteries: Synthesis and Characterization

O. Zakir [1,2,3,*], M. EL Kassaoui [1,4], K. Sayeh [1], A. Nayad [1], O. Mounkachi [4,5], S. Naamane [2], K. El Maalam [2], M. Ait Ali [1]

[1] Laboratory of Molecular Chemistry, Department of Chemistry, Faculty of Sciences Semlalia, University Cadi Ayyad, BP 2390, 40001, Marrakech, Morocco
[2] Durability and Engineering of Materials Center, Moroccan Foundation for Advanced Science, Innovation and Research (MAScIR), Mohammed VI Polytechnic University, Lot 660, Hay Moulay Rachid Ben Guerir, 43150, Morocco
[3] Faculty of Science Semlalia Department of Chemistry, Laboratory of Physical Chemistry of Materials and Environment (LPCME), Cadi Ayyad University, UCA, BP 2390, Marrakech, Morocco
[4] Laboratory of Condensed Matter and Interdisciplinary Sciences, Faculty of Sciences, Mohammed V University, 1014 Rabat, Morocco
[5] College of Computing, Mohammed VI Polytechnic University, Lot 660, Hay Moulay Rachid Ben Guerir, 43150, Morocco

E-mail: o.zakir@gmail.com

Abstract:
Two-dimensional siloxene has attracted considerable attention as a promising anode material for lithium-ion batteries (LIBs), owing to its high theoretical specific capacity, structural flexibility, and substantially reduced volume change during charge/discharge cycling relative to bulk silicon. In this work, siloxene nanosheets were synthesized via chemical exfoliation of a purified calcium disilicide ($CaSi_2$) precursor, obtained after selective removal of residual bulk silicon impurities. The structural, morphological, and vibrational properties of the resulting material were comprehensively characterized using X-ray diffraction, Raman spectroscopy, Fourier-transform infrared spectroscopy, scanning electron microscopy, high-resolution transmission electron microscopy, and atomic force microscopy. Siloxene-based electrodes with varying active material compositions were fabricated and evaluated in CR2032 coin half-cells. Among the formulations tested, the electrode consisting of 60 wt% siloxene, 30 wt% carbon black, and 10 wt% PAA binder exhibited the most favorable electrochemical performance, delivering a reversible discharge capacity of 859.44 mAh/g after 10 cycles at 0.2 C, with a coulombic efficiency of 95.69%. The use of PAA as a binder markedly improved electrode dimensional stability and lithium-ion diffusion kinetics in comparison with PVDF. The optimized electrode also demonstrated good rate capability across a range of applied current densities. These results advance the fundamental understanding of siloxene as a viable high-capacity anode material for next-generation lithium-ion battery systems.

Back to the program

ENERGY STORAGE **Invited Speaker**

Direct recycling of spent Li-ion batteries: innovative processes for sustainable cathode regeneration

Abdelfattah Mahmoud*, Max Larry, Rudi Cloots, Frédéric Boschini, Hamid Oubaha

GREEnMat, CESAM Research Unit, Chemistry Department, University of Liège, Quartier Agora, 13 Allée du 6 Août, 4000 Liège, Belgium

E-mail: abdelfattah.mahmoud@uliege.be

Abstract:
The rapid expansion of the global lithium-ion batteries (LIBs) market has created significant challenges, including a massive shortage of raw materials and a huge quantity of spent batteries. However, because these used batteries contain highly valuable metals, the industry increasingly views them as a vital secondary resource rather than waste. This has created a powerful economic and ecological mandate to develop innovative recycling technologies capable of recovering these materials and securing a sustainable, closed-loop supply chain.
In contrast to conventional high-temperature pyro- and hydro-metallurgical recycling processes, direct recycling of spent LIBs offers a more appealing solution by regenerating electrode active materials without decomposing their crystal structures into constituent elements. This approach not only reduces processing cost, but also lowers the consumption of energy, chemicals and resources required for the materials recovery. By avoiding energy-intensive smelting and leaching steps, direct recycling provides a more sustainable, closed-loop strategy for electrode active materials reuse.
In this talk, I will discuss current strategies and emerging technologies for the direct recycling of end-of-life LIBs. Furthermore, I will present an efficient and sustainable processes for the direct regeneration of spent cathode active materials.

Back to the program

ENERGY STORAGE

A Continuum Electrochemical Modeling Approach for Investigating Transport and Performance Limitations in Lithium-Ion Batteries

Zineb Miftah [1,*], Majid El Kassaoui [1], Ismail Berrada [1], Omar Mounkachi [1,2]

[1] College of Computing, University Mohammed VI Polytechnic, Benguerir, Morocco
[2] Laboratory of Condensed Matter and Interdisciplinary Sciences, Faculty of Sciences, Mohammed V University, 1014, Rabat, Morocco

E-mail: zineb.miftah@um6p.ma

Abstract:
Lithium-ion batteries have become the dominant energy storage technology for a wide range of applications, including portable electronics, electric vehicles, and grid-level energy systems, due to their high energy density, long cycle life, and favorable efficiency. However, their performance and durability are governed by complex, strongly coupled electrochemical and transport phenomena occurring across multiple spatial and temporal scales. These intrinsic complexities make experimental characterization alone insufficient to fully understand and predict battery behavior under various operating conditions.
Continuum modeling has emerged as a powerful approach to bridge this gap by providing a physics-based description of the internal processes governing battery operation. By treating the porous electrodes and electrolyte as continuous media, such models enable the simultaneous description of ionic transport, electronic conduction, and electrochemical reactions within a unified framework. This approach allows for the investigation of key performance-limiting mechanisms, including concentration gradients, polarization effects, and transport limitations, which are difficult to access experimentally.
In our work, we develop a continuum-scale electrochemical model to analyze the dynamic behavior of Li-ion batteries under different operating conditions. The model captures the coupled transport and reaction processes and enables systematic evaluation of the influence of material properties and operating parameters on overall cell performance. Through numerical simulations, we demonstrate how continuum modeling provides critical insights into battery efficiency, rate capability, and degradation trends. Overall, this study highlights the essential role of continuum approaches as predictive and scalable tools for the analysis, optimization, and design of advanced battery systems.

Back to the program

ENERGY STORAGE **Invited Speaker**

Recovery of lithium from spent LIBs and Bayer cake to improve sustainability of battery value chain

Ulla Lassi*, Tuuli Luimula, Petteri Laine, Pekka Tynjälä, Toni Kauppinen

University of Oulu, Finland; Kokkola University Consortium Chydenius, Finland

E-mail: ulla.lassi@oulu.fi

Abstract:
Lithium is a critical raw metal, and essential for lithium-ion batteries (LIBs). EU's Sustainable Batteries Regulation (2023/1542) sets mandatory lithium recovery targets from black mass (BM) of spent batteries, ≥50% and ≥80% by the end of 2027 and 2031, respectively. Lithium can also be recovered from other secondary materials, such as Bayer cake (BaC) from Al production process and from lithium slag (LS, Li-containing calcium silicate slag originated from thermal processing of spent LIBs). Li contents for BM, BaC, and LS were ~5 wt%, 1.6 wt%, and 4.3 wt%, respectively.
Lithium was successfully recycled from BaC and BM using sulfuric acid leaching with optimised leaching temperature, solid to liquid (S/L) ratio, and acid concentration. For the BaC, the highest Li yield of 99.55 % was obtained with S/L ratio of 160 g/L, temperature of 80 °C, and acid concentration of 0.5 M. Li leaching was not selective, and therefore, separate purification step was needed to obtain residual Al concentration below 1 mg/L. For BM, after the traditional sulfuric acid leaching in the presence of H_2O_2, Li yield in metal sulfate solution was 5.9 g/L. For LS, soda leaching process was developed, enabling the integration with primary Li production. It was also observed that extraction temperature and Ca/Li ratio affect mostly the Li yield. Li leaching efficiency over 90% was obtained, with Li concentration of ~10 g/L (Ca/Li ratio of 1.25). For Li recovery, an innovative approach was used, in which instead of traditional sulfuric acid leaching, lithium was recovered using $NiSO_4$ as leaching agent from cathode active material (NMC811). Up to 92.5% lithium yield was obtained from NMC811. Higher Ni content boosted lithium leaching at 150°C. During the early stages of lithium extraction, a nickel sulfate hydroxide hydrate phase $Ni_5(SO_4)_2(OH)_6{\cdot}3H_2O$ was formed on the surfaces of CAM particles. As the delithiation reaction progressed, additional OH- ions were released into the solution, converting the sulfate-rich phase into $Ni(OH)_2$ and re-dissolving the previously precipitated nickel sulfate back into the solution. After the delithiation, resulting powder was successfully used for manganese control during metal leaching in sulfuric acid solution (0.75 M) with an initial manganese concentration of 4.4 g/L.
To conclude, several approaches were shown to extract Li from secondary materials with high yields and Li concentration in the leachate from which Li was recovered by precipitation as LiOH or Li_2CO_3 for re-use in batteries.

Acknowledgments
The research was funded by the European Union's Horizon Europe research and innovation programme under the Grant Agreement No 101137771 (STREAMS), Business Finland (BATCircle3.0, Grant 2196/31/2024), and AKILIT (EU Regional Fund, grant A81278).

Back to the program

ADVANCED MATERIALS and CHARACTERIZATION **Invited Speaker**

Sustainability Standards: A New Era for Photovoltaic Technologies

Nouha Gazbour*, Charles Roux, David Duca

Univ. Grenoble Alpes, CEA, Liten, INES, 73375 Le Bourget du Lac, France

E-mail: nouha.gazbour@cea.fr

Abstract:

The rapid deployment of crystalline silicon photovoltaic (PV) technologies requires not only high efficiency but also improved material sustainability across the entire value chain. This work investigates the influence of European environmental regulations on PV module design, with a specific focus on materials engineering, process optimization, and their impact on Life Cycle Assessment (LCA) results.

Current frameworks, including the Net Zero Industry Act, increasingly constrain PV technologies through carbon footprint thresholds ranging from **< 400 to 830 kgCO_2eq/kWp**. However, LCA outcomes remain highly sensitive to methodological choices. Based on internal analyses, variations of up to **+40 / −30 kgCO_2eq/kWp** arise from database selection, while differences in system boundaries and impact assessment methods contribute an additional **~12–20 kgCO_2eq/kWp**. These discrepancies directly affect the environmental ranking of identical material systems.

From a materials perspective, this study identifies key hotspots along the silicon PV value chain. At the polysilicon and wafer levels, reducing wafer thickness and kerf losses significantly lowers material consumption. At the cell level, decreasing silver usage or implementing metallization alternatives represents a major lever for reducing resource criticality. At the module scale, eco-design strategies—such as lead-free interconnections, increased recycled content, and selection of recyclable encapsulation materials—enable improved environmental performance without compromising device stability.

Furthermore, the impact of material choices on device lifetime is shown to be critical, with variations of approximately **±10 gCO_2eq/kWh**, highlighting the strong coupling between degradation mechanisms, reliability, and environmental performance. Recycling pathways and silicon recovery also play a key role in closing material loops and reducing dependency on critical raw materials.

This work demonstrates that sustainable PV development requires a strong integration of materials engineering with environmental assessment tools. It calls for harmonized LCA methodologies and the adoption of multi-criteria indicators that account for material scarcity, durability, and recyclability. Embedding these parameters at the early design stage is essential to guide the development of next-generation PV modules combining high efficiency, reduced material intensity, and improved circularity.

Back to the program

ADVANCED MATERIALS and CHARACTERIZATION

Synthesis, Characterization and Photovoltaic Performance of Schiff Base Metal Complexes as Sensitizers for Dye-Sensitized Solar Cells (DSSCs)

Abd Elaziz Rahhou [1,2,*], Ali Hasnaoui [2], Nabil Rochdi [1,3], Mustapha Ait Ali [2]

[1] IMED-Lab, Faculty of Sciences and Techniques, Cadi Ayyad University, Bd Abdelkrim Al Khattabi, BP 549, 40000, Marrakech, Morocco
[2] Molecular Chemistry Laboratory, Faculty of Sciences Semlalia, Cadi Ayyad University, BP 2390 Bd My Abdellah, 40000 Marrakech, Morocco
[3] Department of Physics, Faculty of Sciences Semlalia, Cadi Ayyad University, PO Box 2390, 40000, Marrakesh, Morocco

E-mail: a.rahhou.ced@uca.ac.ma

Abstract:
The design of multifunctional organometallic complexes that combine catalytic activity with light-harvesting properties is a promising approach for sustainable energy technologies. In this study, we report the synthesis, characterization, and photovoltaic performance of novel vanadium(V) and copper(II) Schiff base complexes as potential sensitizers for dye-sensitized solar cells (DSSCs).
Two dinuclear water-soluble oxovanadium(V) complexes, $[(L1H)VO(\mu\text{-}O)]_2$ (C1) and $[(L2H)VO(\mu\text{-}O)]_2$ (C2), as well as copper(II) Schiff base complexes were synthesized via the condensation of $VOSO_4$ and Cu(II) salts with tetradentate Schiff base ligands under reflux in methanol. All complexes were fully characterized by elemental analysis, FTIR, ^1H NMR, and UV–Vis spectroscopy, confirming the expected coordination environments.
The optical properties of the vanadium(V) and copper(II) complexes were investigated using UV–Vis absorption spectroscopy in order to evaluate their suitability as sensitizers for DSSC applications.

Back to the program

ADVANCED MATERIALS and CHARACTERIZATION

DFT Investigation of the Structural, Electronic, and Optical Properties of Cubic Tantalate Perovskites $ATaO_3$ (A = Cs, K, Na)

Abdellah Hbab

Ibnou Zohr University, Morocco

E-mail: abdellah.hbab@edu.uiz.ac.ma

Abstract:
Perovskite oxides have attracted considerable attention because of their remarkable structural stability and wide range of physical properties. Tantalate-based perovskites, such as $CsTaO_3$, $KTaO_3$, and $NaTaO_3$, are of particular interest due to their characteristics. These materials are considered promising candidates for applications in optoelectronics, ultraviolet devices, and energy-related technologies. In this work, we report a density functional theory (DFT) study of the structural, electronic, and optical properties of the cubic perovskites $CsTaO_3$, $KTaO_3$, and $NaTaO_3$. The calculations were performed using Quantum ESPRESSO within the PBEsol approximation. The optimized lattice parameters are in good agreement with available experimental data, confirming the reliability of PBEsol for structural predictions. All compounds exhibit insulating behavior with indirect band gaps. The electronic structure analysis shows that the valence band is mainly dominated by O-2p states, whereas the conduction band is primarily composed of Ta-5d states. Optical properties, including the dielectric function, refractive index, extinction coefficient, reflectivity and absorption coefficient, were calculated and analyzed. The results reveal strong optical activity in the ultraviolet region, indicating potential applications in optoelectronic and photocatalytic devices. This study also highlights the importance of beyond-standard DFT approaches for achieving a more accurate description of the properties of tantalate perovskites.

Back to the program

Wednesday, July 1, 2026

2D MATERIALS **Invited Speaker**

Misfit compounds as a platform for engineering doping, charge density waves and topological superconductivity

H. Le Du [1], L. Zullo [1], J. Cordiez, T. Samuely, D. Volavka, P. Samuely, P. Szabo, R. Salvatore [1], G. Marini, D. Pierucci [1], S. Sasaki, F. Pawula, E. Janod, C. Bigi, M. Zonno, F. Bertran, T. Jaouen, P. Le Fèvre, M. Calandra, M. D'Angelo [1], Laurent Cario, M. Hervé [1], **T. Cren** [1,*]

[1] Institut des NanoSciences de Paris, CNRS - Sorbonne University, 4 Place Jussieu, Paris

E-mail: tristan.cren@sorbonne-universite.fr

Abstract:
In the current quest of innovative materials which combine two-dimensionality, strong spin-orbit, valley physics, superconductivity, charge density wave, quantum-spin Hall effect, the transition metal dichalcogenides (TMD) misfit materials appear as extremely promising. They are constituted by sandwiching rocksalt layers, such as LaSe, and TMD layers such as $NbSe_2$. A very large combination of materials is achievable by playing on the stacking. TMD misfits are a new platform that allows achieving unprecedented high doping levels in TMD materials [1,2]. We will show how we have succeeded adjusting finely the chemical potential over a very wide range in $NbSe_2$ using a Pb_xLa_{1-x} rocksalt, and how this can used for stabilizing several charge density wave orders ($2 \times 2, 3 \times 3, \sqrt{3} \times \sqrt{3}$) and tuning the superconducting transition temperature over a wide range [2]. Superconductivity in these compounds exhibits a huge in-plane critical field which is much higher than the paramagnetic limit [3,4] due to a very strong Ising spin-orbit coupling. It was predicted that this huge spin-orbit coupling could lead to non-conventional chiral superconductivity. We will show some hint of a topological superconducting transition in the misfit compounds.

References:
[1] R.T. Leriche et al. Advanced Functional Materials 31, 2007706 (2021).
[2] L. Zullo, G. Marini, T. Cren, M. Calandra. Nano Letters 23, 6658 (2023).
[3] P. Samuely et al. Phys. Rev. B 104, 224507 (2021).
[4] T. Samuely et al. Physical Review B 108, L220501 (2023).

Back to the program

2D MATERIALS **Invited Speaker**

Higher order topological defects in the moiré lattice of a van der Waals magnetic material

E. Gambari [1], S. Meyer [2], S. Guesne [1], P. David [1], F. Debontridder [1], L. Limot [3], F. Scheurer [3], C. Brun [1], B. Dupé [2], T. Cren [1], **M. Hervé** [1,*]

[1] Sorbonne Université – CNRS - Institut des Nanosciences de Paris UMR7588, 4 place Jussieu, Paris 75005, France
[2] Université de Liège Nanomat/Q-MAT Sart Tilman B-4000, Belgium
[3] Université de Strasbourg CNRS Institut de Phsyique et Chime des Matériaux de Strasbourg UMR7504, Strasbourg F-67000, France

E-mail: marie.herve@insp.upmc.fr

Abstract:
Van der Waals materials are emerging as extremely versatile building blocks for many fields of research, both at the fundamental and applied level. They offer tremendous possibilities for fine tuning spintronics, superconducting, nanoelectronics, optical devices. They appear extremely attractive for exploring new exotic physics due to their ability to be staked with an infinite number of combinations that leads to unexpected physical properties. The toolbox of van der Waals heterostructures is continuously growing with for instance the recent discovery of ferromagnetic order down to the monolayer limit in the family of chromium trihalide, CrCl3, CrBr3 and CrI3 (CrX3, X= I, Br, Cl) [1]. Several works have related some observations of moiré structure due to the mismatch between the CrX3 monolayers and their substrate which lead to a wealth of new exotic effects [2, 3]. Combining a chromium trihalide layer with a superconductor might lead for instance to topological superconductivity as recently reported in CrBr3/NbSe2 heterostructures [4]. In this hybrid structure, it was proposed that the mechanisms leading to a topological order in this hybrid structures was intimately related to the presence of a moiré pattern [2]. Another fascinating observation is about the influence of a moiré on the magnetic properties. In the CrX3 family, till now, the magnetization was shown to be essentially colinear, however, in CrI3 double bilayer some hint of non-colinear magnetism was found and was related to the moiré pattern which leads to a non- negligible spatial modulation of the magnetic interaction [3]. In this communication I will present our scanning tunneling microscopy investigation of a CrCl3 monolayer deposited on Au(111) which exhibit a second order moiré pattern. We report the presence of edge dislocations in this moiré pattern (see figure). Based on a comprehensive analytical model, I will show that these well know edge dislocations can be reexamined in the framework of topological concepts where they are described as topological defects analogous to vortices carrying a Berry phase characterized by a Chern winding number. They might therefore be use as a pinning center to host topological spin texture and / or Majorana bound states in CrX3/superconductor heterostructures.

References:
[1] D. Soriano et. al. Nano Lett. 20, 6225 (2020).
[2] S. Kezilebieke et. al. Nano Lett. 22, 328 (2022).
[3] H. Xie, et. al. Nat. Phys. 19, 1150 (2023).
[4] S. Kezilebieke et. al. Nature 588, 424 (2020).

Back to the program

2D MATERIALS **Invited Speaker**

Tuning the thin film interfaces for efficient devices: impact of the geometric organization of the molecules on specific electronic property

Ludovic Tortech

IPCM, Sorbonne Université, 75252 Paris, France
CEA de Saclay, DRF/ IRAMIS/NIMBE/LICSEN, 91191 Gif-sur-Yvette, France

E-mail: ludovic.tortech@sorbonne-universite.fr

Abstract:
Over the last two decades, soft organic materials have attracted considerable attention with the emergence of new electronic devices, following the first 1% organic solar cells [1] in the early 1980s and organic transistors [2] in the 1990s. These devices share a common structural feature: they are based on thin films. The geometrical organization of molecules within these layers can induce a collective electronic behaviour, leading either to the enhancement or suppression of specific electrical and electronic properties.
This presentation will illustrate, through three examples, how the deposition of organic molecules can tune or suppress the electrical properties of thin films. The first example [3] focuses on the deposition of planar molecules such as perylene, where face-on or edge-on orientations can enhance light absorption for an efficient plasmonic effect. The second example [4] is dedicated to spin valves, through the example of brush-deposited sexithiophene inserted between Fe_2O_4 and Co electrodes. Finally, the last example [5] will present the use of small molecules as interfacial layers in organic solar cells (Figure 1).

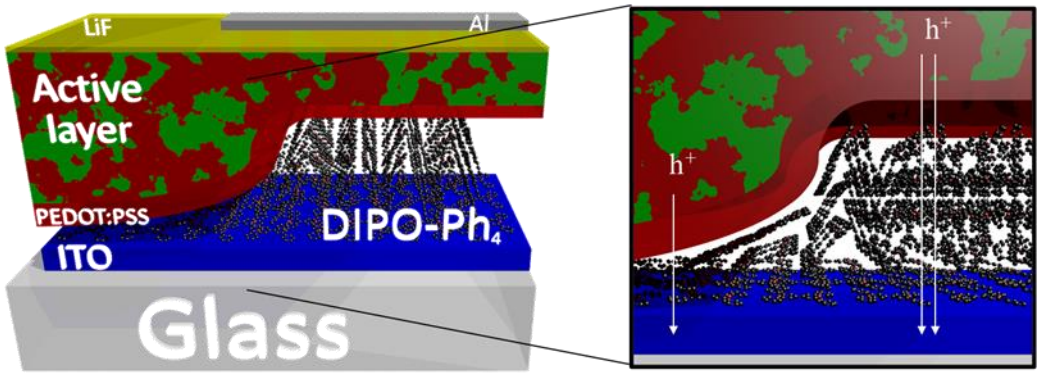


Figure 1: Organic thin film as interfacial layer displaying different organisations lead to a very different conduction property.

References:
[1] C.W. Tang. Appl. Phys. Lett. 48, 183 (1986).
[2] G. Horowitz, D. Fichou, X. Peng, Z. Xu, F. Garnier. Solid State Commun. 72, 381 (1989).
[3] J. Bigeon, S. Le Liepvre, S. Vassant, N. Belabas, N. Bardou, C. Minot, A. Yacomotti, A. Levenson, F. Charra, S. Barbay. J. Phys. Chem. Lett. 8, 5626 (2017).
[4] C. Blouzon, F. Ott, L. Tortech, D. Fichou, J.-B. Moussy. Appl. Phys. Lett. 103, 042417 (2013).
[5] Q. Arnoux, B. Watts, S. Swaraj, F. Rochet, L. Tortech. Nano Res. 11, 2771 (2017).

Back to the program

2D MATERIALS **Invited Speaker**

Charge Density Waves propagation in van der Waals heterostructures

I.-E. Michel [1], A. Karn [2], C. Chacon [2], L. Pai [3], J. Lagoute [2], **Y.J. Dappe** [4,*]

[1] SPEC, CEA, CNRS, Université Paris-Saclay, CEA Saclay, France
[2] Laboratoire Matériaux et Phénomènes Quantiques, CNRS, Université Paris Cité, France
[3] National Taiwan University, Taipei 106, Taiwan
[4] Centre de Nanosciences et de Nanotechnologies (C2N), UMR 9001 CNRS, Université Paris Saclay, Paris, France

E-mail: yannick.dappe@cnrs.fr

Abstract:
Charge Density Wave (CDW) is an important concept in Condensed Matter Physics, at the origin of several physical phenomena (superconductivity, atomic lattice modifications, highly correlated electrons, metal-insulator transition, …). Very recently, important research has been devoted to the study of CDW in 2D transition metal dichalcogenides (TMDs). For example, vanadium diselenide VSe_2 has been widely studied, with a (4x4) CDW phase in its bulk form [1], and a (√3 x √7) CDW phase for its monolayer form adsorbed on a different substrate. Also ScanningTunneling Microscope (STM) experiments show potential manipulation and switch of CDW phases [2].
Here we present a combined experimental and theoretical study of VSe_2 / VTe_2 van der Waals heterostructure. STM images reveal a particular (4x4) CDW phase of VSe_2 in its monolayer form on VTe_2, while Density Functional Theory (DFT) calculations stress the particular role of charge transfer in the propagation of CDW phase from one 2D material to the other. As a result, this study shed light on the potential modulation of CDW phases through charge transfer and more generally electrostatics of the system, with potential applications in future nanodevices.

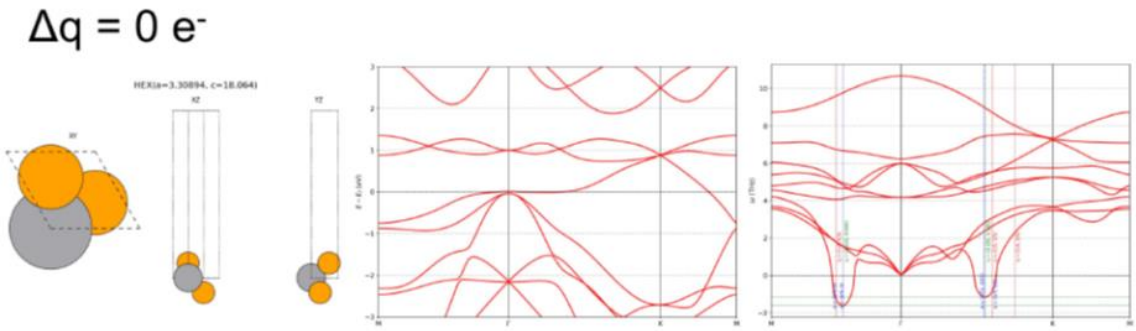


Figure 1: from left to right, unit cell of VSe_2 used for DFT calculations in its neutral form, and calculated electronic and phononic bandstructures, revealing respectively the position of electronic bands of interest and soft phonon modes responsibles for CDW phases.

References:
[1] U. Chazarin et al. Adv. Mater. Interfaces 10, 2201680 (2022).
[2] U. Chazarin et al. Nano Letters 24, 3470 (2024).

Back to the program

2D MATERIALS **Invited Speaker**

Graphene-like 2D carbon nitrides

Vincent Huc [1,*], Yannick Dappe [2], Vincent Derycke [3], Laurie Artero [3], Ariana Filoramo [3]

[1] Université Paris-Saclay-ICMMO, Bâtiment Henri Moissan, 17 avenue des Sciences, 91405 Orsay, France
[2] 10 Boulevard Thomas Gobert - 91120 Palaiseau, France
[3] Centre CEA Paris-Saclay. Site de Saclay. 91190 Gif-sur-Yvette, France

E-mail: vincent.huc@universite-paris-saclay.fr

Abstract:
The discovery of graphene in 2004 sparked an ever increasing interest in 2D materials. Since then, many different families of 2D materials were discovered including both organic and inorganic ones. In this context, 2D carbon nitrides are receiving an ever increasing interest, due to their interesting properties in such diverse area as catalysis, photocatalysis, molecular sieving, etc… Building upon our recently published work [1], new families of carbon nitrides were obtained and characterised (some examples Figure 1). These materials are opening new possibilities in the fields of electronics and catalysis.

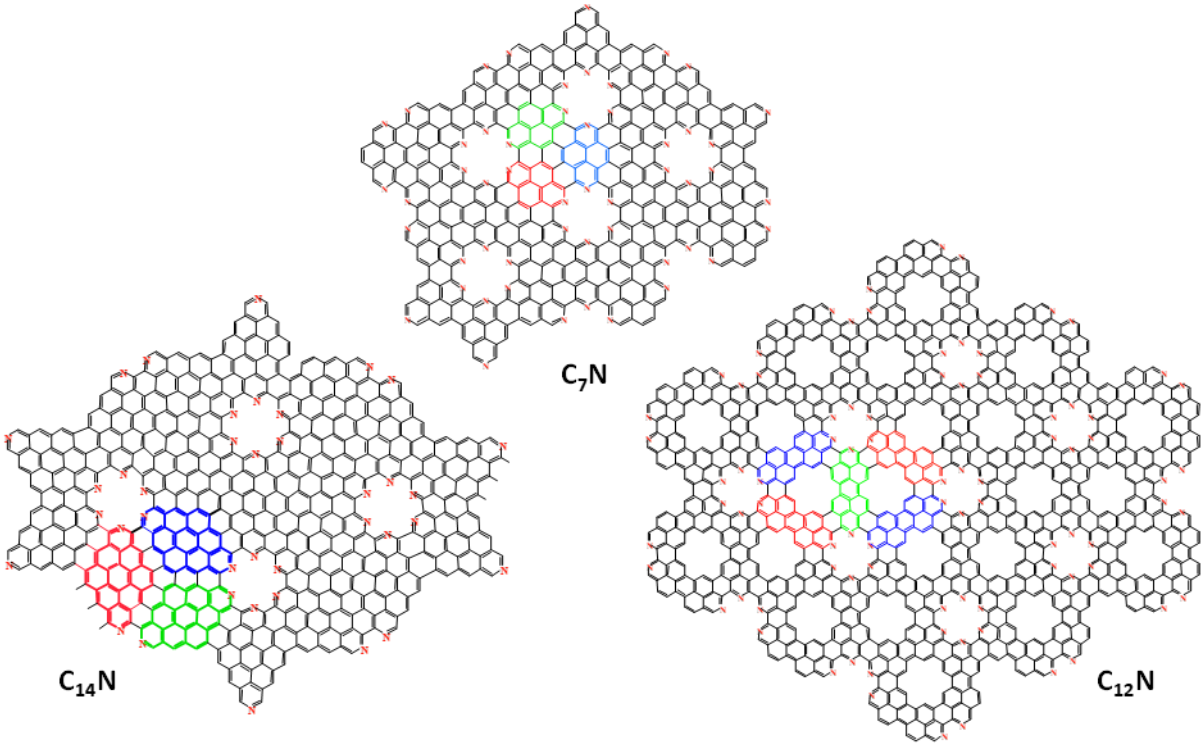


Figure 1: Examples of new families of exended 2D carbon nitrides.

References:
[1] Cora Moreira Da Silva, et al. Scientific Reports 13, 15423 (2023).

Back to the program

2D MATERIALS

Intelligent Molecular Switches for Brain-like Devices

Mohamed Mamlouk*, Yannick Dappe

Centre de Nanosciences et de Nanotechnologies (C2N), UMR 9001 CNRS, Université Paris Saclay, Paris, France

E-mail: mohamed.mamlouk@universite-paris-saclay.fr

Abstract:

Brain-inspired computing represents a paradigm shift toward low-power and adaptive information processing by mimicking the dynamic operation of biological synapses, where ionic fluxes and voltage-dependent neurotransmission regulate signal propagation (*Figure 1*). Emulating such complex behavior at the molecular scale has become feasible through dynamic molecular switches, which couple charge transport with redox and structural reconfiguration processes [1].

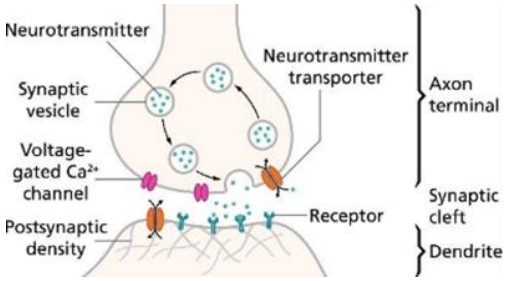


Figure 1: Schematic of a synapses

In artificial molecular synapses, signal modulation arises from voltage-driven protonation/deprotonation and redox processes, analogous to the ionic fluxes that govern neurotransmission in biological systems. This coupling between charge transport and chemical reactivity produces hysteretic current–voltage characteristics and negative differential resistance (NDR), providing an electronic analogue of synaptic plasticity [1]. Here, we investigate how different ionic species (H^+, Na^+, K^+, etc.) modulate the electronic response of molecular junctions. The interaction between these ions and the molecular backbone N-heterocyclic carbene/quinone can induce a mid-gap electronic state within the molecular energy gap, thereby enhancing the tunneling current, widening the hysteresis loop, and reinforcing the overall memory behavior, paving the way for brain-like molecular devices [2].

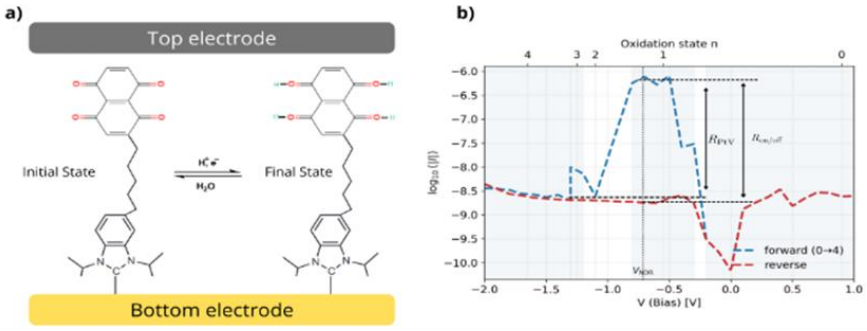


Figure 2: a) The junction consists of Au bottom electrode and the EGaIn. The two ET channels are brisged by slow PCET. b) Electrical characteristics of the Au-HNC-C10-Naphthalene-1,4,5,8-tetrone-Au junction.

References:

[1] Y. Wang, Q. Zhang, H.P.A.G. Astier, et al. Nat. Mater. 21, 1403 (2022).
[2] C. Crudden, J. Horton, I. Ebralidze, et al. Nature Chem 6, 409 (2014).

Back to the program

2D MATERIALS **Invited Speaker**

Characterization of Interfaces between Contact Metals and Monolayer 2D Semiconductor

Chun-Liang Lin

National Yang Ming Chiao Tung University, No. 1001, University Rd. East Dist., Hsinchu City 300093, Taiwan

E-mail: clin@nycu.edu.tw

Abstract:
Transition-metal dichalcogenides (TMDs), as members of the two-dimensional (2D) material family, exhibit strong potential for next-generation semiconductor applications. However, the complex interfacial mechanisms between TMDs and metals, including orbital hybridization and interface dipole redistribution often lead to unfavorable contact resistance, which in turn increase energy consumption and degrades overall device performance. This highlights the need for a comprehensive and systematic investigation of ML-TMD to metal interfaces.
Previously, by using STM metal tip, a semiconductor semimetal transition can be observed on monolayer $PtTe_2$ [1]. Recently, we have studied the interfacial properties of both metal and semimetal to monolayer TMD systems based on a peel and flip method. By using scanning tunneling microscopy/spectroscopy (STM/s), X-ray photoelectron spectroscopy (XPS) and density functional theory (DFT) calculations, the properties of monolayer MoS_2 and WS_2 on a variety of metals are investigated. It uncovers a consistent band-gap-reduction behavior across different contact configurations, arising from orbital hybridization at the interface. In addition, Fermi-level shifts observed in our measurements indicate doping effects induced by interlayer charge transfer.

References:
[1] M.K. Lin et al. ACS Nano 16, 14918 (2022).

Back to the program

Thursday, July 2, 2026

ADVANCED MATERIALS and CHARACTERIZATION **Invited Speaker**

Waste-to-Value Silicon: Pilot-Scale Upcycling of EoL PV Silicon into Si/C Li-ion batteries Anodes

Hamid Oubaha*, Lahcen Fkhar, Nicolas Eshraghi, Audrey Schrijnemakers, Mathieu Borin, Vincent Delaval, Frédéric Boschini, Rudi Cloots, Abdelfattah Mahmoud

GREEnMat, CESAM Research Unit, Chemistry Department, University of Liège, Quartier Agora, 13 Allée du 6 Août, 4000 Liège, Belgium

E-mail: hamid.oubaha@uliege.be

Abstract:

The limited theoretical capacity of graphite restricts the energy density of next-generation lithium-ion batteries (LIBs) required for high-demand applications. Silicon (Si), with nearly tenfold higher theoretical capacity, is a promising alternative. However, its practical deployment remains limited by extreme volume expansion, unstable solid electrolyte interphase (SEI), and loss of electrical connectivity during electrochemical cycling.

While several Si-based anode active material (AAM) technologies have been scaled, most rely on gas-phase synthesis or commercial Si nanoparticles, which are energy-intensive and costly due to high-purity precursor requirements. In contrast, solar-grade Si recovered from end-of-life (EoL) photovoltaic (PV) modules offers a sustainable and cost-effective alternative.

In this work, we demonstrate a scalable process to upcycle PV-derived Si into high-performance Si/C composite anodes (**GREEnSiBat-Si**). Using pilot-scale spray drying, we achieved controlled morphology and consistent quality, reaching technology readiness level (TRL) 6-7. A dual carbon scaffold, combining polymer-derived carbon and carbon nanotubes (CNTs), enhances electronic conductivity and mitigates structural degradation. The resulting anodes deliver high capacity and robust cycling stability, demonstrated at the 2.2 Ah multilayer pouch cell level.

Further integration of graphene oxide coatings and Si/C:SnS_2 hybrid structures demonstrates the versatility of this platform for advanced AAM design [1,2]. This work establishes a practical and sustainable pathway for large-scale valorization of PV waste into high-energy LIB technologies.

References:

[1] 1. N. Eshraghi, H. Oubaha, A. Schrijnemakers, L. Fkhar, J. Bodart, V. Delaval, R. Cloots, F. Boschini, A. Mahmoud. J. Power Sources 661, 238585 (2026).

[2] 2. L. Fkhar, H. Oubaha, A. Schrijnemakers, A. Bekzhanov, D. Cupid, F. Boschini, R. Cloots, A. Mahmoud. J. Energy Storage 162, 122007 (2026).

Back to the program

ADVANCED MATERIALS and CHARACTERIZATION

Design and Functionalization of Schiff Base-Based Materials for Advanced Applications

Khadija Khaldoune*, Ali Hasnaoui, Naima Fdil, Mustapha Ait Ali

Molecular Chemistry Laboratory, Faculty of Sciences Semlalia, Cadi Ayyad University, BP 2390 Bd My Abdellah, 40000 Marrakech, Morocco

E-mail: Khadijakhaldoune451@gmail.com

Abstract:
Schiff base-derived coordination compounds are versatile platforms for the development of functional materials due to their structural tunability and coordination ability. In this work, novel Schiff base ligands were synthesized and complexed with transition metals to form stable coordination systems, characterized by different spectroscopic techniques. Their electrochemical behavior was investigated, revealing redox activity and potential applicability in sensing and catalytic processes. In addition, these compounds were considered for their potential in medicinal and biological applications.

Back to the program

ADVANCED MATERIALS and CHARACTERIZATION

Interfacial Engineering of the ETL/Perovskite Interface Using a Thiophene-Based Capping Layer for Efficient Perovskite Solar Cells

Abderrazak Alihiane [1,*], Walid Riad [2], Mohammed Makha [2], Abdelkader Outzourhit [1,2]

[1] Laboratory of Materials, Energy and Environment (LaMEE), Faculty of Sciences Semlalia, Cadi Ayyad University, Marrakech 40000, Morocco
[2] Material Science and Nanomaterials Department, Mohamed VI Polytechnic University (UM6P), Benguerir, Morocco

E-mail: a.alihiane.ced@uca.ac.ma

Abstract:
Interfacial defects at the electron transport layer (ETL)/perovskite interface represent a major limitation in perovskite solar cells performance, as they promote non-radiative recombination and hinder efficient charge extraction. In this work, an interfacial passivation strategy was employed to reduce trap-state density and to enhance charge transport across the interface using a thiophene-based capping layer. Photoluminescence (PL) measurements confirmed reduction of non-radiative recombination after passivation, leading to improved carrier extraction and reduced recombination losses. As a result, the passivated devices exhibited enhanced photovoltaic performance. This finding highlights the role of thiophene-based interfacial engineering in achieving highly efficient and stable perovskite solar cells.

Acknowledgements:
The author acknowledges the financial support of the National Center for Scientific and Technical Research (CNRST), Morocco, through the Ph.D.-Associate Scholarship (PASS) program. Special thanks to the "Initiative on Energy Research" of University Mohammed VI Polytechnic for the financial support through project "Toward efficient, stable, environmentally friendly, and scalable Perovskite Solar Cells".

Back to the program

ADVANCED MATERIALS and CHARACTERIZATION

Sol-gel Synthesis and Interface Engineering of CZTS Thin Films Using ZnO/TiO_2 Buffer Layers

Sokaina El Ouakili [1,*], Ahmed El Hichou [1], Nabil Rochdi [1,2]

[1] Laboratory of Innovative Materials, Energy and Sustainable Development (IMED-Lab), Cadi Ayyad University, PO Box 549, 40000, Marrakesh, Morocco
[2] Department of Physics, Faculty of Sciences Semlalia, Cadi Ayyad University, PO Box 2390, 40000, Marrakesh, Morocco

E-mail: s.elouakili.ced@uca.ac.ma

Abstract:
Cu_2ZnSnS_4 (CZTS) thin films were successfully synthesized using a sol-gel method and deposited onto ITO substrates via spin coating. The influence of ZnO/TiO_2 buffer layers and post-deposition annealing on the structural, morphological, and electrical properties of the films was systematically investigated. X-ray diffraction analysis confirmed the formation of the kesterite CZTS phase, with slight lattice compression compared to standard values. The incorporation of ZnO/TiO_2 layers led to an increase in crystallite size and improved film uniformity, as observed from morphological studies.
Electrical characterization of the ITO/ZnO/TiO_2/CZTS/Ag structure revealed a pronounced rectifying behavior with an ideality factor close to unity and a low saturation current, indicating diffusion-controlled transport and reduced recombination losses. These results confirm the successful formation of a high-quality p–n heterojunction. In contrast, devices without buffer layers exhibited non-ideal behavior, highlighting the critical role of interface engineering. Overall, this study demonstrates the effectiveness of ZnO/TiO_2 buffer layers in enhancing the performance of CZTS-based heterojunction devices, making them promising candidates for low-cost photovoltaic applications.

Back to the program

Poster Contributions

P01	**Khadija Seyagh**	*Magnetically Recoverable Nanocomposites: A Sustainable Approach for Photocatalytic Degradation of Organic Dyes in Wastewater Treatment*
P02	**Mohammed El-Bassri**	*Monoethanolamine (MEA) Concentration Effect on the Physical Properties of Tin Sulfide (SnS) Thin Films*
P03	**Yassine Bounnaiche**	*Complexing agents' addition effect on the physical properties of electrodeposited Sb_2S_3*
P04	**Mouhcine Ourbaa**	*Nitrogen-annealing-induced interfacial diffusion in RF sputtered SnO_2/Cu/SnO_2 multilayers toward improved photocatalytic performance*
P05	**Noureddine Lebrini**	*Influence of Sn Dopant Concentration on NiS_2 Thin Films Prepared by Spin Coating for Supercapacitor Applications*
P06	**Aymane Ezerraf**	*Machine Learning and DFT-Assisted Design of Eco-Friendly Organic Corrosion Inhibitors for Mild Steel Protection in Acidic Media*
P07	**Rachid Haroudi**	*DFT Investigation of the PtS_2/ZrS_2 Heterojunction for Enhanced Photocatalytic Hydrogen Evolution*
P08	**Adil Mojahid**	*Investigation of the Electronic and Optical Properties of Doped Borophene*
P09	**Ikram Oughaddou**	*Towards Multiscale Modeling of Lithium-Ion Transport in NMC Cathode Materials Using Deep Learning Potentials*
P10	**Oualid Mouktaoui**	*Development of New Chelating Agents for Heavy Metal Complexation*
P11	**Imad Salym**	*Optoelectronic enhancement and exciton control in Si-doped KGeF3 perovskites*
P12	**Jihane Ziraoui**	*Using Waste Jute Bags as Reinforcement to Enhance Geopolymers: An Eco-Friendly Solution for Sustainable Construction*
P13	**Brahim Fakrach**	*A Raman Spectroscopy Study of Double-Walled Carbon Nanotubes at Optimal Interlayer Distance*