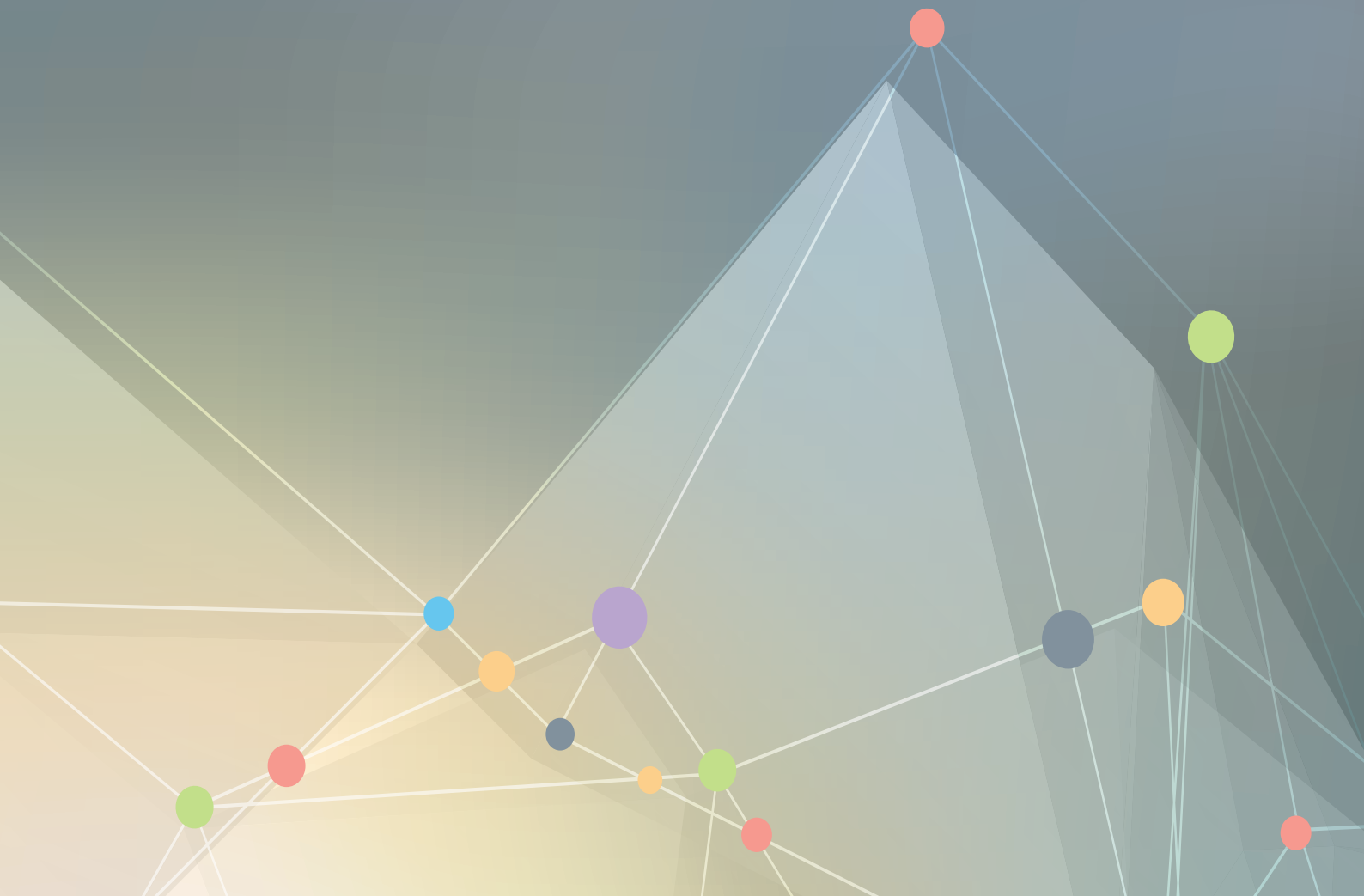


BOOK OF ABSTRACTS

Oral Presentations



2023



Nanomaterials for Energy

(Last update: July 8th, 2022)

Description

- Nanostructured materials offer huge surface to volume ratios and favorable properties for energy-related applications such as solar cells, fuel cells, thermoelectrics, batteries, supercapacitors and hydrogen production and storage systems. In this context, this session focuses on different topics concerning:
- Elaboration and characterization of nanomaterials for (bio)energy production and storage
- New processes of elaboration and implementation in devices (nano-micro systems)
- Phonon, electron, photon and mass transport properties
- Measurement methods, simulation and modelling of nanostructures, nano-structured materials and interfaces
- Limitations and challenges of nanomaterials while being used in energy-related applications

Keywords

nanomaterials: elaboration, characterization, modelling; energy production and storage systems

Scientific committee

Cláudia GOMES DE MORAIS* (Univ. Poitiers – IC2MP, Poitiers)

Liliane GUERLOU-DEMOURGUES (Bordeaux INP – ICMCB, Bordeaux)

Jérôme PACAUD* (Univ. Poitiers – Pprime, Poitiers)

David PORTEHAULT (CNRS – LCMCP, Paris)

Lionel SANTINACCI (CNRS – CINaM, Marseille)

** Session Coordinator*

Friday March 17th

10.30 am – 12.30pm

Main Amphitheater

Program of the session

Chairs: Claudia GOMES DE MORAIS & Jérôme PACAUD

NANOMATERIALS FOR ENERGY

10:30	Electrocatalysis of the oxygen evolution reaction by transition metal oxide nanoparticles	Elena SAVINOVA • Univ. Strasbourg – ICPEES, Strasbourg – France
11:00	Active and Stable NiFe Catalysts supported on TiO _x species for Oxygen Evolution Reaction (OER) in alkaline medium	Victor RAUD • Univ. Poitiers - IC2MP, France
11:15	Composite Mn-Co electrode materials for supercapacitors: Why the precursor's morphology matters !	Ronan INVERNIZZI • Univ. Bordeaux - ICMCB, France
11:30	Nanostructured WO ₃ as photoelectrocatalyst for the selective glycerol valorization	Jesus GONZALEZ COBOS • CNRS - IRCELYON, France
11:45	Characterization of a Kinetic Energy Harvesting System based on Selective Ion Sweeping using Photoluminescent Nanorods	Lilian MAGERMANS • Ecole Polytechnique - LPMC, France
12:00	Tunable dimensions of ZnO nanowires grown by metal-organic chemical vapor deposition and its impact on the physical and piezoelectric properties	Lisa LEGARDINIER • Grenoble INP - LMGP, France
12:15		

Keynote Speakers

NANOMATERIALS FOR ENERGY



Elena SAVINOVA

University of Strasbourg | Professor

Institute for Chemistry and Processes for Energy, Environment and Health

<http://icpees.unistra.fr/catalyse-et-materiaux/ece/personnel/elena-savinova/>

Biography

Elena SAVINOVA received her PhD from the Boreskov Institute of Catalysis of the Russian Academy of Sciences (BIC) in 1988. She has worked as a senior research fellow at the Boreskov Institute of Catalysis (Novosibirsk, Russia), at Technische Universität München (Garching, Germany), and as a visiting researcher at Fritz-Haber-Institut der MPG (Berlin, Germany). Since 2007 she is full professor at the University of Strasbourg. She is head of the group «Electrochemistry and Energy Conversion» at the Institute of Chemistry and Processes for Energy, Environment and Health (UMR7515). In 2006 she was awarded Chair of Excellence in chemistry from the National Research Agency and in 2014 became Fellow of the International Society of Electrochemistry. Her research interests are concerned with interfacial electrochemistry, energy conversion, electrocatalysis and operando spectroscopies.

Electrocatalysis of the oxygen evolution reaction by transition metal oxide nanoparticles

The European Commission launched the European Green Deal with the objective to make Europe climate-neutral by 2050. This plan foresees significant increase in the green hydrogen production by water electrolysis for its use as an energy carrier and feedstock for industry. Last decades have evidenced significant advances in proton-exchange membrane water electrolysis (PEMWE) technology, both in terms of materials and system developments. However, commercial PEMWE systems rely on scarce and Ir for catalyzing sluggish oxygen evolution reaction (OER) occurring at the anode. Recent developments in the field of anion-exchange membranes (AEM) have switched focus of current research towards AEM-based water electrolysis technology (AEMWE), which is compatible with PGM(platinum group metal)-free materials. Yet, development of active and durable PGM-free anode materials for the AEMWE technology still presents a significant challenge.

In this presentation we will discuss electrocatalysis of the OER by transition metal oxides (TMO). We will show that the apparent electrocatalytic activity of PGM-free TMOs is often limited by their low electronic conductivity [1]. To increase the OER current, TMOs are often mixed with conductive binders or supported on conductive supports [1]. We will demonstrate that utilization of such ubiquitous conductive materials as carbons is prohibited at the AEMWE anode due to their oxidative degradation [2]. We will then present two alternative approaches: (i) supporting TMO nanoparticles on high-stability boron doped diamond (BDD) [3], and (ii) development of core-shell nanoparticles comprised of a conductive Fe₃O₄ core and a catalytically active CoFe₂O₄ shell [4]. We will show that confining the active component in a thin (~1-2 nm) shell and taking advantage from the core-shell synergistic interaction allows one to reach an extraordinary OER activity. Finally, we will present the results of operando near edge X-ray absorption fine structure (NEXAFS) spectroscopy [5] and discuss the origin of the synergy between the core and the shell.

Acknowledgements

The author is indebted to I. Filimonenkov, G. Tsirlina, S. Istomin, E. Antipov, G. Kerangueven, L. Royer, B. Pitchon, A. Bonnefont, T. Asset, B. Rotonelli, S. Hettler, R. Arenal, S. Holdcroft and J. Velasco-Vélez.

Keywords:

Water electrolysis; Oxygen evolution reaction; Transition metal oxides; Core-shell nanoparticles; Operando near-edge X-ray absorption fine structure spectroscopy

Keynote Speakers

NANOMATERIALS FOR ENERGY



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Keywords: Hydrogen production, Electrolysis, OER catalysts, Alkaline electrolysis, Ball-milling

Disciplinary field involved: Chemistry

Sustainable Development Goals: Affordable and Clean Energy (Goal 7), Climate Action (Goal 13)

Active and Stable NiFe Catalysts supported on TiO_x species for Oxygen Evolution Reaction (OER) in alkaline medium

Victor Raud^{1,2}, Cláudia Gomes de Morais², Aurélien Habrioux², Jean-Louis Bobet¹, Laurence Pirault-Roy²

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In a context of fight against global warming, hydrogen is seen to be the future energy carrier in the next energetic mix. Hydrogen can be produced by water electrolysis, in particular in alkaline medium, thus making it possible to use using non-noble metals as catalysts. In this case, it's necessary to decrease the cell voltage by developing new materials with high specific surface, high conductivity, and corrosion resistance properties. TiO₂ is an interesting candidate for developing this kind of materials but its low conductivity is a major drawback. To solve this problem, the use of doping elements ^[1] or non-stoichiometric titanium oxides ^[2] is studied. Our research is focused on the development of a new titanium-based support by ball milling using TiO₂ and Ti under hydrogen pressure. The resulting material, a mix of TiO₂, Ti and TiH_x, is then impregnated with different Ni and Fe content with the following formula Ni_{1-x}Fe_x (x = 0.25; 0.5; 0.75 and 1) and finally reduced. The XRD patterns of the catalysts before and after synthesis highlight the transformation of the titanium species into Ti₂O₃ during the reduction step. For Ni_{0.5}Fe_{0.5}, the potential required to drive a current density of 10 mA.cm⁻² is only about 1.52 V vs. RHE and the stability test underlines a good stability of this material even after 7 days running. This new synthesis pathway is more than promising to produce stable, active and corrosion resistant catalysts for OER in alkaline medium.

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Acknowledgment: This work is financially supported by Université de Poitiers and Region Nouvelle-Aquitaine

Keywords: composite; exfoliation and restacking; morphology design; supercapacitors; electrode materia

Disciplinary fields involved: Chemistry, Material science

Composite Mn-Co electrode materials for supercapacitors: Why the precursor's morphology matters !

Ronan Invernizzi,^{1,2} Alexia Lemoine,³ Lénaïc Madec,^{2,3} François Weill,^{1,2} Marie-Anne Dourges,⁴ Céline Tang,^{1,2,5} Pierre Louis Taberna,^{2,6,7} Delphine Flahaut,^{2,3} Jacob Olchowka,^{1,2,6} Liliane Guerlou-Demourgues^{1,2,6}

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7. CIRIMAT, Université de Toulouse, CNRS, Université Toulouse 3 – Paul Sabatier, 118 Route de Narbonne, 31062 Toulouse Cedex 9, France

One of the most promising way to improve the limited performance of the widely used EDLC supercapacitors is to replace one of the carbon capacitive electrode by a pseudocapacitive electrode material such as MnO_2 , which is an abundant and low cost material. This latter involves charge storage through rapid and reversible redox reactions at the surface of the material, which allows to increase the energy density while keeping a high power density. However, to make use of these advantages, the pseudocapacitive electrode material must possess both good ionic and electronic conductivities to perform well. Thus, the development of composite electrode materials combining MnO_2 phase with an electronic conductor appears as a perfectly adapted approach to generate a synergetic effect and compensate the intrinsic poor electronic conductivity of MnO_2 . In this work, an original synthesis strategy based on the exfoliation and restacking of cobalt and manganese layered oxides has been carried out. Three different layered MnO_2 phases with various morphologies (veils, nanoplatelets and microplatelets) were combined with electronic conductor cobalt oxyhydroxides with different platelet sizes (~ 20 nm vs 70 nm wide), to synthesize 6 different composites/nanocomposites. The influence of precursors' morphology on the distribution of the Mn and Co objects within the composites was carefully investigated at the nanoscale by several technics and correlated to the electrochemical performance of the final restacked material. By combining MnO_2 possessing a veil morphology with the smallest cobalt oxyhydroxide nanoplatelets, the most homogeneous distribution between the Mn and Co objects was obtained, leading to a capacity almost two times greater at high rate (19 F.g⁻¹ vs 10 F.g⁻¹ at 500 mV.s⁻¹) compared to the other composites [3].

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Acknowledgment:

AID and Bordeaux INP for financial support (PhD funding and research fees). Région Nouvelle Aquitaine and the French National Research Agency (STORE-EX Labex Project ANR-10-LABX-76-01) for financial support and fruitful discussions. Many thanks to Domitille Giaume, Isabelle Baraille, Catherine Denage, Emmanuel Petit, Eric Lebraud for fruitful discussions and their help in the characterization of the samples for ICP, MEB and XRD.

Keywords: Photoelectrocatalysis, tungsten oxide, glycerol valorization, hydrogen production

Disciplinary fields involved: Chemistry, electrocatalysis, photocatalysis

Sustainable Development Goals* eventually involved in your research: Affordable and clean energy (Goal 7), Responsible Production & Consumption (Goal 12), and Climate Action (Goal 13)

Nanostructured WO₃ as photoelectrocatalyst for the selective glycerol valorization

Jie Yu¹, Jesús González-Cobos¹, Frederic Dappozze¹, Philippe Vernoux¹, Angel Caravaca¹, Chantal Guillard¹

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Nowadays, the need for alternatives to fossil fuels has boosted the worldwide production of glycerol as a co-product of biodiesel production. Therefore, being largely available and cheap, glycerol is an attractive renewable platform molecule for making added-value bio-sourced chemicals like glyceraldehyde (GAD) or dihydroxyacetone (DHA).¹ The photoelectrocatalysis (PEC) is one of the emerging technologies for the glycerol valorization and hydrogen co-generation.² In two previous studies, our group unravelled the outstanding properties of nanostructured WO₃-based materials as photocatalysts for the selective conversion of glycerol,³ and we reported the potential improvement achieved through the photoelectrocatalytic (PEC) route.⁴ Encouraged by these previous results, herein we went a step forward in the development of a device able to simultaneously produce H₂ and valuable C₃ products in a sustainable way, by designing and validating, for the first time, a proton-exchange membrane (PEM) photoelectrolyser using the proposed WO₃ photoanode.

As a result, we report a sustained product generation at the anode of 11.1 and 5.2 mmol m⁻² h⁻¹ for GAD and DHA, respectively, along with 44.0 mmol H₂ m⁻² h⁻¹ at the cathode, under optimum conditions (60 °C and 1.2 V). Indeed, after performing tests under different photo- and electro-catalytic conditions, we confirm the synergistic effect between light irradiation and the external bias. Thus, nanostructured WO₃ is confirmed as a promising base material for the selective generation of target C_{3s} and PEC stands as a realistic technology for the sustainable generation of hydrogen and target biomolecules from organic wastes.

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Acknowledgment:

This work was financially supported by the China Scholarship Council (Grant No. 201906740016).

Keywords: Energy harvesting, nanoparticles, microfluidics

Disciplinary fields involved: Chemistry, Physics, Mechanics

Sustainable Development Goals: Affordable and Clean Energy (Goal 7), Climate Action (Goal 13)

Characterization of a Kinetic Energy Harvesting System based on Selective Ion Sweeping using Photoluminescent Nanorods.

Lilian Magermans¹, Donghoon Lee², Jeongmo Kim¹, Zijun Wang¹, Seok Woo Lee², Thierry Gacoin^{1*}, Jongwook Kim^{1*}

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With the increasing demand for self-powered wearable devices and internet of things (IoT) there is a search for suitable power sources. Kinetic energy is an ideal source due to its abundant availability, such as from human motion. Recently, we demonstrated an electrochemical kinetic energy harvesting system in a hybrid cell consisting of an activated carbon supercapacitor electrode and PBA battery electrode [1]. When flowing electrolyte over the electrodes, ions adsorbed to the supercapacitor electrode will be swept away, whereas ions hosted within the battery electrode lattice are not affected by the flow. This selective ion sweeping at the supercapacitor electrode induces a potential difference between the two electrodes which can be used to generate a current.

In this work we miniaturize the system such that the supercapacitor and battery electrodes are incorporated into a microfluidic channel. Moreover, different channel geometries and electrode materials are explored to optimize selective ion sweeping behavior. To better understand the ion-sweeping phenomena, we must characterize the electrochemical response of the selective ion sweeping device as a function of the flow shear at the electrode surface. This requires flow shear measurements with high spatial and temporal resolution. We have developed such a technique for measuring flow shear in microfluidic channels using the polarized photoluminescence of LaPO₄:Eu nanorods [2]. We can thus characterize the shear flow in our energy harvesting device by adding LaPO₄:Eu nanorods to the electrolyte and collecting their polarized emission under flow. This allows us to study the fundamental relationship between shear flow and ion sweeping and aids in the optimization of the device.

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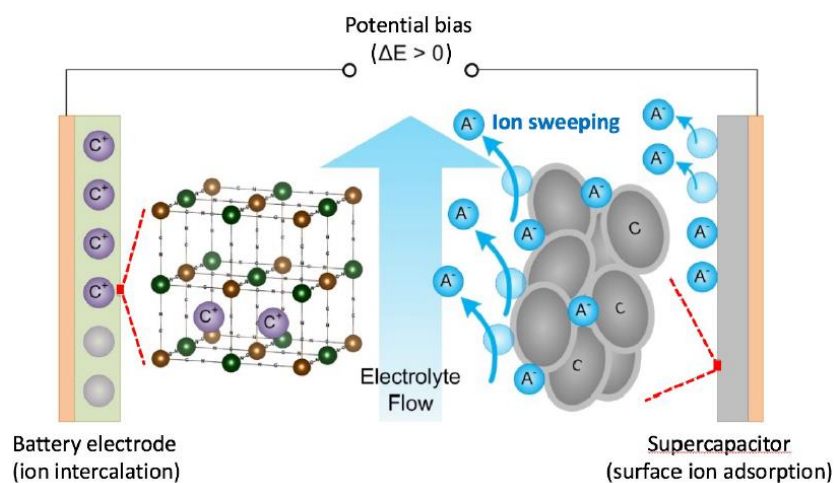


Figure 1: Schematic of energy harvesting hybrid cell

Keywords: Zinc Oxide, Piezoelectricity, Nanowires, Metal-Organic Chemical Vapor Deposition

Disciplinary fields involved: Chemistry, physics

Sustainable Development Goals* eventually involved in your research: Responsible Consumption and Production (Goal 12)

Tunable dimensions of ZnO nanowires grown by metal-organic chemical vapor deposition and its impact on the physical and piezoelectric properties

Lisa Legardinier^{1,2}, Gustavo Ardila², Quang Chieu Bui^{1,2,3}, Isabelle Gélard¹, Thomas Jalabert², Manuel Manrique^{1,3}, Bassem Salem³, Matthieu Weber¹, Carmen Jimenez¹, Fabrice Donatini⁴, and Vincent Consonni¹

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As an abundant and sustainable semiconductor with relatively high piezoelectric coefficients, ZnO nanowires (NWs) have emerged as a promising material for piezoelectric applications [1]. ZnO NWs can be grown by a wide variety of chemical and physical deposition techniques, as a unique ability in the family of semiconducting NWs [2]. The pulsed-liquid injection MOCVD technique deserves a particular attention as a fast growth method that is compatible with large surface area, while still showing the formation of ZnO NWs with a great structural and optical quality [3]. While MOCVD has been assessed when growing ZnO NWs for optoelectronic devices, its potential for piezoelectric devices is still open largely. The NW morphology obtained by MOCVD has shown better piezoelectric performances compared to thin films [3]. Using simulations by finite element method (FEM), it has further been revealed that the dimensions of the NWs could be of critical importance to enhance their piezoelectric performance [4]. The doping concentration and surface trap density are also expected to strongly affect the piezoelectric performance.

In this work, we investigate the growth of ZnO NWs by MOCVD and optimize their dimensions including their diameter and length over a broad range of values by varying the growth time. The physical properties of ZnO NWs including the nature of defects involved and their charge carrier density are assessed by cathodoluminescence and Raman spectroscopy, and point-probe resistivity measurements, respectively. The nature of surfaces is further studied by X-ray photoelectron spectroscopy. Eventually, the impact of the dimensions of ZnO NWs on their piezoelectric performance is assessed experimentally by piezoelectric force microscopy and shortly discussed in the light of FEM simulations.

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Acknowledgment:

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Friday March 17th

2.00 pm – 3.45pm

Main Amphitheater

Program of the session

***Chairs: Stéphane CELERIER
& Liliane GUERLOU-DEMOURGUES***

NANOMATERIALS FOR ENERGY & 2D MATERIALS

14:00	Tailoring nanomaterials for oxygen electrocatalysis	Aurélien HABRIOUX • Univ. Poitiers – IC2MP, Poitiers – France
14:30	Thermally Stable W/TiAlN/TiAlSiN/TiAlSiON/TiAlSiO Selective Solar Absorber Nanofilms for Concentrated Solar Power	Mireia SAINZ-MENCHÓN • Univ. Basque Country - UPV/EHU, Spain
14:45	Mo ₂ CTx MXene supported nickel-iron alloy heterostructure as efficient catalyst for: oxygen evolution reaction	Roald BOULÉ • Univ.Poitiers - IC2MP, France
15:00	Thin film of lanthanum cobaltite LaCoO ₃ for solar thermal collectors	Abdoul Azise BANDE • Univ.Poitiers - Inst. Pprime, France
15:15	Chemical reactivity of layered carbides and borides in molten salts: towards bidimensional MXenes and boridenes	Emile DEFOY • CNRS - LCMCP, France
15:30	The use of noble gas implantation to improve the thermoelectric properties of ScN and CrN thin films	Hugo BOUTEILLER • Univ.Poitiers - Inst. Pprime, France

Keynote Speakers

NANOMATERIALS FOR ENERGY



Aurélien HABIROUX

University of Poitiers | Researcher

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Biography

Aurélien HABIROUX is 40 years old. He obtained his PhD at University of Poitiers in 2009. He completed a postdoctoral fellowship at CEA Saclay. He is an associate professor at University of Poitiers since 2011. He has his expertise in electrocatalysis. His research interest is focused on designing and characterizing electrocatalysts for hydrogen evolution, oxygen reduction and oxygen evolution reactions in alkaline medium. He has been coordinating several research projects aiming at developing heterostructured catalysts for the positive electrode of high energy density metal-air batteries (Zn/air, Al/air). He is deeply involved in the design of nanocatalysts composed of 3d transition metal-based active phases (oxides, hydroxides, sulfides) supported onto 2D materials (MXene, graphene derivatives). He works on the understanding of the role played by the active phase/substrate interaction on the electrocatalytic activity. He is also interested in scrutinizing and explaining the dynamics of electrochemical interfaces (surface reconstruction phenomenon, interactions in the double layer) upon working conditions.

Tailoring nanomaterials for oxygen electrocatalysis

Electrocatalysis is involved in many electrochemical energy storage and conversion devices (electrolyzers, fuel cells, metal-air batteries,...) that will implement the future energy grid. The design of efficient electrodes allowing increasing the rate of electrochemical reactions is required to enhance the electrical performances of the above-mentioned devices. Performances of electrodes depend on a complex entanglement between the intrinsic properties of the catalyst (chemical composition, crystal structure, exposed facets, partial charges on surface atoms, morphology) and the characteristics of the electrode itself (conductivity, porosity).

This presentation focuses on the different steps allowing the rational design of electrocatalysts:

- Identification of potentially efficient surfaces
- Synthesis and characterization of nanocatalysts
- In-depth conceptual understanding of electrocatalytic processes by establishing the relationship between the physico-chemical properties of the nanocatalyst and its electrochemical behavior (activity, durability).

This scientific approach will be mainly illustrated by investigating 3d transition metal-based heterostructured catalysts designed for oxygen evolution and reduction reactions in alkaline medium [1-10]. The tailoring of cheap, efficient and stable materials for oxygen electrocatalysis remains a major challenge in modern electrochemistry.

Keywords:

Oxygen electrocatalysis; 2D materials; Heterostructured catalysts; 3d transition metal

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Keywords: selective absorbers, solar energy, CSP, thin film, coatings

Disciplinary fields involved: Physics, Chemistry

Sustainable Development Goals eventually involved in your research: Affordable and clean energy (Goal 7), Climate Action (Goal 13)

Thermally Stable W/TiAlN/TiAlSiN/TiAlSiON/TiAlSiO Selective Solar Absorber Nanofilms for Concentrated Solar Power

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A spectrally selective absorber coating was developed based on a W/TiAlN/TiAlSiN/TiAlSiON/TiAlSiO tandem structure of films of about 50 nm thick deposited on stainless steel by magnetron sputtering. The structure is especially tailored to effectively absorb solar radiation while suppressing infrared emission at high temperatures. In this work, the spectral directional emissivity of the structure has been measured from 100 °C to 600 °C. The total hemispherical emissivity does not show a significant temperature dependence. The structure presents a suitable combination of high solar absorptance ($\alpha=0.954$) and low thermal emittance ($\epsilon = 0.07$) with a cut-off wavelength of around 1.75 μm , which conforms to the requirements of an effective photothermal converter. A gradient in refractive indices, from metallic to transparent, ensures a high absorbing nature. W is found to function as an infrared reflector as well as a diffusion barrier. No unfavourable alteration in the phases or composition of the sample were found after subjecting it to 600 °C in vacuum, which is indicative of thermal stability at operating temperatures.

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Keywords: MXenes, Ni/Fe nanoalloy, composites, oxygen evolution reaction, electrolyser

Disciplinary fields involved: Electrocatalysis, Material Science

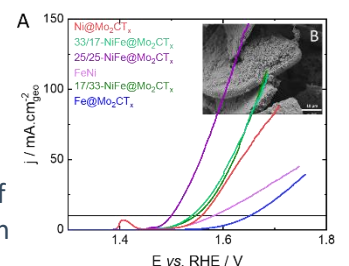
Sustainable Development Goals* eventually involved in your research: Climate Action (Goal 13)

Mo₂CT_x MXene supported nickel-iron alloy heterostructure as efficient catalyst for: oxygen evolution reaction.

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Rechargeable metal-air batteries and electrolyzers are needed to reduce greenhouse gas emissions and the consumption of fossil fuels in the new energy grid [1]. The elaboration of electrocatalysts is a key point in the conception of these systems in order to improve the kinetics of the reactions implied, in particular the oxygen evolution reaction (OER) [2]. By polyol-assisted solvothermal synthesis route, non-noble composites of Ni_xFe nanoalloys supported onto a highly electron conductive 2D transition metal carbide, Mo₂CT_x MXene, were obtained without degrading the MXene phase. Structural and morphological properties as well as composition of the composite materials were determined using several physical and chemical techniques. These latter properties have been correlated to the activity of the different materials towards oxygen evolution reaction in alkaline medium. The presence of MXene has a twofold interest: it allows the formation of a nanostructured metallic Ni_xFe nanoalloy during the synthesis and it favors the interfacial charge transfer during OER. By tuning the Ni/Fe ratio in the composite composition it was possible to obtain an OER catalyst exhibiting an outstanding activity (1.50 V vs. RHE at 10 mA.cm⁻²) combined with an amazingly low Tafel slope value of 34 mV.dec⁻¹. This material also exhibited an excellent stability during 168 h under harsh conditions. *In situ* Raman experiments were performed using the most efficient catalyst and it was shown that a nickel oxyhydroxide phase, possibly containing Fe element, is the active phase for the OER [3].



A. Linear polarization curves recorded in a nitrogen-saturated 1 mol.L⁻¹ KOH electrolyte with Ni@Mo₂CT_x, 33/17-NiFe@Mo₂CT_x, 25/25-NiFe@Mo₂CT_x, Fe/Ni, 17/33-NiFe@Mo₂CT_x, Fe@Mo₂CT_x catalysts using a rotating disk electrode set at 1600 rpm and a scan rate at 5 mV.s⁻¹.
B. SEM micrographs of 25/25NiFe@Mo₂CT_x.

References:

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Keywords: -

Disciplinary fields involved: -

Thin film of lanthanum cobaltite LaCoO_3 for solar thermal collectors

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In the past, we demonstrated the feasibility of optimized VO₂ thermochromic solar collectors whose stagnation temperature can be reduced by more than 35°C, while keeping the high performance of the system [1][2]. The aim of the present work is to elaborate and optimize a new generation of more effective solar collectors based on thermochromic perovskite-type nano-films of LaCoO₃. Thermochromism is the aptitude of materials to reversibly change their properties versus temperature due to structural modifications. Such change occurs at a specific temperature called metal-insulator transition temperature (*TMI*) and thus, thermochromic materials are IR transparent (insulator) below *TMI* and IR reflective (metal) above. LaCoO₃ exhibit complex and temperature dependent behavior leading to a thermochromic effect and an unsharpened transition accompanied by a drastic change in emissivity. This makes it an excellent candidate for passive thermal regulation. However, due to the structural and chemical complexity of such

systems, their design is challenging. For this work, we present the synthesis of LaCoO₃ thin films deposited on silicon substrates obtained from a magnetron sputtering machine (PVD). Then, the optical and electrical behavior of two films with different thicknesses has been performed by X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR) and scanning electron microscopy (SEM). To finish, with ellipsometric spectroscopy measurements, a comparison of these optical properties simulation and an

estimation of the band gap energy has been made for LaCoO₃ thin films.

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Keywords: MBenes, molten salt

Disciplinary field involved: Chemistry

Sustainable Development Goals* eventually involved in your research: Ensure sustainable production patterns

Chemical reactivity of layered carbides and borides in molten salts: towards bidimensional MXenes and boridenes

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MXenes are bidimensional metal carbides or nitrides that present many interesting properties for photocatalysis, electrocatalysis, and magnetic shielding, among others.[1] Boridenes are a related family of 2D nanomaterials made of transition metal borides, which emerge as analogues of MXenes. They are expected to exhibit new properties, especially for electrocatalysis.[2]

The rare occurrences of boridenes have been obtained from the parent phases MAB where A (Al) atoms are interleaved between the transition metal boride layers. The A atoms can be etched by treatment in fluorhydric acidic or basic aqueous solutions, thus leading to the exfoliation of the material.[3] These harsh conditions are hardly suited to poorly stable MAB phases and boridenes. On the other side, a large knowledge has been acquired on the chemical exfoliation of MAX phases to yield MXenes, either in acidic or basic aqueous solutions.[1] More recent works have been focused on the exfoliation in molten salts.[4] However, the mechanisms underlying this new way to functionalize MXenes are still poorly understood and the method has never been investigated for boridenes.

In order to address the challenge raised by the synthesis of boridenes, we are investigating the chemical reaction of MAX and MAB phases in molten salts. We will present our investigations on the reactivity of $\text{Mo}_2\text{Ga}_2\text{C}$ and Fe_2AlB_2 in oxidative molten salts to achieve their delamination. By monitoring the reactions with synchrotron-based *in situ* X-ray diffraction, we could shed light on the exfoliation mechanisms. Finally, we will show how to etch partially or completely Fe_2AlB_2 and $\text{Mo}_2\text{Ga}_2\text{C}$ by tuning synthesis conditions.

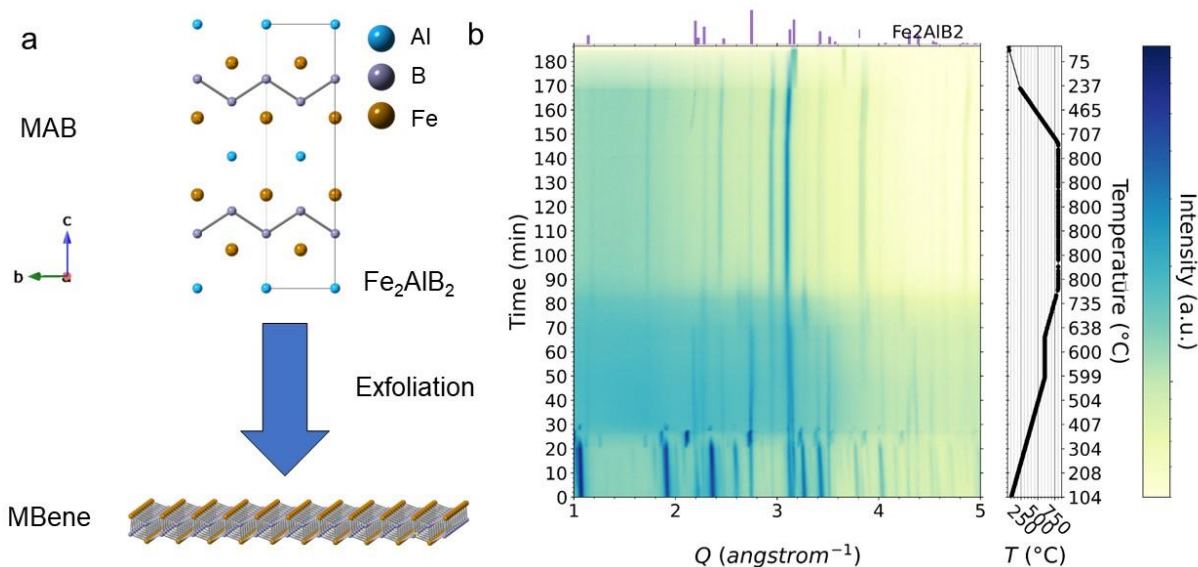


Figure 1 : a) Scheme of the exfoliation of Fe_2AlB_2 into Fe_2B_2 . b) In situ XRD patterns of Fe_2AlB_2 reacting with an eutectic mixture of $\text{CdCl}_2/\text{NaCl}$.

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Acknowledgment: ESRF and SOLEIL support. H2020 program (ERC CoG project GENESIS).

Keywords: Thermoelectric, Nitrides, implantation, thin films, defects

Disciplinary fields involved: Physics, Chemistry, Energy

Sustainable Development Goals* eventually involved in your research: Affordable and clean energy (Goal 7)

The use of noble gas implantation to improve the thermoelectric properties of ScN and CrN thin films.

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Nitride-based semiconductors, such as ScN and CrN, exhibit interesting transport properties for thermoelectric (TE) applications generally used to convert wasted heat into electricity. However, their efficiency has yet to be improved to allow their development at a larger scale. Their performance is expressed by the figure of merit $zT = S^2 T / \rho (k_e + k_l)$, S being the Seebeck coefficient, ρ the resistivity, k_e and k_l the electronic and lattice contributions of the thermal conductivity. In this work, ion implantation was used to introduce defects to increase the phonon scattering and thus reduce the lattice thermal conductivity, k_l . The ion implantation results in the generation of a large concentration of Frenkel pairs, that tends to recombine and/or condense to form various types of defects. Thin films of ScN and CrN were deposited, at respectively 950°C and 600°C, on c-plane Al₂O₃ by using magnetron sputtering. The films were implanted at room temperature with noble gases (Ar, He) by using a multi-energy process. For example, in ScN films, the implantation of argon at a high damage regime, results in the formation of Ar-vacancies complexes. These defects act as carrier traps, reducing the charge carriers mobility and strongly affecting the thermoelectric properties of the film. In particular, the thermal conductivity is found to be reduced by a factor of four and the Seebeck coefficient is strongly enhanced (see Fig. 1).¹ The modifications under implantation of the TE properties of both nitride-compounds, currently in progress, will be presented and compared.

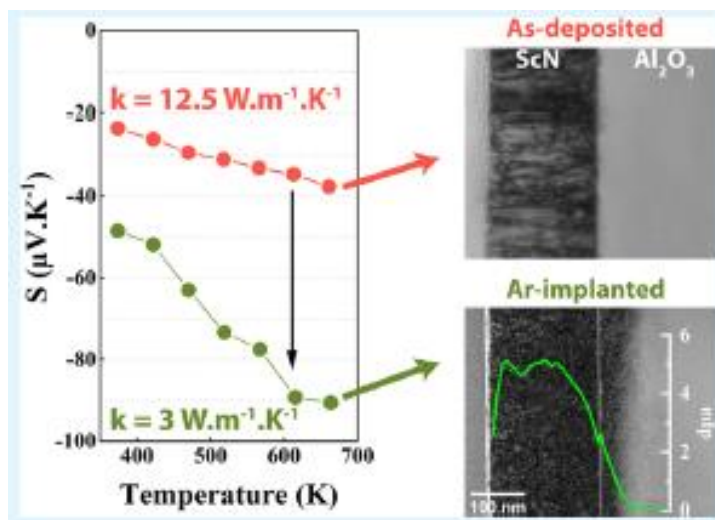


Figure 1: Effects of Ar-implantation on the structural and TE properties of ScN films

Reference:

¹R. Burcea, J.-F. Barbot, P. O. Renault, D. Eyidi, T. Girardeau, M. Marteau, F. Giovannelli, A. Zenji, J.-M. Rampoux, S. Dilhaire, P. Eklund and A. le Febvrier, ACS Appl. Energy Matter. 5, 11025 (2002)

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