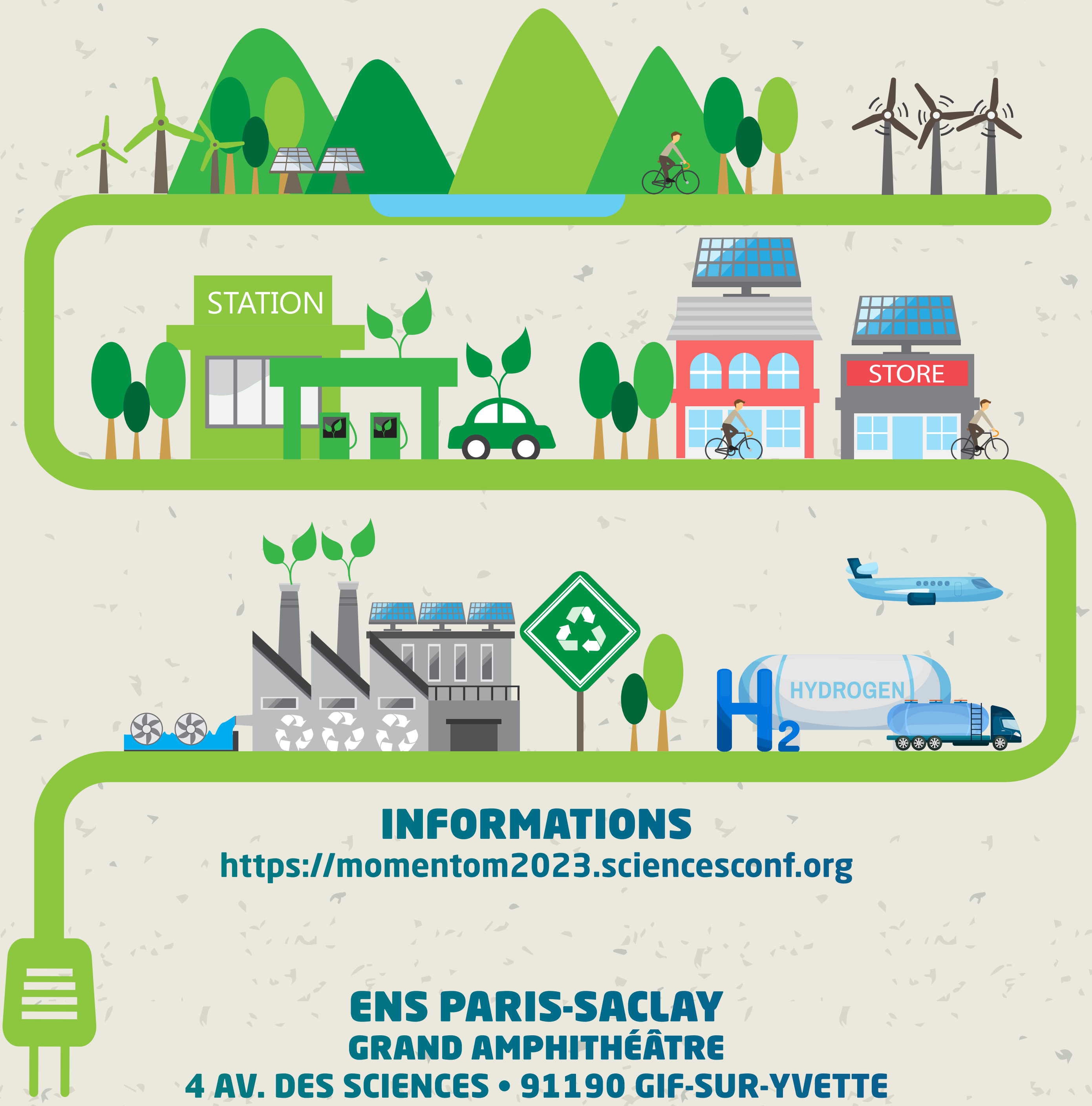
8-10 MARCH 2023

3rd MOMENTOM INTERNATIONAL CONGRESS

ENERGY AT THE CROSSROADS:

Accelerating innovation in the age of disruption



INFORMATIONS

https://momentom2023.sciencesconf.org

ENS PARIS-SACLAY

GRAND AMPHITHÉÂTRE

4 AV. DES SCIENCES • 91190 GIF-SUR-YVETTE

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université PARIS-SACLAY
INSTITUT DE L'ÉNERGIE SOUTENABLE université PARIS-SACLAY
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Maison des Sciences de l'Homme PARIS-SACLAY
ENSTA IP PARIS

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Patrick Schembri,
UVSQ, Université Paris-Saclay

Virginie Tallio,
Université Paris-Saclay, IES

FOREWORD

Dear attendees,

On behalf of the Organization committee of the 3rd MOMENTOM International Congress: Energy at the crossroads, we are glad to welcome you on the campus of the University Paris-Saclay. This congress has been organized on the initiative of the Institute for Sustainable Energy of the University Paris-Saclay. The Institute for Sustainable Energy (IES) is an interdisciplinary program of the University of Paris-Saclay. It brings together research teams from more than 41 laboratories representing about 450 researchers and lecturers.

The aim of this Congress is to share knowledge and the most recent scientific advances, from fundamental to applied research, towards the energy transition. In addition, Human and Social Sciences, in relationship with the society apprehension in our changing world, will be one of the topics of this congress.

Our thanks go to worldwide renowned scientists who accepted to participate to this congress as well as all the contributors and attendees.

We are thankful to the constant support of the University Paris-Saclay and MSH Paris-Saclay, and particularly indebted to the sponsors of this Congress.

We wish you all fruitful scientific discussions to tackle the challenges of the Energy of tomorrow.

Loïc Assaud, Hynd Remita, Guilhem Dezanneau, Emmanuelle Deleporte, Patrick Schembri, Magali Gauthier, Marc Petit, Virginie Tallio

Steering committee of the Institute for Sustainable Energy

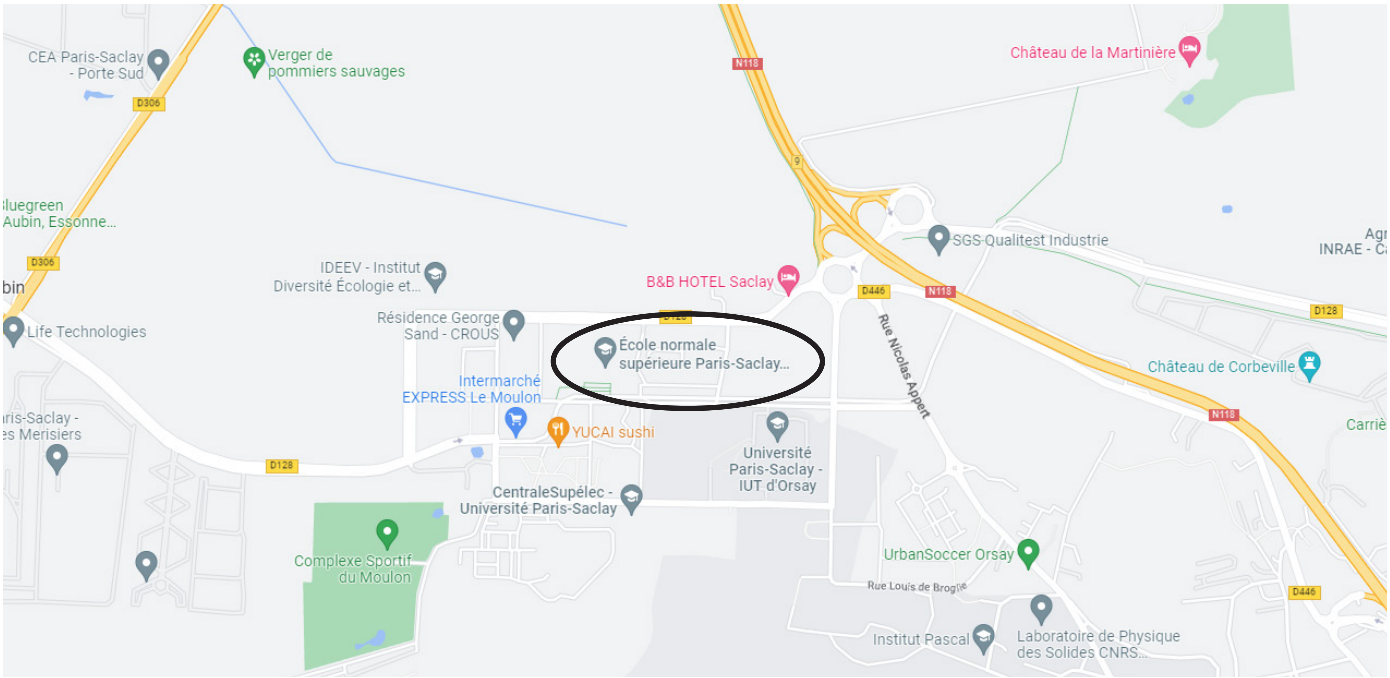
PRACTICAL INFORMATION

The Congress will take place at the ENS Paris-Saclay.

The Congress will be held in the rooms Room 1B26, Room 1B36, and Grand Amphithéâtre.

The coffee breaks, lunches and the cocktail on the 8th of March will be held at Emmy Noether Hall.
The different congress rooms will be clearly indicated.

Address: ENS Paris-Saclay, 4, avenue des Sciences, 91400 ORSAY, France.



To reach ENS:

BY TRAIN:

- International and national trains: Railway station MASSY TGV, then take the bus 91.06 (Christ de Saclay) or 91.06 (St Quentin en Yvelines). Bus stop: Moulon
- Regional trains (RER): RER B Le Guichet station, then take bus 9 (Christ de Saclay/Gare de Jouy en Josas/ Campus HEC). Bus stop: Moulon or Bus 9106 (Gare de Massy Palaiseau), Bus stop: Université Paris Saclay

RER B or RER C Massy-Palaiseau station, then take one of the following buses : 91.06 (Christ de Saclay) or 91.10 (St Quentin en Yvelines) Bus stop: Moulon or 91.06 (Gare du Guichet), Bus stop: Université Paris-Saclay.

BY BUSES: lines 91.06 (Christ de Saclay/Gare de Massy Palaiseau), 91.10 (St Quentin en Yvelines-Orly), 9 (Christ de Saclay/Gare de Jouy en Josas/Campus HEC). Bus stop: Moulon
Line 7 (Plateau de Moulon-Corbeville). Bus stop : Université Paris-Saclay
Line 11 (Parc Orsay Université-Gare de Gif-sur-Yvette). Bus stop: Centralesupélec

BY CAR: Through N118
You can park at the «Digiteo» parking. The access (there is a road sign) is via Raimond Castaing street.

BY AIRPLANE: There are two airports in Paris: Roissy-Charles de Gaulle and Orly.
From Roissy-Charles de Gaulle, take the RER B (St Rémy les Chevreuse) to Massy-Palaiseau or Le Guichet.
From Orly, take Orlyval to Antony and then take the RER B (St Rémy les Chevreuse) to Massy-Palaiseau or Le Guichet.

BY CAR-POOLING: There are several applications proposing car-pooling. The most known is Blablacar.

SUSTAINABILITY ENGAGEMENTS OF THE IES

The engagements towards sustainability are of very high interest at the Université Paris-Saclay. They are detailed in the Charte Développement Soutenable[1], endorsed on the 6th of July 2021.

The mission of the Institute for Sustainable Energy (IES) is to connect academics working on sustainable ways to produce, store, convert, distribute and use energy, and to support industrials, start-ups, and territorial stakeholders towards the energy transition. In that regard, it is strongly committed to support the sustainability engagements of the Université Paris-Saclay.

GOODIES

It has been decided to considerably diminish the number of goodies given at the congress, and the communication supports. You will find at the end of this leaflet a few pages to take notes. There will be only a few abstract books available at the counter. You can otherwise download the abstract book on the congress website.

CARBON FOOTPRINT

As a matter of fact, travel is the most environmentally costly when organizing a conference, especially when participants are travelling by plane. Nevertheless, the IES acknowledges that some trips can only be done by airplane.

Several carbon mitigation programs exist. Please consider to mitigate your carbon footprint by giving to one of these programs. The IES is aware of the multiple flaws of carbon mitigation[2] but it is considered as well that, when airplane travel is the only solution, mitigating the carbon footprint by giving to such programs is acceptable.

This program has been chosen on the basis that its positive carbon mitigation impact is not done at the expense of other environmental and/or social impacts.
https://CO2solidaire.org/

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[1] https://cirrus.universite-paris-saclay.fr/s/r7L3RdRsiB7z4QB

[2] https://www.cirad.fr/les-actualites-du-cirad/actualites/2021/compensation-et-neutralite-carbone

PROGRAM: DAY 1

Emmy Noether Hall	
8:30 - 9:30	Welcome coffee
Grand Amphithéâtre	Chairwoman / Chairman: Hynd Remita / Loïc Assaud
9:30 - 10:00	Introductive words: UPSaclay, IES, MSH
10:00 - 10:45	**PLENARY #1:** Hydrogen from Water electrolysis for a Changing World: Elena BARANOVA
10:45 - 11:15	**KEYNOTE #1:** Reinforcement learning for electrical markets and the energy transition: Damien ERNST
11:15 - 11:35	**ORAL #1:** Chalco-POM based catalysts: from fundamentals to hydrogen evolution real-life application: Emmanuel CADOT
11:35 - 11:55	**ORAL #2:** Status and perspectives of photovoltaics: Jean-Paul KLEIDER
11:55 - 12:10	Short presentations: booths
Emmy Noether Hall	
12:10 - 14:00	Lunch
Grand Amphithéâtre	Chairwoman: Magali Gauthier
14:00 - 14:45	**PLENARY #2:** Sodium-ion Batteries: challenges and opportunities for an alternative sustainable energy storage technology: Ivana HASA
14:45 - 15:15	**KEYNOTE #2:** Geologic hydrogen: sources, fluxes and relationships with deep microbial activity and abiotic organic synthesis: Bénédicte MENEZ
15:15 - 15:45	**KEYNOTE #3:** Synchrotron Radiation at the Crossroads of the Sustainable Energy Science from Today to Tomorrow: Valérie BRIOIS
Emmy Noether Hall	
15:45 - 16:15	Coffee Break

3 PARALLEL SESSIONS:

Grand Amphithéâtre	**SESSION 1: ENERGY PRODUCTION - PHOTOVOLTAICS** Chairman: Emmanuel Cadot
16:15 - 16:30	**ORAL #3:** Routes for low cost III-V solar cells: Lise WATRIN
16:30 - 16:45	**ORAL #4:** Solid-state monolithic dye-sensitized solar cell exceeding 10 % of power conversion efficiency using a copper-complex HTM and a carbon counter-electrode : Fatima SANTOS
16:45 - 17:00	**ORAL #5:** High bandgap triple mesoscopic perovskite solar cell: Sookyung KANG
17:00 - 17:15	**ORAL #6:** Study of the formation of 2D/3D perovskite heterostructures for solar cells: Thomas CAMPOS
17:15 - 17:30	**ORAL #7:** Promising Ultra-wide Bandgap Spinel ZnGa2O4 for Energy Storage and Conversion: Zeyu CHI
Room 1B26	**SESSION 2: ENERGY STORAGE - BATTERIES / SUPERCAPS** Chairman: Fabien Miomandre
16:15 - 16:30	**ORAL #8:** Deep eutectic solvents as sustainable electrolytes for supercapacitors: Xavier MASCARENHAS
16:30 - 16:45	**ORAL #9:** Functionalizing graphene with tetrazine derivatives to desing new materials for supercaps: Margarita BOSMI
16:45 - 17:00	**ORAL #10:** A multiscale study of the electronic and ionic transport processes influencing the performance of Lithium-ion batteries: Julius AKINRIBIDO
17:00 - 17:15	**ORAL #11:** A study of sulfide-based solid electrolytes (SSEs) sensitivity towards humidity: gas evolution quantification and degradation mechanisms investigation: Ivan LETEYI MFIBAN
17:15 - 17:30	**ORAL #12:** Fundamental understanding of concentrated aqueous electrolytes for batteries: Malaurie PAILLOT
17:30 - 17:45	**ORAL #13:** Multi-scale study of lithium diffusion in garnet-type solid electrolyte: Neutron powder diffraction and NMR spectroscopy analysis: Said YAGOUBI
Room 1B36	**SESSION 3: ENERGY AND SOCIETY** Chairman: Pierre Guibentif / Patrick Schembri
16:15 - 16:30	**ORAL #14:** Alternative scenario for the energy transition: Jean-Marc SALOTTI
16:30 - 16:45	**ORAL #15:** Local narratives and energyscapes. Energy transition seen from the margins of a coal region: Elena APOSTOLI CAPPELLO
16:45 - 17:00	**ORAL #16:** Measuring the ecological impacts of digital organisations: Organisational learning and indirect effects: Cedric GOSSART
17:00 - 17:15	**ORAL #17:** Testing the impacts of disaggregated renewable energy sources on economic growth: evidence of spatial spillover effects for developing countries: Katia RADJA
17:15 - 17:30	**ORAL #18:** The impacts of combining incentives on carpooling for commuting in Paris Metropilitan area: Fawaz SALIHOU
Emmy Noether Hall	
17:45 - 19:45	Poster session #1 + Cocktail

PROGRAM: DAY 2

3 PARALLEL SESSIONS:

Grand Amphithéâtre

SESSION 1: ENERGY NETWORKS Chairman: Marc Petit

9:00 - 9:15 **ORAL #19:** Evaluation of industrial hubs designs to enable the infrastructure for a hydrogen market: Gabriela NASCIMENTO DA SILVA

9:15 - 9:30 **ORAL #20:** From energy technology complexity to socio-technical approach: the bioenergy example: Clément LASSELIN

9:30 - 9:45 **ORAL #21:** Use of reversible pump-turbines (RPT) as an alternative to expand «submotorized» hydropower plants (HPP) in Brazilian Electric System - Case Study of Foz do Areia: Murilo CARDOSO DE MIRANDA

9:45 - 10:00 **ORAL #22:** Scalability of an Integrated-PEC for high efficiency Hydrogen production: Angela R. A. Maragno

Room 1B26

SESSION 2: ENERGY CONVERSION - HYDROGEN Chairman: Johnny Deschamps

9:00 - 9:15 **ORAL #23:** Bandgap tuning of Graphdiyne to promote photogenerated charge separation and Photocatalytic Hydrogen Production: Mohamed Nawfal GHAZZAL

9:15 - 9:30 **ORAL #24:** Highly Porous Iridium Oxides Electrocatalysts for Proton Exchange Membrane Water Electrolyzers: Jennifer PERON

9:30 - 9:45 **ORAL #25:** Ruthenium nanocatalysts for electrocatalytic hydrogen evolution reaction: Karine PHILIPPOT

9:45 - 10:00 **ORAL #26:** Challenge and prospects for the development of hydrogen and renewable Gases in France: Clothilde MARIUSSE

Room 1B36

SESSION 3: ENERGY AND CO_2 CONVERSION Chairwoman: Anne Dolbecq

9:00 - 9:15 **ORAL #27:** Density Functional Studies on Photocatalytic Methane Coupling over Au/TiO_2: Dorota RUTKOWSKA-ZBIK

9:15 - 9:30 **ORAL #28:** Selective electrochemical reduction of CO to n-propanol and ethanol by nitride-derived bimetallic catalysts: Hong Phong DUONG

9:30 - 9:45 **ORAL #29:** Shaping the Electrocatalytic Performance of Metal Complexes for CO_2 Reduction: Philipp GOTICO

9:45 - 10:00 **ORAL #30:** Forming multiple C-C bonds upon electrocatalytic reduction of CO_2 by molecular transition metal macrocycles: Si Thanh DONG

Emmy Noether Hall

10:15 - 10:45 **Coffee Break**

Grand Amphithéâtre Chairwoman: Yara Hodroj

10:45 - 11:30 **PLENARY #3:** The challenges of rare earths in the energy transition: Stéphane GOUTTE

11:30 - 12:00 **KEYNOTE #4:** Offshore energy hubs: Nicolaos A. CUTULULIS

12:00 - 12:05 **DIM MaTerRE:** Anne DOLBECQ

Emmy Noether Hall

12:05 - 14:00 **Lunch**

INNOVATION SESSION

Grand Amphithéâtre Chairman / Chairwoman: Stanilas Pommeret / Elsa Couderc

14:00 - 14:30 **PLENARY #4:** Vertically Aligned Carbone Nanotubes – a new material for energy, from the lab to mass production: Pascal BOULANGER

14:30 - 15:30 Airthium, an engine to decarbonize the planet: Andrea KLOCHKO

Innovation across organizational and disciplinary boundaries at Lemon Energy: enhancing industrial energy performance based on data: Ana ROCHA

Low-electricity Hydrogen Production with Methane Pyrolysis Catalyzed by NanoPulsed Plasma: Erwan PANNIER

SoY PV: the photovoltaic innovation in action: Daniel LINCOT / Jean-Michel LOURTIOZ

H_2YAM: Combustion engines, the only viable and scalable means of decarbonizing maritime mobility immediately: Alexandre MARC

15:30 - 16:30 Round Table : **Energy at the crossroads**

Emmy Noether Hall

16:30 - 18:00 **Poster session #2**

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20:00 - 23:00 **GALA DINNER IN PARIS**
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PROGRAM: DAY 3 AM

Grand Amphithéâtre Chairwoman: Emmanuelle Deleporte

9:30 - 10:15 **PLENARY #5:** Perovskite Photovoltaics for Electricity and Fuel Generation from Sunlight: Michael GRÄTZEL

10:15 - 10:45 **KEYNOTE #5:** Cybersecurity in the Energy sector: Challenges, Perspectives and Policy Approaches: Arnault BARICHELLA

Emmy Noether Hall

10:45 - 11:15 Coffee Break

3 PARALLEL SESSIONS:

Grand Amphithéâtre **SESSION 1: BIO-INSPIRED ENERGY PRODUCTION** Chairman: Philipp Gotico

11:15 - 11:30 **ORAL #31:** Microbial electrochemical technologies for taking advantage of the energy and carbon content of organic waste to fuel the bioeconomy sector: Théodore BOUCHEZ

11:30 - 11:45 **ORAL #32:** Microalgae for CO_2 capture: Catherine EVEN

11:45 - 12:00 **ORAL #33:** Development of the Biofuel industry in Europe: interactions with the oil industry and the agricultural supply through a modeling approach: Frederic LANTZ

12:00 - 12:15 **ORAL #34:** Bio-Inspired Bimetallic Cooperativity Through a Hydrogen Bonding Spacer in CO_2 Reduction: Chanjuan ZHANG

Room 1B26 **SESSION 2: ENERGY PRODUCTION - ELECTROCATALYSIS / PHOTOELECTROCATALYSIS** Chairwoman: Dorota Rutkowska-Zbik

11:15 - 11:30 **ORAL #35:** Solar to chemical energy conversion - what is the potential of photocatalysis?: Wojciech MACYK

11:30 - 11:45 **ORAL #36:** Sulfur-doped carbon nitride hybrid materials tested under green light for photoelectrocatalytic benzylamine oxidation and oxygen evolution reactions: Pablo JIMENEZ-CALVO

11:45 - 12:00 **ORAL #37:** Synthesis developments and performances of non-noble metal ORR electrocatalysts by ammonia induced CO_2 laser pyrolysis of liquid droplet aerosol: Henri PEREZ

12:00 - 12:15 **ORAL #38:** Tuning the syngas composition obtained via electrochemical reduction of CO_2 by in situ potential cycling: Catia AZENHA

Room 1B36 **SESSION 3: ENERGY PRODUCTION AND STORAGE - HYDROGEN** Chairman: Guilhem Dezanneau

11:15 - 11:30 **ORAL #39:** Conducting Polymer-Based Heterojunction for Photocatalytic Hydrogen Generation: Srabanti GHOSH

11:30 - 11:45 **ORAL #40:** Corrosion of metallic bipolar plates and porous transport layers in proton exchange membrane water electrolyzer anodes: Michel PRESTAT

11:45 - 12:00 **ORAL #41:** Development of a High-Throughput Approach for the Research of Materials for Protonic Ceramic Cells: Giulio CORDARO

12:00 - 12:15 **ORAL #42:** Hydrogen storage in clay materials: Pascale LAUNOIS

Emmy Noether Hall

12:30 - 14:00 Lunch

PROGRAM: DAY 3 PM

Grand Amphithéâtre Chairwoman: Hynd Remita

14:00 - 14:45 **PLENARY #6:** Structure-Reactivity Relationship for Pt-Rare Earth Nanoalloy Electrocatalysts for Fuel Cell Cathodes: Sara CAVALIERE

14:45 - 15:15 **AWARDS CEREMONY & ACKNOWLEDGEMENTS** Chairman: Ally Aukauloo

3 PARALLEL SESSIONS:

Grand Amphithéâtre

SESSION 1: ENERGY PRODUCTION - SOLAR FUELS

Chairman: Macyk Wojciech

15:15 - 15:30 **ORAL #43:** Analysis of Low Temperature Combustion (LTC) process in internal combustion engines: Fadila MAROTEAUX

15:30 - 15:45 **ORAL #44:** Bifunctional earth-abundant catalysts for solar to hydrogen fuel production: Maria MENDEZ

15:45 - 16:00 **ORAL #45:** Unveiling the Mechanism of the Photocatalytic Reduction of CO_2 to Formate Promoted by Porphyrinic Zr-Based Metal-Organic Frameworks: Amanda Lyn ROBINSON

16:00 - 16:15 **ORAL #46:** Synthesis of p-Silicon/Agx Cu100-x Photocathodes applied to light-assisted CO_2 reduction: Encarnacion TORRALBA

Room 1B26

SESSION 2: ENERGY HARVESTING - MICRODEVICES

Chairman: Remith Pongilat

15:15 - 15:30 **ORAL #47:** Diamond semiconductor: its challenging n-type doping: Marie-Amandine PINAULT-THAURY

15:30 - 15:45 **ORAL #48:** Influence of GaN NW diameter on their piezo-conversion properties: Effect of the surface charges: Quang-Chieu BUI

15:45 - 16:00 **ORAL #49:** Micro-device optimization for energy harvesting applications: Ann-Lenaig HAMON

16:00 - 16:15 **ORAL #50:** Unlocking the photophysics of mesoporous graphitic-carbon nitride (mpg-CN): Jokotadeola ODUTOLA

Room 1B36

SESSION 3: ENERGY PRODUCTION AND STORAGE - HYDROGEN

Chairwoman: Natalia Zugravu

15:15 - 15:30 **ORAL #51:** On Robust Optimization, Blackouts and the Law: Dirk LAUINGER

15:30 - 15:45 **ORAL #52:** Predator-Prey model of a technological renewable-based energy transition: Diana MONROY

15:45 - 16:00 **ORAL #53:** A meta-analysis of the concept of “green jobs”: the search for sustainable development paths in developing countries: Alexandre MATHIEU

16:00 - 16:15 **ORAL #54:** Damping analysis of Floating Offshore Wind Turbine (FOWT): a new control strategy reducing the platform vibrations: Matteo CAPALDO

POSTER SESSION: DAY 1

P#1	Perazio Alessandro	Acidic Electroreduction of CO_2 to Multi-Carbon Products with Continuous CO_2 Recovery from Carbonate
P#2	Plantevin Olivier	Strain and Optoelectronic tuning in Mixed Halide Perovskites with Ion Irradiation
P#3	El Khoueiry Maria	Characterization of molecular catalysts by Atomic Force Microscopy combined to Scanning Electrochemical Microscopy for the Hydrogen Evolution Reaction
P#4	Naciri Yassine	Compositional, Structural, and Surface Characterization of Titanium doped Imogolite Clay Nanotubes: Implications for Photocatalytic Hydrogen Production
P#5	Segura Yutzil	Copper-based nanoparticles for CO_2 electroreduction
P#6	Zafar Sharyal	Decentralized Control of EVs in Smart Grid using Multi-Agent Multi-Armed Bandits
P#7	Dias Fernandes Marie-Sophie	Direct Synthesis and Electrochemical Characterization of Nasicon-Type Li2NaV2(PO4)3 Cathode
P#8	Mary Caroline	Doping influence on g-C3N4 based heterojunction for hydrogen production by water splitting under solar irradiation
P#9	Meziani Narimane	Effect of hydration on the properties of a superionic conductor M2Ti2O5.$(H_2O)x$
P#10	Stephan Emma	Electrical behavior and stability under real outdoor working conditions of triple-mesoscopic perovskite solar cells.
P#11	El Semaan Elio	State estimation of low voltage networks using machine learning techniques
P#12	Ihlal Ahmed	Experimental investigations on atmospheric water harvesting using composite desiccant-based solar collector
P#13	Bach Alexandre	Fault location on MV distribution grids with distributed measurements
P#14	Ullah Wahid	Graphdiyne quantum dots: new metal free co-catalyst for efficient photocatalytic hydrogen generation
P#15	Attia Mahmoud	Investigations of diffusion and NMR properties in LLAZO through a multiscale simulations approach linked to experimental data
P#16	Rocha Ana	Innovation across organizational and disciplinary boundaries at Lemon Energy: enhancing industrial energy performance based on data analysis
P#17	Smith Adrien	Metalloporphyrins bearing imidazolium groups for CO_2 reduction
P#18	Xi Qingyang	Molecular engineering of hole transporting molecules for high efficient and enhanced thermal stability perovskite solar cell
P#19	Lopez Girlie Eunice	Photocatalytic Oxygen Reduction to Hydrogen Peroxide from Oxygen and Water by Metal- free Nano-Polypyrrole
P#20	Rashid Haroon	Polymeric porphyrin-based material for the activation and reduction of CO_2
P#21	Khan Alisha	Porous Composite Nanomaterials Based On MOFs For Green Hydrogen Production
P#22	Emile Emery	Power Grid Structure for the Energy Transition
P#23	Mendez Medrano Ana Andrea	Enhancement of Photocatalytic Hydrogen Generation on TiO_2 by AuPd nanoalloys
P#24	Nakamae Sawako	Thermogalvanic Energy Conversion Improvement in Ionic Liquids Redox Solvation and Coordination Chemistry
P#25	Harvey Catherine	Towards the Electrolysis of Seawater by Iridium and Iridium Mixed Based Oxide Nanoclusters for the Generation of the Hydrogen Energy Carrier
P#26	Scola Joseph	Interfacial properties of a ZnO-polymer nanocomposite for PENG applications
P#27	Stanescu Dana	Intrinsic photoanode band engineering: surface segregation mediated enhanced solar water splitting efficiency in Ti-doped hematite nanorods
P#28	Julius Akinribido	A multiscale study of the electronic and ionic transport processes influencing the performance of Lithium-ion batteries

POSTER SESSION: DAY 2

P#29	**Watrin Lise**	Routes for low cost III-V solar cells
P#30	**Matmati Hanah**	3 generation of green gas: from the circular economy of the territory to the resilience of gas networks
P#31	**Quach Vien-Duong**	Artificial strong metal-support interaction on plasmonic core-shell nanostructures for photo(electro)catalytic reaction
P#32	**Votat Sébastien**	Bioremoval of dyes in a microbial fuel cell by the fungus Trichoderma harzanium : a sustainable approach in energy production
P#33	**Chevillard Amaury**	GaN nanowire-based piezoelectric devices for energy harvesting: Impact of the NW/polymer matrix composite
P#34	**Wang Xingze**	Heterometallic (MIV/MII) MOFs as a versatile platform for the photocatalytic overall water splitting reaction
P#35	**Pinault-Thaury Marie-Amandine**	Ionic analysis of phosphorus doped-diamond homoepilayers grown with different carbon isotopic abundances
P#36	**Pinault-Thaury Marie-Amandine**	Locally Ion Implantation and Annealing Effects in Diamond
P#37	**Bui Thanh-Tuan**	Molecular engineering of hole transporting molecules for high efficient and enhanced thermal stability perovskite solar cell
P#38	**Haake Matthieu**	Selective Aqueous Electrocatalytic CO_2-to-CO Reduction with a Cobalt-based Molecular Cathode
P#39	**Wang Cong**	Structure-Engineered TiO_2: Harvesting Light for Photocatalytic H_2 Production
P#40	**Le Pivert Marie**	ZnO nanostructures based photocatalytic civil engineering materials development for urban pollution remediation
P#41	**Delachaux Valentin**	Why are photovoltaic/thermal solar collectors (PVT) yet on the way to be a key technology of buildings energy transition, especially for DHW preparation?
P#42	**Benyahia Raihana**	Nickel based anodes for the electro-oxidation of urea and synthetic urine in alkaline media
P#43	**El Sied Moataz**	The way to 100% MW scale renewable power systems: future challenges and promising solutions
P#44	**Xie Peigen**	Smart building simulation and control
P#45	**Dubouis Nicolas**	How R&D Can Help us Transform into a Clean H_2 Economy
P#46	**Chatelet Corentin**	Vertically aligned carbon nanotubes on aluminum foils: one-step synthesis from bio-sourced precursors and electrochemical characterization
P#47	**Ferreira Lauro**	Operation of Power Diodes at Cryogenic Temperature
P#48	**Duong Viet Dung**	Semiconducting conjugated oligomers for photo-driven water oxidation
P#49	**Kumar Ashutosh**	Thermoelectric Properties of high-entropy rare-earth cobaltates
P#50	**Matmati Hanah**	3rd gas revolution: challenges and prospects for the development of renewable gases
P#51	**Pugliese Eva**	Photo-induced Fe(III)-hydroperoxo generation for oxygen atom transfer reaction
P#52	**Yuan Xiaojiao**	Molecular imprinted butterfly-shaped micromotors for selective target recognition
P#53	**Lhostis Florian**	High-rate CO_2 reduction to formic acid using bismuth-based electrocatalysts
P#54	**Bathia Ankush**	New insights on the charge storage mechanism of thin films electrode materials by Raman spectroscopy

ABSTRACTS OF THE PLENARY AND KEYNOTE SESSIONS

PLENARY SESSIONS

ELENA BARANOVA

Hydrogen from Water electrolysis for a Changing World

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To accelerate the transition to the low carbon future based on renewable energy, e.g., solar and wind energy, more effort is required to ensure flexible storage and usage options of this intermittent energy. Converting and storing the excess renewable electrical energy into chemicals is an essential constituent in this challenge. Hydrogen is a unique chemical and fuel that can play a key role in the transition to low-carbon technologies. One promising path for green hydrogen production is water electrolysis. Hydrogen generation by water electrolysis can potentially satisfy renewable energy storage and transportation with high efficiency and low cost. Two primary commercially available technologies for water electrolysis are liquid alkaline systems, which have a long history in large-scale installations using Nickel-based electrodes and Proton Exchange Membrane (PEM) water electrolyzers that have a compact design, operate at high current densities but employ expensive Platinum Group Metal (PGM) catalysts. These two technologies have several benefits but also technical challenges and require considerable total cost reduction for large-scale hydrogen generation.

An emerging technology for hydrogen production is an alkaline membrane water electrolysis (AMWE) promises to use an anion exchange membrane (AEM) to combine the benefits of alkaline and PEM electrolyzers to produce hydrogen at high current densities, high efficiency using low-cost, non-PGM catalysts.

Nanostructured Ni-based catalysts are promising non-noble metal catalysts for both anodic (oxygen evolution reaction, OER) and cathodic (hydrogen evolution reaction, HER) reactions in AEM water electrolyzers due to their high activity, stability in alkaline media and low cost. In an AEMWE, Ni nanoparticles form a catalytic layer bound together using an anion exchange ionomer (AEI), providing hydroxide ion transport throughout the layer. AEMWE technologies show promising performance using non-PGM catalysts for both OER and HER. This talk will discuss the opportunities for green hydrogen generation in AEM water electrolysis and the technical challenges related to electrode materials, membrane, ionomer, and gas-diffusion layer (GDL) that need to be solved to design commercial systems for hydrogen production at a lower cost using renewable energy.

BIOGRAPHY

Elena Baranova is a Full Professor in the Department of Chemical and Biological Engineering and a Director of Nexus for Quantum Technologies (NexQT) Institute at the University of Ottawa, Canada. She received her Ph.D. from École Polytechnique Fédérale de Lausanne (EPFL) in 2005. She was an NSERC post-doctoral fellow with the National Research Council (NRC), Canada (2005-2007) before joining University of Ottawa in 2008 as a tenure-track Assistant Professor. Her field of research is Electrochemical Engineering, Energy and Catalysis. Dr. Baranova has authored over 130 publications, three book chapters and holds one US patent. She is an Executive Editor of the Journal of Chemical Technology and Biotechnology, JCTB (SCI, Wiley) and a Member of the Editorial Board of the Journal of Solid State Electrochemistry (Springer Nature).

PLENARY SESSIONS

IVANA HASA

Sodium-ion Batteries: challenges and opportunities for an alternative sustainable energy storage technology.

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The increasingly growing demand of lithium-ion batteries (LIBs) for electromotive and stationary storage application, has been raising concerns about the future and long-term availability and cost of the critical raw material employed in LIB production, such as cobalt, nickel, lithium, graphite and copper [1]. In this scenario, sodium-ion batteries (SIBs) have the potential to become the next green, low cost, environmentally friendly electrochemical storage system. Indeed, owing to their potential lower cost and higher sustainability compared to the current lithium-based technology, SIBs have the potential to dominate the future stationary energy storage market filling the gap between clean energy production and utilization, and the electrified transport sector [2].

Due to the similarity in and the operating principles, a transfer of knowledge from LIBs to SIBs has allowed a rapid progression of the latter. Indeed, SIBs have already demonstrated great potential with several companies working toward their commercialisation [3]. However, to meet the requirements for practical application, development and optimization of novel electrode materials and electrolytes is required.

This presentation gives an overview on the journey toward the development of SIBs linking chemistry and electrochemistry of the employed materials with key performance indicators of cells approaching commercialization. Challenges on the transition from lab to scaled-up processes and the development of industrially relevant cell prototype are also presented.

BIOGRAPHY

Ivana Hasa is Assistant Professor of Electrochemical Materials in WMG at the University of Warwick. She is a chemist by background and for the past ten years her research activities have been focused on the development and characterization of battery materials and their implementation in cell prototypes. She completed her PhD in 2015 on the design and characterization of sodium-ion battery materials at Sapienza University of Rome (Italy). She has gained broad experience in electrochemical energy storage systems during her postdoctoral appointments at the Lawrence Berkeley National Laboratory (California, USA) and at the Helmholtz Institute Ulm (Germany).
Her research activities in WMG are directed towards the understanding of the processes governing sodium-ion batteries. At the Energy Innovation Centre, she is working toward the development and scale up of new battery chemistries from concept to full proven cell prototypes.

References

[1] The Faraday Institution, Faraday Insights - Lithium, Cobalt and Nickel: The Gold Rush of the 21st Century, (2020) 1–6.

[2] I. Hasa, S. Mariyappan, D. Saurel, P. Adelhelm, A.Y. Koposov, C. Masquelier, L. Croguennec, M. Casas-Cabanas, Challenges of today for Na-based batteries of the future: From materials to cell metrics, J. Power Sources. 482 (2021) 228872.

[3] A. Bauer, J. Song, S. Vail, W. Pan, J. Barker, Y. Lu, The Scale-up and Commercialization of Nonaqueous Na-Ion Battery Technologies, Adv. Energy Mater. 8 (2018) 1–13.

PLENARY SESSIONS

STÉPHANE GOUTTE

The challenges of rare earths in the energy transition

Stéphane GOUTTE
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Under the Paris Agreement scenario, keeping the world below a 2°C rise in temperature relative to pre-industrial levels will require the decarbonisation of the energy system at an unprecedented scale. This accelerated transition to mitigate climate change will need a growing supply of critical raw materials, such as rare earth elements (REEs). Rare earths are a group of 17 chemicals, that possess unique properties of value in catalysts, optical materials, magnets, batteries, and lighting applications, amongst others. Regarding the energy transition, four REEs are of interest: neodymium, praseodymium, dysprosium, and terbium. Often used in permanent magnets called neodymium-iron-boron magnets (NdFeB), these rare earths are critical elements in the manufacturing of wind turbines and hybrid/electrical vehicles. Their use benefits green technologies by increasing, efficiency, power density and reducing weight.

However, a balance problem is rising in the REEs market. Demand is growing, driven by developed economies eager to achieve their energetic transition plans, but also by other expanding sectors such as ICT or defence. Supply is geospatially concentrated, the majority of REE mining and purification, as well as most permanent magnet production, are concentrated in China. Even if REEs mining projects are booming worldwide, most processing unities facilities remain in China, and the development of new ones is at issue due to environmental concerns and the long-time frames for their development. In other words, western economies aim to diversify their REEs supply chain to reduce their dependency on Chinese importations and respond to their growing demand, whereas they struggle to find sustainable mining and processing plants.

Substitute to NdFeB magnets and recycling of REEs in retired wind turbines and electric cars might offer a solution to the supply shortage. But, as of today, all forecasting studies have shown a short-term mismatch between REEs supply and clean energy ambitions.

BIOGRAPHY

Stéphane Goutte has two PhDs, one in Mathematics and one in Economics. He is full professor at Université Paris-Saclay, UVSQ, France. He is adjunct professor at University of Calgary, Canada. He received his Habilitation for Supervising Scientific Research (HDR) in 2017 at University Paris Dauphine. He is a Senior Editor of Energy Policy (JEPO), a Senior Editor of Finance Research Letters (FLR); an Associate Editor of International Review of Financial Analysis (IRFA) and Research in International Business and Finance (RIBAF); a Subject Editor of Journal of International Financial Markets, Institutions and Money (JIFMIM). His interests lie in the area of mathematical finance and econometric applied in energy or commodities. He has published more than 70 research papers in international academic review. He has also been a Guest Editor of various special issues of international peer-reviewed journals and Editor of many handbooks. He is expert of the High Council for Evaluation of Research and Higher Education (Hcéres) and member of the Graduate School of Economy and Management of University Paris-Saclay.

PLENARY SESSIONS

PASCAL BOULANGER

Vertically Aligned Carbone Nanotubes a new material for energy, from the lab to mass production

Dr. Pascal BOULANGER, Dr. Thomas GOISLARD1

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Energy transition is the challenge of the century. It will require great innovations and new materials to face minerals scarcity and CO_2 intensive mining production processes. In this context, nanotechnologies have already played a major role in opening new doors with less material needed and more efficient products and processes. Amongst new nanomaterials, nanocarbons have been at the center of many discoveries with fullerenes, nanotubes and more recently graphene. In particular, Vertically Aligned Carbon NanoTubes (VACNT) have demonstrated outstanding potentialities as novel material to elaborate multifunctional materials for a wide range of applications such as membranes, composites but also for energy conversion and storage.

Through NAWATechnologies's story, a breakthrough born here in Saclay, its founder will describe the various steps that lead the company to be the world leader in VACNT production and what challenges the company is still facing :the first steps to demonstrate the proof of concept, the intermediate step to validate the manufacturing process up to the coming production and commercialization. As a pioneer in Deeptech, NAWA had to face challenges that nobody addressed before and for which scientific knowledge is the key.

Basics of the use of VACNT as a component of nano-3D “Ultra-Fast Carbon Electrode” for next generation of supercapacitors and lithium batteries as well as a reinforced material for fibers enhanced composite materials will be highlighted by our recent results.

We will present our vision on how this new generation of material can lead to better applications in the field of energy and transportation, cheaper, safer, more reliable, with the added advantage of being more environmentally friendly.

BIOGRAPHY

Mathematician/physicist by training, Pascal is graduated from ENSEA and Ecole Superieure d’Electricité. He defended his PhD in applied mathematics for signal processing 1986 and worked for 25 years as a researcher at the French Atomic Energy Commission (CEA) in various sectors, nuclear energy but also very early on in solar energy and renewable energies, contributing to the development programs of the European Commission. He travels the world to evaluate photovoltaic projects as an expert and then worked for 4 years at the Banque Publique d’Investissement (now BPI France) to finance innovation in small and medium-sized companies. Back at the CEA in 2005, he held management positions at IRAMIS -Institut Rayonnement Matiere de Saclay) at CEA for 5 years in the nanoscience field, But he quickly decided to «go back to the lab» on a business creation project that has given birth to NAWATechnologies in 2013.

Pascal is founder of NAWATechnologies and technical director.

ABSTRACTS OF THE PLENARY AND KEYNOTE SESSIONS

PLENARY SESSIONS

MICHAEL GRAETZEL

Perovskite Photovoltaics for Electricity and Fuel Generation from Sunlight

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Metal halide perovskites of the general formular ABX3 where A is a monovalent cation such as caesium, methylammonium or formamidinium, B stands for divalent lead, tin or germanium and X is a halide anion, have shown great potential as light harvesters for thin film photovoltaics This new and revolutionary generation of solution-processable thin film solar cells emerged directly from dye sensitized solar cells about 10 years agi [1-4]. Amongst a large number of compositions investigated, the cubic α-phase of formamidinium lead triiodide (FAPbI3) has emerged as the most promising semiconductor for highly-efficient and stable perovskite solar cells (PSCs). Maximizing the performance of α-FAPbI3 has therefore become of vital importance for the perovskite research. Using formate ions as pseudo-halides to mitigate lattice defects and to augment film crystallinity, we attain a power conversion efficiency (PCE) of 25.6 % (certified 25.2%) with a cell architecture of n-i-p configuration. We further enhanced light capture and largely suppressed non-radiative recombination by SnO_2 quantum dots as electron transport layer and an amphiphilic ammonium passivating agent at the perovskite hole conductor interface enabling PSCs with a PCE of 25.7 % (certified 25.4 %) [5] as well as intense electroluminescence reaching external quantum efficiencies of 12.5 %. Recently we have achieved a new record for the operational stability of perovskite solar cells by maintaining over 95 % of their initial stability during 3'300 hours of continued full solar light exposure at 75° C [6]. Our findings provide a facile access to solution processable films with unprecedented opto-electronic performance. These fundamentally new concepts have been applied to solar driven generation hydrogen from water as well as converting CO_2 to CO or ethylene. Combining perovskite photovoltaics in a tandem with silicon has allowed reaching a solar to hydrogen conversion efficiency of close to 19 %. The current research status of this field will be presented.

BIOGRAPHY

Michael Graetzel is a Professor at EPFL, where he investigates systems that generate electricity and chemical fuels from sunlight. Michael graduated with a doctoral degree in natural science (Dr.rer.nat) from the Technical University of Berlin and was a postdoctoral fellow at the University of Notre Dame, USA. After a brief return to Berlin, where he obtained his Habilitation (Dr. habil) at the Free University he moved to Lausanne, where he joined the EPFL faculty as a Professor of physical chemistry. There, he started his pioneering research on colloidal semiconductor nanocrystals and their use for solar energy conversion and storage which generated several new research fronts worldwide. The large impact of his studies is documented by over 45'000 publications and over 3000 patents that appeared in the photovoltaic domain alone.

Michael is well known for his discovery of mesoscopic dye-sensitized solar cells (DSCs) named after him "Graetzel cells", which in turn engendered perovskite solar cells constituting the most exciting breakthrough in the recent history of photovoltaics. Their advent triggered a second revolution in photovoltaics. Michael played a pivotal role in the stunning rise of PSCs, making key contributions to their phenomenal increase in efficiency from < 4 % to > 25 % within the last decade and to the dramatic improvement of their operational stability enabling practical applications. Today's prevalent and most efficient PSC embodiments borrowed their design concept and choice of components from Michael's solid state version of the DSC He is one of the laureates of the 2022 Rank Prize in Optoelectronics (UK) for "pioneereing the development of new solar cell technology based on perovskite semiconductors, which promises to play a key role in the future of solar power to the benefit and well-being of mankind.»

PLENARY SESSIONS

Michael received numerous prestigious awards, including the. BBVA Foundation Frontiers of Knowledge Award in Basic Science, Marcel Benoist Prize, August Wilhelm von Hofmann Memorial Medal of the German Chemical Society, Global Energy Prize, Rusnano Prize, Zewail Prize and Medal in Molecular Science, Leonardo da Vinci Medal of the European Academy of Science, Paracelsus Prize of the Swiss Chemical Society, Ordre de mérite du canton de Vaud, Switzerland, King Faisal International Science Prize, Samson Prime Minister's Prize for Innovation in Alternative Fuels (Israel), First Leigh-Ann Conn Prize in Renewable Energy (USA) Paul Karrer Gold Medal, Switzerland, Albert Einstein World Award of Science, Swiss Electric Research Award, Wilhelm Exner Medal, Gutenberg Research Award, Galileo Galilei Award, Balzan Prize, Galvani Medal, Millennium Technology Prize, Balzan Prize, the Harvey Prize and the Calveras Award for Leapfrog Photovoltaics (NREL,USA). He received honorary doctor's degrees from 12 European and Asian Universities.

Michael is an elected member of the Swiss Academy of Technical Sciences, the German Academy of Science (Leopoldina), the Royal Society (UK), the Chinese Academy of Science. the Royal Spanish Academy of Engineering and several other learned societies. He is a honorary member of the European Academy of Science, the Société Vaudoise de Sciences Naturelles and the Israeli Chemical Society. His over 1800 publications had a major impact on the renewable energy research field. A recent bibliometric ranking by Stanford University places Michael first amongst 100'000 world-wide leading scientists across all fields of science. According to the Web of Science (2022), he is currently the most highly cited chemist in the world.

References

1. B.O'Regan and M Grätzel, A low-cost, high-efficiency solar cell based on dye-sensitized colloidal TiO$_2$ films, Nature 1991, 353 ,737-740. https://doi.org/10.1038/353737a0
35'200 citations

2. M.Grätzel et.al. Lead Iodide Perovskite Sensitized Mesoscopic Solar Cell with Efficiency Exceeding 9%, Scientific Reports 2012, 2, 591. https://doi.org/10.1038/srep00591
7'800 citations

3. M.Grätzel et.al, Sequential deposition as a route to high-performance perovskite sensitized solar cells, Nature 2013, 499, 316–319. https://doi.org/10.1038/nature12340.
9'400 citations.

4. M.Grätzel, Light and shade of perovskite solar cells, Nature Mater 2014, 13, 838–842
https://doi.org/10.1038/nmat4065
1'670 citations.

5. M.Grätzel et.al Conformal quantum dot-SnO$_2$ layers as electron transporters for efficient perovskite solar cells. Science 2022, 375, 302-306 DOI: 10.1126/science.abh1885.

6. M.Grätzel et.al. Science 2022, DOI: 10.1126/science.abh1885

ABSTRACTS OF THE PLENARY AND KEYNOTE SESSIONS

PLENARY SESSIONS

SARA CAVALIERE

Structure-Reactivity Relationship for Pt-Rare Earth Nanoalloy Electrocatalysts for Fuel Cell Cathodes

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The widespread adoption of proton exchange membrane fuel cells (PEMFCs) strongly relies on a significant enhancement of electrocatalyst mass activity for the sluggish oxygen reduction reaction (ORR) and stability in the fuel cell operating conditions. With this aim, carbon supported Pt-based nanoalloys are widely developed allowing to reduce the noble metal loading in PEMFC cathodes while keeping a high activity. Alloys of Pt with rare-earth metals (REM) have been demonstrated as one of the most promising candidates with high ORR activity and durability with respect to pure Pt and Pt-alloys with late transition metals1,2. However, Pt-REM synthesis by conventional chemical methods is challenging, since REM have very low reduction potentials and high oxygen affinity leading to the formation of oxides rather than alloys.

In recent work, we prepared a series of carbon supported Pt-REM nanomaterials with a solid-state method3, characterized them by physico-chemical techniques and evaluated them towards the ORR in acidic medium. In particular, we have undertaken a systematic investigation of the influence of the type of rare earth metal (Y, Gd, Nd), of the Pt:REM ratio4, and of the post-synthesis treatment5, on the structural, morphological and electrochemical properties of the prepared electrocatalysts. The nature of the carbon support used during the synthesis also played a crucial role driving the formation of different phases and morphologies of particles. Operando synchrotron-based wide-angle X-ray scattering and X-ray absorption spectroscopy were used to investigate structural evolution of the nanoalloys during the electrochemical experiments, providing evidence for the structural transitions and strain dynamics that govern the electrocatalytic activity towards the ORR.

In this presentation we will give an overview of the results obtained on these carbon-supported Pt-REM nanostructured electrocatalysts and of the challenges to be tackled for their application at the cathode of proton exchange membrane fuel cells.

1. Greeley, J. et al. Nat. Chem. 1, 552–6 (2009).
2. Campos-Roldán, C. A., Jones, D. J., Rozière, J. & Cavaliere, S. ChemCatChem 14, (2022).
3. Hu, Y., Jensen, J. O., Cleemann, L. N., Brandes, B. A. & Li, Q. J. Am. Chem. Soc. 142, 953–961 (2020).
4. Campos-Roldán, C. A. et al. ACS Catal. 11, 13519–13529 (2021).
5. Campos-Roldán, C. A. et al. Nanoscale Adv. 4, 26–29 (2022).

The research leading to these results has received funding from the IMMORTAL project, which receives funding from the Fuel Cells and Hydrogen 2 Joint Undertaking (now Clean Hydrogen Partnership) under Grant Agreement No. 101006641. This Joint Undertaking receives support from the European Union’s Horizon 2020 research and innovation programme, Hydrogen Europe and Hydrogen Europe Research.

BIOGRAPHY

Sara Cavaliere is Professor at the University of Montpellier, Charles Gerhardt Institute for Molecular Chemistry and Materials. She received her PhD in Chemistry and Materials Science in 2006 in Versailles, France.

Her work aims at developing advanced nanostructured materials to enhance performance and durability of electrochemical energy conversion and storage devices, including fuel cells and electrolysers. Current research directions include the development of new electrolyte and electrode materials for proton and anion exchange membrane fuel cells and water electrolysers. In particular, the group is dealing with design and preparation of nanostructured and nanofibrous materials e.g. obtained by electrospinning, and new membrane-electrode assembly architectures. Techniques for metal deposition and surface functionalisation are also implemented to prepare materials with improved properties relevant to the targeted applications.

In 2017 Prof. Cavaliere was awarded the CNRS bronze medal and appointed junior member of the Institut Universitaire de France. She co-authored over 70 scientific papers with a h-index of 28, 2 patents, 5 book chapters, and edited one book.

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KEYNOTE SESSIONS

DAMIEN ERNST

Reinforcement learning for electrical markets and the energy transition University of Liège

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In this talk, Professor Damien will talk about reinforcement learning, a subfield of artificial intelligence, and the many applications these techniques could have in solving decision-making problems related to energy markets and the energy transition. He will present, among other things, recent research results obtained using such RL techniques for the design of intelligent agents for intraday electricity trading. He will also present a new class of reinforcement learning algorithms that can calculate what are the optimal investments to be made in new complex energy systems, such as renewable energy communities or remote renewable energy hubs.

BIOGRAPHY

Damien Ernst received the M.Sc. and Ph.D. degrees in engineering from the University of Liège, Belgium, in 1998 and 2003, respectively. He is currently Full Professor at the University of Liège and Visiting Professor at Télécom Paris. His research interests include electrical energy systems and reinforcement learning, a subfield of artificial intelligence. He is also the CSO of Haulogy, a company developing intelligent software solutions for the energy sector. He has co-authored more than 300 research papers and two books. He has also won numerous awards for his research and, among which, the prestigious 2018 Blondel Medal. He is also regularly consulted by industries, governments, international agencies and the media for its deep understanding of the energy transition.

KEYNOTE SESSIONS

BÉNÉDICTE MENEZ

Geologic hydrogen: sources, fluxes and relationships with deep microbial activity and abiotic organic synthesis

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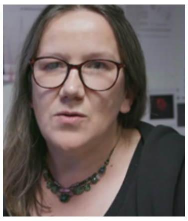
Molecular hydrogen (H_2) forms widely on Earth through well established processes, including for the major ones, (i) large-scale reduction of water during the oxidation of ferrous iron in silicate or sulfide minerals; this mainly occurs in oceanic hydrothermal systems operating from low temperature and low pressure (LT-LP) at mid ocean ridges to great depths in subduction zones; (ii) radiolytic splitting of water molecules (via ⊠, ⊠, or ⊠ radiations induced by the decay of radioactive elements) in sediments as well as oceanic and continental rocks; H_2 production via water radiolysis proceeds at all temperature and pressure conditions under which water is stable, even when it is ice, vapor, or bound in hydrated salts; (iii) degassing of magma at low pressures that favor SO_2 and H_2 production at the expense of H_2O + H_2S; and (iv) reaction of water with surface radicals during the mechanical breaking of silicate rocks; H_2 can hence be generated continually or episodically during slip events in orogenic belts, subduction zones, continental rifts, passive margins, spreading centers, transform faults, and fracture zones (i.e., up to high temperature and high pressure).

Although some of these mechanisms have been identified for decades, the current challenges that hinder the exploitation of natural (or geologic) hydrogen are, among others, to understand if the yields associated with these long-standing geological processes are high enough for H_2 to constitute a sustainable resource, and if this hydrogen is produced continuously or if it is formed punctually and accumulates in reservoirs not yet identified in the Earth's crust. Another major challenge is related to the fact that H_2 is a reductant capable of supporting a large diversity of microbial metabolisms in oxic as well as in anoxic conditions. Knowing now that the first kilometers of the subsurface, where natural H_2 is generated, are home to more than 70% of the terrestrial microorganisms for which H_2 represents a choice energy resource, it becomes crucial to evaluate the impact of this deep microbial activity on the potentially exploitable emissions of natural H_2 as well as on the underground storage of this resource as it is envisaged in the years to come. In addition, the strong reducing power of H_2 gives it the capacity to initiate abiotic (i.e., purely chemical) organic synthesis in the lithosphere. This process is now acknowledged to lead to the non-biological production of various organic compounds with diverse composition and structure depending on the redox conditions under which they were formed and the minerals they are associated with. Competing with hydrogenotrophic (i.e., H_2-consuming) autotrophic microbial activity at a temperature compatible with the development of life, which similarly transforms inorganic carbon compounds, such as carbon mono- and di-oxide (CO and CO_2, respectively), into organic compounds, abiotic organic synthesis can nonetheless occur up to very high pressure and temperature and has the potential to similarly impact natural H_2 emissions.

In this keynote we will review all these concepts to identify the current knowledge barriers to exploration and exploitation of natural $H_2$and the geological storage of this gas.

BIOGRAPHY



Pr Bénédicte Ménez is a geobiologist with expertise in high resolution microimaging techniques that allow to characterize microbe-mineral interactions over time and to identify traces of life within rocks. She received her PhD degree in Geochemistry (with Honors) from Paris Diderot University in 1999. After a two-year postdoc at the Commissariat à l'Energie Atomique (CEA, France), she first joined the French National Center for Scientific Research (CNRS) as a Research Scientist and the Institut de physique du globe de Paris (IPGP) in 2001 and was recruited as Full Professor from Paris Diderot University in 2011. She dedicated the first 10 years of her career at developing innovative and interdisciplinary approaches with the aim to unlock some of the barriers hampering the study of deep biosphere, now acknowledged to host >70% of the Earth's microbial life. These developments were funded by several national or international projects she led or participated to as co-PI and were rewarded by several awards. Since then, she has been working at the interface between (bio)geochemistry, mineralogy, petrology, microbiology and molecular ecology with the aim to study the deep biosphere hosted in the oceanic lithosphere and its relationship with the origin of life. She has headed the geomicrobiology group of IPGP between 2010 and 2019 and was one the former Directors of the Centre of Research on CO_2 geological storage funded by IPGP-TOTAL-SCHLUMBERGER and the ADEME agency.

KEYNOTE SESSIONS

VALÉRIE BRIOIS

Synchrotron Radiation at the Crossroads of the Sustainable Energy Science from Today to Tomorrow

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Energy-related materials used for production and storage are complex and heterogeneous systems in which interfaces play a key role. Those systems are dynamical over a wide range of temporal scales and are organized over multi length scales, each scale having to be characterized to gain a full understanding of their functioning. The SOLEIL Synchrotron Radiation facility located on the Saclay plateau provides access to powerful techniques, such as X-ray Absorption Spectroscopy (XAS) or X-ray microscopy (XRM) to cite only few of them, for gaining chemical and structural information on the systems with micron to sub-micron meter spatial resolution in in situ or operando conditions with sub-second time resolution. A few examples of the current studies carried out at SOLEIL in the field of batteries [1] and catalysts used for H_2 production [2] or greenhouse mitigation [3] will be first presented.

Understanding the formation of Solid Electrolyte Interface in Na-ions batteries or solving the large-scale fabrication and durability of perovskite solar cells are recognized to make practical implementation still problematic for large scale deploying of clean energy technologies. In the recently published Conceptual Design Report for the upgrade of the current 3rd SOLEIL generation facility into a 4th generation [4], the opportunities offered by the expected increase in brightness and coherence of the SOLEIL-II source have been discussed. Coherent-based imaging techniques with improved spatial and temporal resolution will be available providing a powerful lever to overcome the aforementioned bottlenecks, as briefly discussed in the perspective and conclusion section of this keynote.

BIOGRAPHY

Valérie Briois received her PhD from the Paris VI University (Paris) in 1991. She worked at LURE (1991-2004) and now at SOLEIL, the French Synchrotron Radiation facilities. CNRS Research Director, she is the head of the ROCK quick-EXAFS beamline at SOLEIL. She works on the operando quick-EXAFS characterizations of catalysts and contributes to the spread of MCR-ALS applied to quick-EXAFS analysis. Her current research activities are focused on hydrodesulfurization and ethanol steam reforming catalysts.

References

[1] Wernert, R., Iadecola, A., Stievano, L., Carlier, D., Croguennec, L. Chemistry of Materials., 35(2): 617–627. (2023).

[2] Passos, A.R., La Fontaine, C., Pulcinelli, S.H., Santilli, C.V., Briois, V. PCCP - Physical Chemistry Chemical Physics., 22(34): 18835-18848. (2020)

[3] Beheshti-Askari, A., Al Samarai, M., Morana, B., Tillmann, L., Pfänder, N., Wandzilak, A., Watts, B., Belkhou, R., Muhler, M., DeBeer, S. ACS Catalysis., 10(11): 6223–6230. (2020).

[4] Conceptual Design Report for SOLEIL-II,
https://www.synchrotron-soleil.fr/fr/actualites/avant-projet-sommaire-pour-lupgrade-de-soleil

KEYNOTE SESSIONS

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Offshore energy hubs

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Europe has set very ambitious targets for deployment of offshore wind power, which will form the backbone of power generation in a decarbonized power system. To facilitate a cost-efficient connection of such massive amounts of offshore wind power, Denmark is revolutionizing the grid connection concept for offshore wind. In 2020, the Danish Parliament decided to develop and build two energy islands: one on the natural island of Bornholm in the Baltic Sea and a second as an artificial island in the North Sea. Other countries, like Belgium, have announced their own plans of building energy islands.

The talk with give an update on the status of the development of the energy islands, addressing the challenges but also the innovation opportunities that come with these massive infrastructure projects, including the connection with green hydrogen production.

BIOGRAPHY

Nicolaos A. Cutululis is Professor in Offshore Wind Power Integration, based in the Department of Wind and Energy Systems at the Technical University of Denmark. He holds a M.Sc. (1998) and a Ph.D (2005) in Automatic Control.

His main research area is integration and operation of wind power moving towards 100% RES power systems, with a special focus on offshore wind and HVDC. He has authored/co-authored extensively in his research field and is currently serving as Chief Editor for Wind Energy Science journal, associated editor for IEEE Trans on Sustainable Energy and Deputy Subject Editor for IET RPG.

He is scientific director in the DTU TotalEnergies Excellence Center of Clean Energy (DTEC). He is active in shaping the wind and power research agenda at European level, being a MB member of EERA JP Wind and Ex-co member for ETIPWind. He is also co-chairing the SET Plan IWG drafting the first Implementation Plan for HVDC. He represents Denmark in IEA Wind Task 25 – Design and Operation of Power Systems with Large Amounts of Wind Power.

KEYNOTE SESSIONS

ARNAULT BARICHELLA

Cybersecurity in the Energy sector: Challenges, Perspectives and Policy Approaches

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As digitization accelerates in our societies, cybersecurity has become an increasingly important issue that touches on nearly all sectors and activities. The energy sector possesses its own particular characteristics, which are complementary but often different from those in other sectors. Information and communication technologies (ICTs) have only gradually been integrated into energy infrastructure. Yet, the need to rationalize production, distribution and consumption processes to manage an increasing amount of data, has contributed to the progressive deployment of ICTs. This digitization has allowed for important efficiency gains by optimizing the supply chain. At the same time, the deployment of ICTs has also considerably increased the risk of cyberattacks. The energy sector has evolved from relatively isolated industrial systems to an open network relying on technologies connected with the Internet.

Cybersecurity includes both protection from computer viruses intended to cause physical and material damage, as well as from hacking and theft of personal data for commercial profit. Moreover, the strategically critical role of the energy industry for all vital State functions (defense, communications and healthcare for example) has turned this sector into an increasingly privileged target for cyberattacks, often in relation to geopolitical confrontations. This is partly because it is often difficult to attribute with precision responsibility for a cyberattack, which allows a State to rely on mass spying or to cause major damage while remaining undetected. Thus, Russia is the prime suspect behind a series of devastating cyberattacks over the last few years that have hit the energy sector in Ukraine, along with Europe and North America. These include the Black Energy and NotPetya viruses targeting Ukraine in 2015 and 2017 respectively, or the Colonial Pipeline hacking impacting the US in 2021, amongst others. Due to the globalization of trade and digital technologies, cyberattacks aimed at Ukraine subsequently spread globally.

In order to manage these growing threats, countries around the world have progressively put in place a number of regulations, laws and institutions to protect the energy industry from cyberattacks. In is notable how each country or group of countries has tended to develop a particular approach to cybersecurity in this sector. For instance, the US has adopted a strategy of 'security in depth' focusing on strict and detailed regulations in specific fields, implemented by institutions possessing coercive powers. By contrast, the EU has chosen a more flexible and holistic strategy, favoring the protection of a wide range of different sectors (low-carbon technologies, data and privacy, etc.), whilst providing member states with broad autonomy in the implementation process. As the digitization of critical infrastructure accelerates, cybersecurity in the energy sector will be of seminal importance in the years to come. This is especially the case due to the unstable context of international relations, where a notable increase in cyberattacks has accompanied the rise in tensions between the great powers, as highlighted by the current war in Ukraine.

BIOGRAPHY

Arnault Barichella is completing his PhD in Political Science at Sciences Po Paris with the Center for European Studies and Comparative Politics. He obtained his Masters' degree in European Affairs from Sciences Po Paris, and received a BA degree in Modern History from Oxford University. Arnault was a Visiting Fellow at Harvard in 2018-19, affiliated with the Department of Government.

EVENTS OF THE CONGRESS

INNOVATION SESSION (MARCH, 9TH)

One of the afternoons will be dedicated to Innovation. During this afternoon, several events will take place around the idea of Innovation and Entrepreneurship.

POSTER AWARDS

Two Poster sessions are organized during the congress. They will take place on the 8th and the 9th of March, in the Emmy Noether Hall. At the end of the congress, five Poster Awards and one Innovation Poster Award will be granted to the best contributions.

STUDENT WORKSHOPS

Different workshops are organized for the University Paris-Saclay Graduate Schools students.
Registration is compulsory and places are limited.
Registration can be done at momentom2023@sciencesconf.org.

Comment écrire pour un public non-spécialiste et partager ses recherches avec le plus grand nombre ?

Cet atelier, animé par un journaliste de *The Conversation*, permet aux chercheuses et chercheurs d'approfondir leur connaissance de ce média et de s'approprier des outils de vulgarisation.

Dans un premier temps, l'intervenant détaille des outils concrets de vulgarisation, basés sur des exemples d'articles publiés sur le site. Des outils pour trouver le bon angle, intéresser, simplifier sa recherche sans la dénaturer et construire un article accessible.

Puis chacun est invité à dire un mot de ses recherches, voire à proposer une idée d'article. Le journaliste aide à affiner les angles afin d'aboutir à une proposition de papier pour *The Conversation*. L'objectif est qu'à l'issue de cet atelier, un maximum de participants puissent proposer un article et, à terme, être publiés dans *The Conversation*.

Open science: Publications to Data and Numerical Identity

This workshop is divided into two parts: open science and insights into numerical identity.
In the first part, we will see what open science is, what its implications are for researchers, what their obligations (with respect to institutions or funding agencies) are, what benefits they will have and how to train oneself (in the context of Université Paris-Saclay).

For the second part, we shall focus on your numerical ID (ORCID, for instance), the use of different platforms (both academic ones, like ResearchGate, or professional ones, like LinkedIn) and how you appear on the web.

The objective of this workshop is to train the future researchers with respect to the different aspects of open science, the implementation of recommendations to the full extent, and whom to contact in case of specific problems.

Pourquoi penser design pour un monde soutenable ?

Cet atelier est proposé par Design Spot. Le design est une approche globale et systémique qui aborde une problématique par l'interaction d'une solution avec son environnement. Celui-ci permet de répondre à un besoin par la forme pour en maximiser l'efficacité.

Dans cet atelier, nous vous proposons de comprendre son fonctionnement et de l'expérimenter à travers des objets du quotidien. Venez expérimenter la pensée «design» au service d'un développement soutenable !

THE GALA DINNER

The gala dinner will take place at the Train Bleu, in Paris. Places are limited. Attendance is free and upon registration.

Le Train Bleu is a gastronomic restaurant at the Gare de Lyon, and one of the most famous in Paris. Built in 1900 for the Universal Exhibition, the Buffet de la Gare becomes Le Train Bleu in 1963. Its rooms still have the original features of La Belle Epoque, and some of them are classified as Monument historique.

ORALS
SESSION

ORAL #1

ChalcoPOM-based catalysts: from fundamentals to hydrogen evolution real-life application

Serge AlBacha,1 Loic Assaud,2 Bruno Fabre,3 Nathalie Leclerc,3 Clément Falaise,3 Emmanuel Cadot*3

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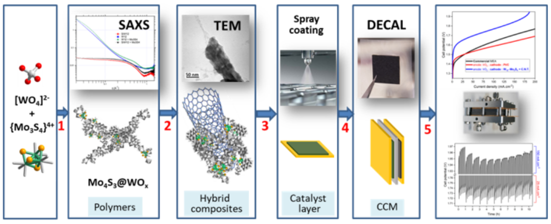

Fig. 1 Successive steps integrating chalco-POM polymer within PEM electrolyser technology : **1**- acidic condensation of the tungstate anions in the presence of the $\{Mo_3S_4\}$ clusters leading to large $Mo_3S_4@WO_x$ polymers; **2-** design of carbon-based composites where the large “chaotropic polymers” interface with the exposed carbon surface (CNTs, GO, carbon dots, …); **3-** processing the colloidal composite aqueous suspension as catalytic ink for the fabrication of large surface area electrodes; **4-** CCM fabrication through the so-called DECAL process; **5-** Integrating Pt-free CCM into PEM electrolyser.

Molecular engineering of efficient HER catalysts is an attractive approach for controlling the spatial environment of specific building units selected for their intrinsic functionality required within the multistep HER process.1 As the {Mo-S} cores has been identified as one as the most promising HER electrocatalysts, we demonstrated that the covalent association between the {Mo3S4} core and tungsten-containing redox-active polyoxometalates (POM) produces a striking synergistic effect featured by high HER performance.2 Various experiments carried out either in homogeneous or in heterogeneous conditions showed that this synergistic effect arises from the direct connection between the {Mo3S4} cluster and the POM unit. In addition, we report that this effect is retained when the Chalco-POM based catalyst is transferred within photocatalytic device or deposited as co-catalyst (cocat) onto a microstructured p-type silicon. Using drop-casting procedure to immobilize cocat onto the silicon interface using electrostatic incorporation into a poly(3,4-ethylenedioxythiophene) (PEDOT) led the excellent HER performance of this photoelectrochemical system. At last, an innovative and straightforward approach consists to polymerize monomeric tungstate anions under acidic conditions in the presence of the HER-active cluster [Mo3S4(H_2O)9]4+ to yield highly insoluble {Mo3S4}-containing polymers, abbreviated Mo3S4@WOx. Herein, we showed that Mo3S4@WOx inorganic polymers exhibit strong propensity to interface with carbon-based nanomaterials e.g. nanotubes, graphene oxide or carbon black to be integrated as electrode active component within PEM electrolyser cells. Preliminary results showed that synergistic effect between the catalytic unit and the WOx polymer was retained leading to highly stable and efficient HER cathodes (see Figure 1).

(1) Hou, Y et al. Nature Materials 2011, 10 (6), 434–438.
(2) Tourneur, J. et al. J. Am. Chem. Soc. 2019, 141 (30), 11954–11962.

BIOGRAPHY

Emmanuel Cadot is Professor at the University of Versailles Saint Quentin where he is developing his research project within the MIM research team at the Lavoisier Institute of Versailles UMR-CNRS 8180. His long-term research project concerns polyoxometalate chemistry with particular emphasis on their functionalization by chalcogenide clusters and their applications in the field of energy conversion processes.

ORAL #2

Status and perspectives of photovoltaics

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Photovoltaics (PV) must be considered as a major contributor for tomorrow's electricity supply. PV has become a fast-growing market; the cumulative PV installations have been growing by 30% every year in the last ten years, and the 1 TWp milestone of cumulative installed solar capacity has been passed in 2022. At the same time, prices decreased at a rate of about 15% per year. Today's module prices are around 0.2 €/Wp, while the levelized cost of electricity for large PV systems is in the range of 0.02-0.10 €/kWh (20-100 €/MWh). With 95% of the market, silicon technologies hold an undisputed leading place in PV industry. The average PV conversion efficiency of industrially available silicon modules is around 20.4%, however the best silicon module efficiency is at 24.4% and the best solar cell efficiency is at 26.8%, which shows that some improvements are still possible at the industrial level to increase the module efficiency and to approach the best cell efficiency. On the other hand, the theoretical limit of silicon solar cell efficiency from thermodynamic laws (known as the Shockley-Queisser limit) is at 32.3%, and calculations considering the unavoidable Auger recombination losses point toward a limit efficiency of 29.4%. Taking into account that all losses will never be fully avoided in the real world, it is believed that it will be very difficult for silicon solar cells to go beyond efficiencies of 28%. This shows that improvements at the cell level are now very limited. To go beyond the 30% efficiency target and even beyond the Shockley-Queisser limit, the most attractive route is that of tandem solar cells employing silicon as the absorber in the bottom subcell and a semiconductor with larger bandgap as the absorber in the top cell. While record efficiency of 32.8% was reached for GaAs/Si mechanically stacked tandem cells, a lot of research has been focusing in recent years on hybrid (organic-inorganic) perovskites which have experienced impressive progress in their performance within less than 10 years, and a record of 31.3% was reached last year for monolithic perovskite/Si tandem (on a 1 cm2 area cell).

In this presentation, I will give an overview of the status of the PV market and of the various technologies. I will then describe the current trends in tandem solar cells that are scheduled to enter the market in the next decades. They are at the focus of the research all over the world, including in France within the French CNRS Photovoltaic Federation (FedPV).

BIOGRAPHY

Jean-Paul Kleider graduated from the SUPELEC school of engineering in 1984 and obtained his PhD in physics at the University Pierre et Marie Curie in 1987. He has been holding a researcher position at CNRS since 1988. Since 2015, he has been leading the department of Materials at Laboratoire de Génie Electrique et Electronique de Paris (GeePs).
Since 2020 he is Director of FedPV, the French CNRS Federation of Photovoltaics.
His main research interests and activities are in the electrical and optoelectronic characterization of semiconductor materials and in device physics for photovoltaics, including theoretical analysis and numerical modelling.

ORAL #3

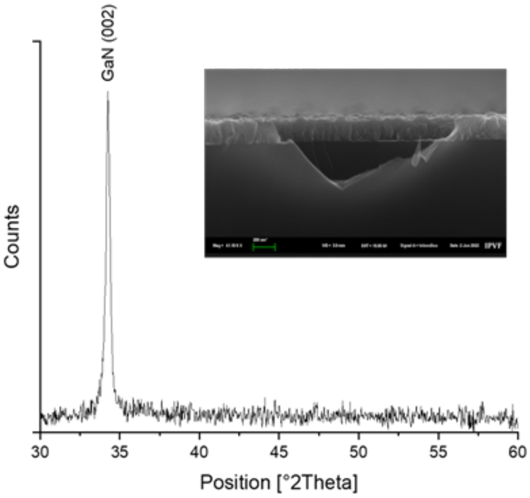

Figure 1 XRD spectrum of a GaN thin film grown by PECVD
(inset shows a SEM cross section image of a hole in the c-Si substrate resulting from Ga diffusion)

Routes for low cost III-V solar cells

Lise Watrin1,2*, François Silva2, Cyril Jadaud2, Pavel Bulkin2,
Jean-Charles Vanel2,
Erik V. Johnson2, Karim Ouaras2, and Pere Roca i Cabarrocas1,2

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Solar cells based on III-V materials have reached the highest efficiency of any technology available today, i.e. up to 47% under concentration1. Nevertheless, their cost is a hundred times higher than that of c-Si solar cells2. Most of this cost difference comes from i) the III-V or Ge substrate required to grow a single crystal layer and ii) the growth process.

In a previous study we have shown how the use of a virtual substrate can tackle the first part of the challenge3. This innovative substrate is composed of a crystalline silicon wafer coated with an ultrathin (20 nm) epitaxial layer of germanium. Thus, costs can be drastically reduced as Si wafers are much more affordable than those made of III-V or Ge semiconductors, mainly due to the greater abundance of Si in the earth's crust4. In addition, the silicon can be used directly as a bottom cell in a tandem architecture, further increasing the efficiency/cost ratio.

In this work we focus on the development of a new strategy for the epitaxial growth of III-V materials by using Plasma-Enhanced Chemical Vapor Deposition (PECVD) technique, with the aim of drastically reducing the processing costs in comparison with usual semiconductor deposition techniques such as Molecular Beam Epitaxy (MBE) and Metal Organic Chemical Vapor Deposition (MOCVD). Indeed, plasma assistance allows us to work at lower temperatures, thus reducing thermal stresses and hopefully defects but also the well-known issue of gallium mixing with silicon at high temperature (meltback etching in litterature5). Moreover, PECVD enables low pressure operation, which reduces drastically the precursor consumption i.e. the main source of cost in a deposition process6. Some works showing the feasibility of such an approach were published in the 1980s7 and the subject is again attracting interest8 due to the strong growth of the photovoltaic market. Here we will present the results of the GaN thin films grown by PECVD in terms of deposition conditions (temperature, pressure, plasma power, precursor flow rates…) and the crystalline (Fig. 1), morphological and compositional properties of the films obtained. Finally, we will show that the so-called meltback etching effect is reduced by the low temperature used in PECVD (inset Fig. 1).

In sum, these results open the prospect of a more affordable method for the production of III-V materials, thus addressing the important issue of costs for III-V photovoltaic industry with the possibility of obtaining large-scale epitaxial films, thanks to a low-cost substrate and deposition process.

[1] Geisz, J.F., France, R.M., Schulte, K.L. et al., Nature Energy, 2020, Volume 5, 326-335.
[2] Smith, Brittany L., Michael Woodhouse, Kelsey A. W. Horowitz, Timothy J. Silverman, Jarett Zuboy, and Robert M. Margolis, CO: National Renewable Energy Laboratory, 2021.
[3] Monalisa Ghosh, Pavel Bulkin, François Silva, Erik V. Johnson, Ileana Florea, Daniel FunesHernando, Alexandre Tanguy, Charles Renard, Nicolas Vaissiere, Jean Decobert, Iván García, Ignacio Rey-Stolle, Pere Roca i Cabarrocas, Solar Energy Materials and Solar Cells, 2022, Volume 236,111535.
[4] Horowitz, Kelsey A., Remo, Timothy W., Smith, Brittany, and Ptak, Aaron J., A Techno-Economic Analysis and Cost Reduction Roadmap for III-V Solar Cells. United States: N. p., 2018.
[5] Hiroyasu Ishikawa, Kensaku Yamamoto, Takashi Egawa, Tetsuo Soga, Takashi Jimbo, Masayoshi Umeno, Journal of Crystal Growth, Volumes 189–190, 1998.
[6] Horowitz, Kelsey A., Remo, Timothy W., Smith, Brittany, and Ptak, Aaron J. A Techno-Economic Analysis and Cost Reduction Roadmap for III-V Solar Cells. United States: N. p., 2018.
[7] K.P. Pande and A.C. Seabaugh, J. Electrochem.Soc.: Solid-State Science And Technology, Volume 131, 1357, 1984.
[8] Uvarov, A.V.; Gudovskikh, A.S.; Nevedomskiy, V.N.; Baranov, A.I.; Kudryashov, D.A.; Morozov, I.A.; Kleider, J.-P., J. Phys. D: Appl. Phys., 2020, Volume 53, 345105.

BIOGRAPHY

My name is Lise Watrin, I graduated from a double degree program between an engineering diploma in Materials and Nanotechnologies and a research Master's degree on Quantum Devices, co-habilitated by Ecole Polytechnique and Université de Paris.

I am currently preparing a PhD funded by the Institut Photovoltaique d'Ile de France (IPVF) at Ecole Polytechnique on III-V growth by PECVD for application to solar cells.

I am passionate about the field of energy and more particularly about photovoltaic energy and its challenges in the energy transition.

ORAL #4

Solid-state monolithic dye-sensitized solar cell exceeding 10 % of power conversion efficiency using a copper-complex HTM and a carbon counter electrode

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Faculty of Engineering, University of Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal
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Indoor photovoltaics (iPVs) are becoming a reliable asset to cover the needs in cordless power for the exponentially increasing number of Internet of Things (IoT) devices operating indoors. Several PV technologies have been proposed as iPVs, but up to now only the third-generation PV cells, such as dye-sensitized solar cells (DSSCs), organic solar cells (OPVs) and perovskite solar cells (PSCs) reached the milestone of 30 % power conversion efficiency (PCE) under ambient light. Critical requirements for iPVs include being safe and environmentally friendly, without employing toxic materials. DSSCs devices with Cu-based complex hole transport materials (HTM) and organic sensitizers do not use toxic materials, which turn DSSCs one of the safest and sustainable options for iPVs [1]. Besides, DSSCs have a versatile architecture [2], and present a low-cost and simple fabrication process [1].

DSSCs using a Cu(II/I)-based electrolyte recently reached a new landmark PCE of 15.2 % under 1 sun illumination using a hydroxamic acid derivative pre-adsorbent prior to co adsorption with two organic sensitizers [3]. An advantage of the DSSCs employing copper based electrolytes is the possibility to form a solid-state HTM by slow evaporation of the electrolyte solvent; up to now, 11.7 % is the record PCE for a solid state DSSC [4]. It is important to mention that these devices employ a PEDOT:PSS counter-electrode, which has stability issues during long-term operation [5]; and were fabricated in the conventional configuration, with two conductive transparent substrates, complicated for production in series modules, and costly.

In this work we present for the first time solid-state monolithic dye-sensitized solar cells (M-DSSCs) using a copper-complex HTM and a carbon-based counter-electrode. The monolithic structure uses a single conductive transparent substrate, reducing the material costs by 20 30 % [6] and being straightforward for module design [7]. The mesoporous TiO_2 photoanode and the graphite/carbon black counter-electrode are deposited in the same substrate, and a TiO_2 insulating/spacer layer is used to electrically separate them. The sensitization was carried out using Y123 organic dye, while [Cu(tmby)2(TFSI)2/1]2+/+ were the selected copper complexes for the electrolyte solution. Since these M-DSSCs are thicker than the conventional DSSCs using a PEDOT:PSS catalyst, the vacuum was used to facilitate the infiltration of the electrolyte solution through all the layers; this procedure was crucial to form a stable solid-state copper complex HTM after acetonitrile evaporation. The best-performing device displayed a PCE of 10.4 % under 1-sun, and 26.1 % and 28.5 % under 600 lx and 1000 lx indoor light, respectively (Figure 1a); this device is stable for 1000 h under natural aging and artificial light-soaking (Figure 1b). The sequential deposition of the main components of the M DSSCs in a single conductive transparent substrate using only commercial materials turns these devices very attractive for the market-scale production of iPVs.

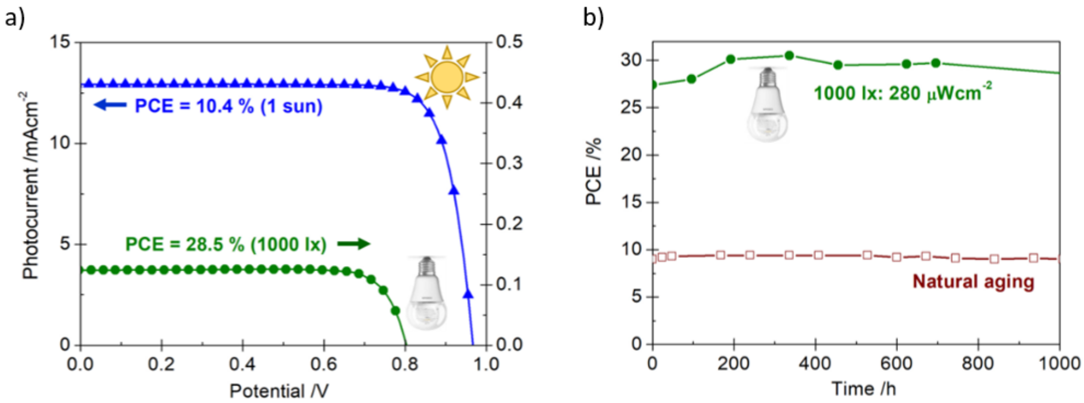

Figure 1 - I-V characteristics for the best-performing M-DSSC under 1-sun and 1000 lx artificial light (a); PCE *vs* time for M-DSSCs under natural aging and continuous artificial light-soaking (b).

Acknowledgements:
The research leading to these results has received funding from: i) project 2SMART, with reference NORTE-01-0145-FEDER-000054, supported by Norte Portugal Regional Operational Programme (NORTE 2020), under the PORTUGAL 2020 Partnership Agreement, through the ERDF; ii) project HopeH$_2$, with reference POCI-01-0145-FEDER-030760, funded by FEDER funds through COMPETE2020 – Operational Programme for Competitiveness and Internationalization (POCI) and by national funds (PIDDAC) through FCT/MCTES; and iii) LA/P/0045/2020 (ALiCE), UIDB/00511/2020 and UIDP/00511/2020 (LEPABE), funded by national funds through FCT/MCTES (PIDDAC).

References:

[1] Pecunia, V., Occhipinti, L. G., Hoye, R. L. Z., Emerging Indoor Photovoltaic Technologies for Sustainable Internet of Things. Adv. Energy Mater. 2021, 11, 2100698. DOI: 10.1002/aenm.202100698.
[2] Muñoz-García, A.B., Benesperi, I., Boschloo, G., Concepcion, J.J., Delcamp, J.H., Gibson, E.A., Meyer, G.J., Pavone, M., Petterson, H., Hagfeldt, A., Freitag, M., Dye-sensitized solar cells strike back. Chem. Soc. Rev. 2021, 50, 12450–12550. DOI: 10.1039/D0CS01336F.
[3] Ren, Y., Zhang, D., Suo, J., Cao, Y., Eickemeyer, F.T., Vlachopoulos, N., Zakeeruddin, S.M., Hagfeldt, A., Grätzel, M., Hydroxamic acid preadsorption raises efficiency of cosensitized solar cells. Nature 2022. DOI: 10.1038/s41586-022-05460-z.
[4] Zhang, W., Wu, Y., Bahng, H.W., Cao, Y., Yi, C., Saygili, Y., Luo, J., Liu, Y., Kavan, L., Moser, J.E., Hagfeldt, A., Tian, H., Zakeeruddin, S.M., Zhu, W., Grätzel, M., Comprehensive control of voltage loss enables 11.7% efficient solid-state dye-sensitized solar cells. Energy Environ. Sci. 2018, 11, 1779. DOI: 10.1039/C8EE00661J.
[5] Kamppinen, A., Aitola, K., Poskela, A., Miettunen, K., Lund, P.D., Stability of cobalt complex based dye solar cells with PEDOT and Pt catalysts and different electrolyte concentrations. Electrochim. Acta, 2020, 335, 135652. DOI: 10.1016/j.electacta.2020.135652.
[6] Kroon JM. Energy Research Center report. 2005;ECN-C-05-078;1-41.
[7] Santos, F., Ivanou, D., Mendes, A., The renaissance of monolithic dye-sensitized solar cells. Mater. Today Commun. 2022, 32, 104030. DOI: 10.1016/j.mtcomm.2022.104030.

BIOGRAPHY

Fátima Santos holds a BSc and a MSc in Chemical Engineering from the University of Porto. In June 2022, she obtained her PhD degree in Chemical and Biological Engineering at the same institution. Her PhD thesis was related to the development of highly efficient and stable monolithic dye-sensitized solar cells (M-DSSCs); during her PhD, she reported the worldwide record efficiencies of iodide and cobalt-mediated M-DSSCs, as well as highly stable M-DSSCs by cell full glass encapsulation. In the last 5 years, she worked in the research and development field on LEPABE/ALiCE research group, has been involved in 2 R&D projects funded by EU agencies, and published 8 original research articles. Fátima Santos started recently a position as a junior researcher on LEPABE/ALiCE, and she is currently developing solid-state M-DSSCs to power IoT devices.

ORAL #5

High bandgap triple mesoscopic perovskite solar cells

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Today's development of the hydrogen fuel automotive industry is strongly limited by the lack of processes and technologies able to provide sufficient amounts of hydrogen at acceptable costs without polluting the environment or increasing the CO_2 footprint. A very promising solution has been found in the use of solar energy, in combination with photovoltaic devices, to perform water splitting to produce hydrogen in an ecological manner. While the use of expensive catalysts and multi-junction solar cells has shown potential for high performance and a good solar to hydrogen (STH) conversion efficiency, the cost of such produced hydrogen stays prohibitive. Various low-cost PV cells including silicon, perovskite and dye-sensitised solar cells have been investigated as a means of supplying the additional bias to the photoelectrodes made of earth-abundant elements to achieve spontaneous water splitting.1,2,3,4 Impressive STH efficiencies that were not previously possible have been reported in the last few years. Among the PV devices, solution-processed organohalide perovskite cells are excellent candidates for tandem configurations with photoelectrodes due to their inexpensive solution processing, high efficiencies, bandgap tunability and optical transparency.5,6 While the performance characteristics of perovskite devices are very well suited for water splitting, their extreme sensitivity to water makes them very difficult to use, directly, as photoelectrodes. Printable perovskite solar cells based on MAPbI3 in a TiO_2/ZrO_2/Carbon triple-layer mesoporous scaffold have shown simple fabrication process7 and impressive stability.8 In addition, the hydrophobic mesoporous carbon layer protects the perovskite absorber from moisture penetration. In this communication, we will discuss the development of high bandgap perovskite solar cells using triple mesoscopic architecture (figure 1) as a stable solution and their potential application in water splitting.

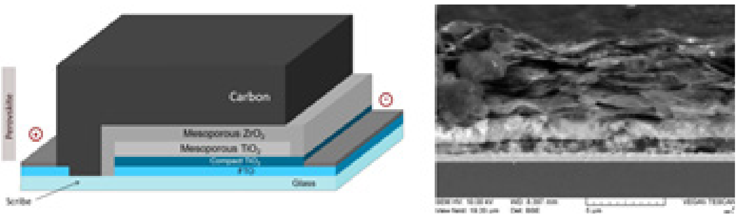

Figure 1. Triple mesoscopic architecture and SEM cross section

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[1] M. Grätzel et al., Nano Lett. 2015, 15, 3833.

[2] J. H. Park et al., Nano Energy 2015, 13, 182

[3] J. S. Lee et al., ACS Nano 2015, 9, 11820

[4] S. Yang et al., J. Mater. Chem. A 2017, 5, 19091

[5] M. Grätzel et al., Science 2014, 345, 1593

[6] S. I. Seok et al., Science 2017, 356, 1376

[7] H. Han et al., J. Nanophotonics 7 (2013) 073090-073090.

[8] G. Grancini et al., Nat. Comm., 8, 15684, (2017).

ORAL #6

Study of the formation of 2D/3D perovskite heterostructures for solar cells

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Perovskite-based solar cells, using 3D perovskites as the active layer, have achieved efficiencies of 25.7% [1]. Many improvements have been made on the intrinsic and extrinsic stabilities of this material against exposure to light, temperature, oxygen and humidity, but the stability of 3D perovskites remains one of the main issues in order to develop the industrialisation of this technology. [2]

Many approaches have been studied to improve the stability of perovskite-based cells, with particular attention paid to the interfaces. [3] In this perspective, the use of 2D perovskites and their addition to 3D perovskites, forming an heterostructure of 2D/3D perovskites, is a promising way to obtain perovskite-based solar cells [3] and tandem silicon-perovskite cells [4] more stable and efficient.

In this work, we study the spin-coating synthesis of a 2D/3D perovskite heterostructure by depositing a solution containing a “spacer” cation, 4-fluorophenethylammonium iodide (4-FPEAI) on an triple-cation 3D perovskite. This process forms a thin layer of 2D perovskite on the 3D perovskite surface.

An improvement in the efficiency and stability of the photovoltaic cells is obtained by adding 2D perovskite and forming the 2D/3D structure. A study of the 2D perovskite formation mechanisms is carried out through the analysis of the structural, chemical and optoelectronic properties of the structure, while varying several synthesis parameters. We reveal the presence of bromine in the 2D phase and conclude on the existence of a second mechanism, besides the most commonly accepted mechanism, involving the excess of lead iodide (PbI2) contained in the 3D perovskite. Thus, we demonstrate how the stoichiometry of the 3D perovskite affects the composition of the 2D layer formed on top. [5]

This study gives a better understanding of the synthesis mechanisms of 2D/3D heterostructures, helping the development of new, more efficient and functional material for photovoltaic cells applications.

REFERENCES :

[1] Min, H. et al. Nature 2021, 598 (7881), 444–450. DOI : 10.1038/s41586-021-03964-8.

[2] Cheng, Y. et al. Energy Environ. Sci. 2021, 14, 3233–3255. DOI : 10.1039/D1EE00493J

[3] Grancini, G. et al. Nat. Commun. 2017, 8, 15684. DOI : 10.1038/ncomms15684.

[4] Kim, D. et al. Science 2020, 368(6487) : 155-160. DOI : 10.1126/science.aba3433.

[5] Campos, T. et al. J. Phys. Chem. C 2022, 126 (31), 13527–13538. DOI : 10.1021/acs.jpcc.2c04957.

BIOGRAPHY

Thomas Campos obtained a master degree in Material Science at Troyes University of Technology (UTT) in 2019. He then started his PhD in Physics at Paris-Saclay University under the supervision of Pr. Emmanuelle Deleporte. He works on the study of 2D/3D hybrid halide perovskite heterostructures for perovskite solar cells. His main focuses are the solution-processed synthesis of thin-film perovskite materials and the characterization of the physical properties of this material (structural, morphological, optoelectronic, etc.), as well as the fabrication of perovskite solar cell devices.

Promising Ultra-wide Bandgap Spinel ZnGa2O4 for Energy Storage and Conversion

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Globally, energy production is mainly based on the consumption of fossil fuel resources which leads to environmental pollution. To reduce CO_2 emissions, it is essential to turn to use renewable energy, to increase the efficiency of energy conversion and transmission by relying on new technologies and new materials. Spinel zinc gallate (ZGO - ZnGa2O4) is arguably a ternary oxide semiconductor with an ultra-wide bandgap (~5 eV). Different from binary semiconductors, ZGO has three distinctly coordinated elements, which can result in different properties of the materials by changing their sites. This phenomenon is known as the self-doping effect [1]–[3]. Since highly conductive ZGO has been recently highlighted [4]–[6], it becomes a very promising candidate for implementations in energy storage (solar cells), energy conversion applications (ultra-high-power electronics) and catalysis (water splitting). Understanding and controlling the conductivity is then crucial.

Due to the self-doping effect, we have recently demonstrated that p- and n-type ZGO epilayers can be obtained by adjusting the growth conditions during metal-organic chemical vapor deposition (MOCVD). The intrinsic conductivity can be controlled up to 10 orders of magnitude (conducting n-ZGO, ρ = 3.2 ×10-2 Ω·cm at 300 K, highly resistive p-ZGO, ρ = 6 ×106 Ω·cm at 490 K) [7]. Further research is required to better comprehend and control the conductivity. Indeed, several factors can influence the final electrical properties such as growth temperature, total pressure in the growth chamber, cation precursors' ratio, oxygen flow, for instance.

The objective of this work is to deepen the investigation of the surface and in-depth chemical composition of the ZGO spinel thin films obtained by XPS on their electrical transport and optical properties. Particular attention is given to the deposition parameter (Zn precursor's flow and oxygen) influence. A preliminary study of photosensitivity for the p-type ZGO, as well as water splitting for n-type ZGO will be also presented.

ZnGa2O4 thin films were grown by MOCVD at 720 °C and 25 torr, the TEGa flow was fixed at 27.3 µmol/min, the DEZn flow was tuned from 14.0 to 21.0 µmol/min. After the growth, the oxygen flow was kept for some samples while it was cut for the others. By the means of the structural, morphological, chemical, optical characterizations combined with electrical transport measurements, we conclude that the oxygen plays an important role in the conductivity. Keeping the oxygen flow after the growth made the native conductivity of the ZnGa2O4 thin film to become resistive p-type (105 Ω▯cm at 550 K) from n-type (10-1 Ω▯cm at 300 K), with no significant modification of the bandgap (~ 4.6 eV at 300 K). The influence of the DEZn flow on the properties of the samples is limited. Besides, the preliminary study of the UV photosensitivity of the p-type ZnGa2O4 thin film showed that the current can be increased by 3 orders of magnitudes after turning on the UV lamp (IUV/Idark = 103) though without any metallization. Conductive ZGO material was also tested as electrode for hydrogen production and showed promising results.

REFERENCES :
[1] R. Pandey, J. D. Gale, S. K. Sampath, and J. M. Recio, 'Atomistic Simulation Study of Spinel Oxides: Zinc Aluminate and Zinc Gallate', Journal of the American Ceramic Society, vol. 82, no. 12, pp. 3337–3341, 1999, doi: 10.1111/j.1151-2916.1999.tb02248.x.
[2] T. R. Paudel, A. Zakutayev, S. Lany, M. d'Avezac, and A. Zunger, 'Doping Rules and Doping Prototypes in A2BO4 Spinel Oxides', Adv. Funct. Mater., vol. 21, no. 23, pp. 4493–4501, Dec. 2011, doi: 10.1002/adfm.201101469.
[3] Y. Shi et al., 'Self-Doping and Electrical Conductivity in Spinel Oxides: Experimental Validation of Doping Rules', Chem. Mater., vol. 26, no. 5, pp. 1867–1873, Mar. 2014, doi: 10.1021/cm404031k.
[4] D. C. Look, K. D. Leedy, R.-H. Horng, M. D. Santia, and S. C. Badescu, 'Electrical and optical properties of degenerate and semi-insulating ZnGa2O4 : Electron/phonon scattering elucidated by quantum magnetoconductivity', Appl. Phys. Lett., vol. 116, no. 25, p. 252104, Jun. 2020, doi: 10.1063/5.0014827.
[5] Y.-S. Shen, W.-K. Wang, and R.-H. Horng, 'Characterizations of Metal-Oxide-Semiconductor Field-Effect Transistors of ZnGaO Grown on Sapphire Substrate', IEEE J. Electron Devices Soc., vol. 5, no. 2, pp. 112–116, Mar. 2017, doi: 10.1109/JEDS.2017.2653419.
[6] W.-K. Wang, K.-F. Liu, P.-C. Tsai, Y.-J. Xu, and S.-Y. Huang, 'Influence of Annealing Temperature on the Properties of ZnGa2O4 Thin Films by Magnetron Sputtering', Coatings, vol. 9, no. 12, p. 859, Dec. 2019, doi: 10.3390/coatings9120859.
[7] Z. Chi et al., 'Bipolar self-doping in ultra-wide bandgap spinel ZnGa2O4', Materials Today Physics, vol. 20, p. 100466, Sep. 2021, doi: 10.1016/j.mtphys.2021.100466.

ORAL #8

Deep Eutectic Solvents for Supercapacitors

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The growing need to store enormous amounts of energy and power, driven by the decarbonization revolution and the transition to renewable energy, has created a demand for new and improved storage technologies to cost-effectively supply future necessities of the grid. Devices like supercapacitors are exceptional at supplying and absorbing power bursts. They offer high power densities and last for thousands of cycles, with little to no degradation due to the nature of the non-Faradaic or fast Faradaic reactions. Currently, most supercapacitor electrolytes are either aqueous or ionic liquids. Aqueous electrolytes are clean, cheap, durable, safe and capable of high power densities, but as they are water-based, they degrade at high temperatures and potentials (above 1.2V). Ionic liquid electrolytes can potentially provide high energy densities, but they are more expensive, toxic, polluting, and less conductive than aqueous electrolytes. Herein, deep eutectic solvents (DES) are explored as a solution to maintain the wide voltage window of ionic liquid electrolytes and meet the clean and safe expectations of aqueous electrolytes. DES are made from a simple atom-efficient synthesis at a specific ratio and temperature. Considerably cheaper than ionic liquids, these solvents can sustain a wide range of potentials and safely deliver high capacitances even at high temperatures.

This work explores the use of choline chloride-based DES as an electrolyte medium for supercapacitors. Additives such as urea are explored to improve the stability and of these solvents. Cyclic voltammetry and supercapacitor cycling are performed to measure the performance of different DES relative to each other. The infinite possibilities to combine different species and prepare new and innovative DES, resulting in different electrolyte-electrode interactions can result in a maximization of the efficiency improving greatly the supercapacitor technology. Therefore, although the DES studies that have been presented by our research group, in the future we will carry on relentlessly to find the best combination of DES that can bring the highest energy densities at the lowest cost of storage.

BIOGRAPHY

Xavier Mascarenhas began an engineering degree in micro and nanotechnologies in 2013 at the Universidade Nova de Lisboa, Faculdade de Ciências e Tecnologias, where he started to learn about concepts such as material science, chemistry, physics and electronics. In 2019 he completed his Masters' thesis on the development of a nanostructured molybdenum disulphide interlayer to protect lithium-sulphur batteries from degrading. Because he loved what he did in his thesis, he decided to further develop his experience in energy storage devices by joining the Vasco da Gama Collaborative Laboratory in Porto, Portugal in 2020, where he is working on deep eutectic solvents, sodium ion batteries and the economics of energy storage. Eager to learn and dedicated to finding cost effective solutions, this motivated worker wants to make a difference.

ORAL #9

Functionalizing graphene with tetrazine derivatives to design new materials for supercaps

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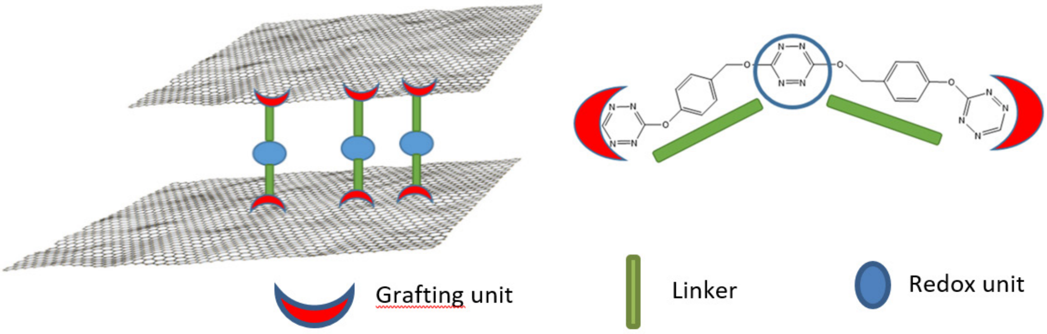
Energy storage has become a more and more important issue in the present general context of sustainable energy sources coupled to increasing mobility and use of portable devices. Therefore the synthesis of more complex and smart architectures of materials has been the aim of much interest from the scientific community. Molecular materials offer the opportunity to chemists to design these new architectures from well-chosen molecular units using all the reaction pathways of the so-called ‘chimie douce’, in particular simple reactions performed in mild experimental conditions. The most interesting results are often obtained with hybrid structures or composites since they allow a synergetic combination of the properties of each component.
In that framework we performed the chemical modification of functional graphene sheets (FGS), a variety of graphene obtained by exfoliation of graphite, and used the ability of tetrazine units to be grafted on the sp2 backbone in a controlled way through inverse demand Diels-Alder reaction1-4. This allowed us to generate new functionalities on graphene leading to nanocomposites with conducting polymers or modified graphene incorporating redox active bridges between graphene sheets (see scheme below). These materials have been designed to enhance the charge storage ability of graphene in view of making supercapacitors with high energy storage performances.



REFERENCES :
1. Rus, Y.B., Qu Y., Bosmi M., Galmiche L., Audebert, P., Miomandre, F. Efficient functionalization of reduced graphene oxide by 3-(pyridin-2-yl)-1,2,4,5-tetrazine and design of hybrids with silver nanoparticles for electrocatalysis, Mat. Chem. Phys. 291 (2022) 126607.
2. Rus, Y.B., Galmiche L., Audebert, P., Miomandre, F. Influence of the electrolytic medium on the performance and stability of functionalized graphene-polypyrrole nanocomposites as materials for supercapacitors, Synth. Met. 254 (2019) 22
3. Y. Li, G.Louarn, V. Alain-Rizzo, L. Galmiche, P. Audebert, F. Miomandre Polypyrrole-Tetrazine Modified Graphene Nanocomposites as New Materials for Supercapacitors, Carbon 105 (2016) 510-520.
4. Li Y., V. Alain-Rizzo*, L. Galmiche, P. Audebert, F. Miomandre, G. Louarn, M. Bozlar, M. Pope, D. Dabbs, I. Aksay, Functionalization of Graphene Oxide by Tetrazine Derivatives: A Versatile Approach toward Covalent Bridges between Graphene Sheets, Chem. Mater. 27 (2015) 4298-4310.

ORAL #10

A multiscale study of the electronic and ionic transport processes influencing the performance of Lithium-ion batteries

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The use of low-cost and highly efficient lithium-ion batteries in electric vehicles is critical to enabling the essential transition to carbon-free energy systems in the transportation sector. As a result, several research projects are focusing on the optimization of existing materials as well as the search for novel materials and elaboration methods. However, an all-inclusive challenge is the several kinetic setbacks that limit rate processes in advanced lithium-ion batteries. These multiscale interfacial barriers exponentially affect the optimum electronic and ionic transfers in conducting networks of the composite electrode. Several studies have used electrochemical impedance spectroscopy and dc conductivity measurements to access the variations of the charge transport across model electrodes, but these low-frequency methods only provide macroscopic interfacial information and overall conductivity measurements.

By using broadband dielectric spectroscopy (BDS) over a wide frequency range from 102 Hz to 1010 Hz, we are able to characterize the influence of the different interfaces on the frequency-dependent charge transfers in two active materials used in the composite positive electrode of electric vehicle grade battery1,2: NMC532 (LiNi0.5Mn0.3Co0.2O$_2$) and NMC811 (LiNi0.8Mn0.1Co0.1O$_2$) using multiple electrode models, both in the dry (ex-situ) and wet states (with electrolyte). The Nyquist fittings of the obtained dielectric permittivity and conductivity data provided a multiscale description of the electronic and ionic transport across the composite electrode and the influence of material variations. The initial results reveal a higher frequency and lower interfacial activation barrier for the nickel-rich electrode NMC811, projecting the material to have a better rate performance.

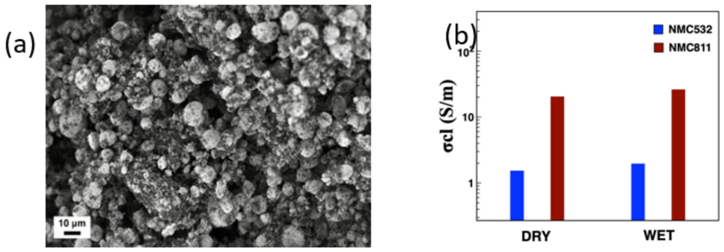
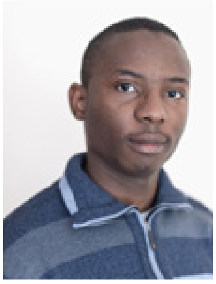


Fig. 1. (a) SEM image of NMC811 electrode mix with 5% carbon black. (b) Cluster conductivity σcl in dry and wet electrodes at room temperature.

1. K.-A. Seid, J.-C. Badot, C. Perca, O. Dubrunfaut, P. Soudan, D. Guyomard, B. Lestriez, *Adv. Energy Mater.* **2015**, *5*, 1400903.

2. A. Agrawal, O. Dubrunfaut, L. Assaud, S. Franger, B. Lestriez, J. C. Badot, *J. Phys. Chem. C* **2021**, *125*, 17629.

BIOGRAPHY



Julius Akinribido is a first-year PhD Student at the Institut de Chimie Moléculaire et des Matériaux d'Orsay (ICMMO), Université Paris-Saclay. He holds a joint Erasmus international master's degree from Université Paris-Saclay in Chemistry and from the University of Porto in Nanomaterials Science and Technology. He is deeply committed to research and collaborations that will improve the efficiency and accessibility of advanced energy storage systems.

Julius Akinribido's current thesis: "Study and Modelling of Limiting Phenomena in Lithium-ion Batteries Electrodes", is being carried out under the multidisciplinary direction of Prof. Sylvain Franger and Dr Loïc Assaud from ICMMO and Olivier Dubrunfaut and Jean-Claude Badot from the Group of electrical engineering – Paris, CentraleSupélec, and Institut de Recherche de Chimie Paris, Chimie ParisTech-PSL respectively.

ORAL #11

A study of sulfide-based solid electrolytes (SSEs) sensitivity towards humidity: gas evolution quantification and degradation mechanisms investigation

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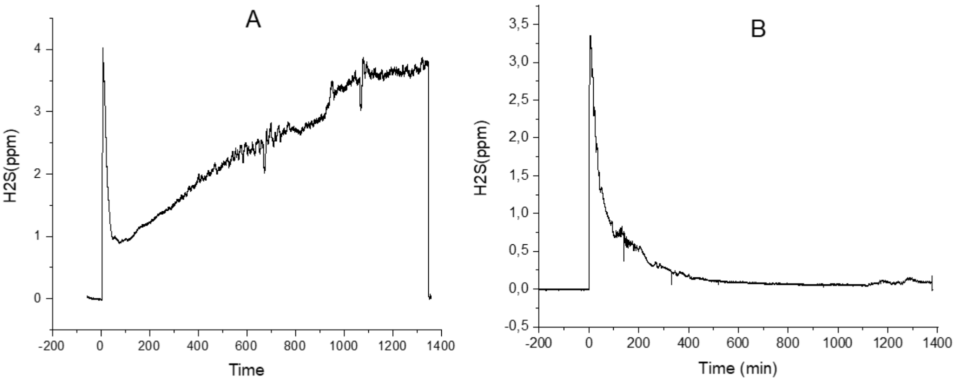
Lithium-ion batteries (LIBs) have been widely used for several energy storage applications (electronic devices, electric vehicles). However, their high flammable organic liquid electrolyte keep them from usage in high energy density batteries. A very promising alternative to LIBs are all-solid-state batteries (ASSBs) containing a sulfide-based solid electrolyte (SSE). SSEs have two main advantages, high ionic conductivity and deformability [1, 2]. However, their main disadvantage is their high sensitivity towards humidity. In fact, SSEs can react with very low concentrations of water (down to a few tens ppm vol.), leading to the destruction of their structure and release of toxic H_2S gas [3].

The aim of the present work is to characterize the reactivity of commercial SSEs (Li6PS5Cl, Li6PS5Br, Li7P3S11, Li3PS4, Li10GeP2S12) towards humidity in realistic dry room conditions. To do so, it is focused on two main aspects:

- Accurate quantification of gases generated by these SSEs when reacting with moisture via a home-made flow-through setup. The developed flow-through setup is more efficient than closed-type setups commonly used and described in literature [3, 4]. Indeed, it avoids overconcentration of detected gases frequently encountered when using closed-type setups;
- Investigation of SSEs degradation mechanisms thanks to characterizations of pristine and humidity-exposed SSEs.

Gas quantification experiments carried out for 22 hours on 1 g of SSE samples exposed to a dry room atmosphere (dew point, d. p. - 40°C) revealed two types of H_2S evolution profiles depending on SE structure (Fig. 1): A peak followed by a growing evolution of H_2S was found forLi7P3S11 and Li3PS4. We assume in this case a surface reaction between SSE and water molecules that result in the formation of a poor passivating layer on SSE particle surfaces. The passivating layer formed is inefficient in preventing humidity diffusion into the bulk of SSE powder, leading to a continuous SSE degradation.

A peak followed by a low plateau of H_2S evolution was found for Li6PS5Cl, Li6PS5Br and Li10GeP2S12. In this case, the passivating layer formed on the surface of SE powders as a product of reaction with traces of water is efficient. It drastically reduces humidity diffusion into SSE powder bulk, generating very low amounts of H_2S after the initial peak (diffusion-dependent plateau on the curve).



REFERENCES :
[1] Energy Storage Mater. 2018, 14, 58–74; [2] Nano Energy 2021, 83, 105858; [3] Solid State Ion. 2011, 182 (1), 116–119; [4] Chem. Mater. 2020, 32 (6), 2664–2672.

Fundamental understanding of concentrated aqueous electrolytes for batteries

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Aqueous electrolytes, studied since the 1990s, are a way to solve the current problems of Li-ion batteries in terms of safety, cost and environmental impact. However, their energy density is limited by the narrow thermodynamic stability window of water (1.23 V). The concept of concentrated aqueous electrolytes has completely changed this vision with the discovery of the so-called water-in-salt electrolyte (WISE), obtained by dissolving a large amount of salt in water. These electrolytes can be depicted as few water molecules surrounded by cations and anions forming ion pairs. This change of solvation structure compared to classical electrolytes (salt solvated by water) increases the stability window. Nevertheless, there is no comprehensive view of concentrated aqueous electrolytes and fundamental questions remain [1]. To what extent is water limiting the stability window, how does the increase in molality affect the organization in solution, or what is its influence on reaction mechanisms are all paths to explore. While these electrolytes pave the way for efficient aqueous Li-ion batteries, Li salts providing a high solubility are few and limited to toxic and costly imides. Aqueous rechargeable magnesium batteries (where Mg is more abundant and inexpensive) are a promising alternative to move towards greener and safer batteries.

Studying these electrolytes by radiolysis provides an accelerated chemical approach to evaluate the influence of water activity and the long-term stability of the electrolyte solutions [2]. The degradation process with radiolysis is much shorter than the electrochemical one and mimics the products of salt and solvent degradation observed during long battery operation [3]. We will show how we are using radiolysis combined with electrochemistry experiments and spectroscopic analyses to study different water-in-salt electrolytes and propose degradation mechanisms. This is essential to get a deeper understanding of the reaction at stake and assess the viability of these electrolyte solutions.

REFERENCES :
[1] D. Aurbach, Z. Lu, A. Schechter, Y. Gofer, H. Gizbar, R. Turgeman, Y. Cohen, M. Moshkovich, E. Levi, Nature, 2000, 407, 724.
[2] D. Ortiz, I. Jiménez Gordon, J.-P. Baltaze, O. Hernandez-Alba, S. Legand, V. Dauvois, G. Si Larbi, U. Schmidhammer, J.-L. Marignier, J.-F. Martin, et al., ChemSusChem, 2015, 8, 3605.
[3] F. Varenne, J. P. Alper, F. Miserque, C. S. Bongu, A. Boulineau, J.-F. Martin, V. Dauvois, A. Demarque, M. Bouhier, F. Boismain, et al., Sustainable Energy Fuels, 2018, 2, 2100.

ORAL #13

Multi-scale study of lithium diffusion in garnet-type solid electrolyte: Neutron powder diffraction and NMR spectroscopy analysis

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Abstract Lithium solid-state batteries are emerging as one of the most promising solution to safety issues and energy density limitations of current lithium-ion batteries. One of the challenges for the development of all-solid-state batteries is to increase the ionic conductivity of solid electrolytes while ensuring good mechanical strength at the interfaces with the electrodes. Indeed, the control and improvement of ionic conduction properties requires precise knowledge of the atomic structure as well as the mechanisms that govern the diffusion of lithium. Lithium-stuffed garnet oxides (doped-$Li_7La_3Zr_2O_{12}$) are promising candidates as solid-state electrolytes. In this talk, we present details of lithium disorder in garnet electrolyte from Rietveld refinement of high-resolution neutron data at room and high temperature. The ionic transport of Li ions was determined by applying an anharmonic Gram–Charlier development of the atomic displacement factors of lithium atoms. Three-dimensional diffusion paths of lithium are observed in garnet crystal structure from neutron data (Figure 1). This result is in good agreement with the calculations obtained by the Bond-Valence Energy Landscape (BVEL) method. To complete the study, the combination of solid-state NMR and electrochemical impedance spectroscopy (EIS) were used to understand the dynamics at several scales.

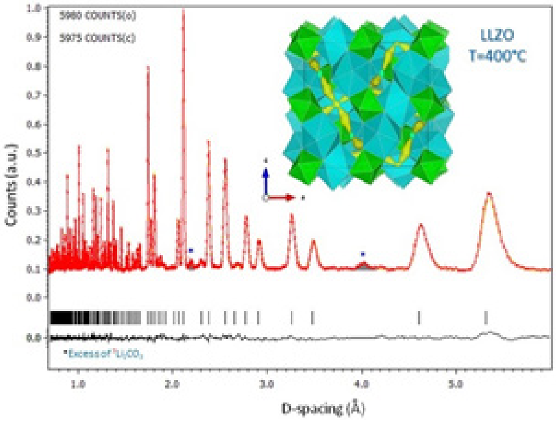

Figure 1: Crystal structure of LLZO at 400°C obtained by Rietveld refinement from neutron data

ORAL #14

Alternative scenario for the energy transition

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The ADEME study on the 2050 French energy transition is a comprehensive source on which we must rely in order to define the strategy to follow (ADEME 2021). Each of the 4 ADEME scenarios contains interesting proposals, but it is scenario 4 that seems to us the most realistic and acceptable for the population as it is not based on a drastic reduction of energy needs. The major difficulty is to find the energy sources that will replace fossil fuels without imposing unpopular laws for the reduction of the needs. The energy mix we propose is slightly different from that of ADEME Scenario 4, which suffers from several drawbacks (Salotti 2022). We recommend priority investment in the photovoltaic / STEP (Station de Transfert d'Energie par Pompage) coupling, especially in cities and isolated villages located on hills or mountains, taking care to preserve our forests and our landscapes as much as possible, with a target to be specified, which could be around 200 TWh per year (ADEME proposes 180 TWh). This idea, which has been neglected for complex political and legal reasons, has been successfully implemented in several places, such as Corsica. As STEP and photovoltaic systems are relative low-tech, affordable and with good recycling rates, they can easily be implemented by many actors in many places, and the subsidiarity principle can be implemented for the decision. Importantly, the laws also have to be changed to allow local investments and ease the decision process to implement the STEP/solar panels solution, eliminating administrative issues and adapting EDF controls and responsibilities. Concerning nuclear energy, we propose to increase its capacity as the ADEME foresees, but this will not be easy and, above all, it will take time, because many power plants are at the end of their life, and the potential sites are not numerous.

As the energy agency clearly explains, a massive development of biomass is expected, in particular through the valorization of waste of all kinds as well as through the production of biogas and biofuels. However, as the production of energy from waste is not profitable, it can only be implemented by taking the French energy sector out of the globalization of trade. For the biomass production, we propose to go even further by developing, in a reasonable way, the bioethanol sector as a fuel for some categories of cars. Compared to ADEME scenario 4, an additional 60 TWh of biomass could be produced. This option is even more appropriate in the context of the war in Ukraine and the drastic reduction of natural gas imports, which reduces electricity production in Europe and makes it difficult to convert all cars to electricity. An important issue is to develop biofuels taking all agricultural surfaces into account, especially the ones dedicated to food production. This problem is tightly linked to the ecological footprint of the French people upon the French territory, and poses the question of demographic limits. It can be noted that in the 3 other ADEME scenarios, an important decrease in energy consumption is expected, even though the trend is stationary and the population is slowly growing, mainly because of a positive migration balance. ADEME did not integrate in its model demographic parameters, but it is clearly a key variable of the problem. These efforts have to be made in conjunction with a strong CCS (carbon capture and storage) strategy at large scales, as suggested in ADEME scenario 4 (ADEME 2021, Salotti 2022).

(ADEME 2021) Transitions 2050, Choisir Maintenant, Agir pour le Climat, ADEME éditions, novembre 2021. Voir également les autres rapports (feuilletons) associés.

(Salotti 2022) J.M. Salotti, "Neutralité Carbone et Stratégie Energétique 2022", Rapport de recherche Auctus_2022_07_10_002, pages 1-17. Available at: https://hal.science/hal-03774530/

ORAL #15

Local narratives and energyscapes. Energy transition seen from the margins of a coal region

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Drawing on methodological and theoretical frameworks from political anthropology and from interdisciplinary approaches to energy transition, from SHS and STS (Sovacool, Baker, Martiskainen & Hook, 2019) we discuss how mechanisms of exclusion and exploitation typical of extractivist production systems are used, contested or replicated in energy transition discourses.

We situate our study on the island of San Pietro, just off the western coast of the Sulcis coal region in Southern Sardinia (Italy). San Pietro’s inhabitants claim to be special in their community’s way of life, language and economic background, with its sailors, trade and tourism. While the island is also currently engaging in a number of initiatives related to renewables, it is geographically and functionally part of the Sulcis. This region has a long history of coal mining, and is still going through a deep economic crisis, albeit with new projects for major infrastructure associated with decarbonization schemes.

Our study shows that, despite the ongoing transition towards renewables, energy discourses used in this area replicate cultural and structural forms of violence that tend to exclude or exploit the local communities (experimentation, financialization, colonization and dispossession). These discourses are resisted and subverted in San Pietro, making room for individuals and their community to embark on a genuine sustainable transition. Drawing on methodological and theoretical frameworks used in political anthropology and social psychology, we argue that an ‘-emic’ approach is needed to interpret situated energyscapes (Appadurai, 1996; Lempinen, 2019) that are culturally rooted, and contribute to the stability of their local systems (they are not just about technological and policy innovations). Moving from these premises, we examine the echo of extractivist and dispossession processes in local discourses and practices, and the ways in which they contribute to community and even family dynamics in a unique spatial setting: a small island on the edge of a CCIR in transition.

Measuring the ecological impacts of digital organisations: Organisational learning and indirect effects

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Instruments used by organisations to measure their ecological impacts, such as life cycle assessments (LCA), suffer from several limits, especially when applied to general purpose technologies (Bresnahan, 2010) such as digital ones. Indeed, the ecological impacts of digital technologies occur at different levels (direct, indirect, structural), can be both negative and positive (Hilty, 2008) and offset each other, especially in the presence of rebound effects (Gossart, 2015). We argue that a more reliable account of these impacts implies relying on participatory indicators inspired by post-normal science (Funtowicz & Ravetz, 2018), i.e. constructed with the participation of multiple stakeholders and in an open fashion (e.g. with open crowdsourced data). Such an instrument, developed along the lines of consequential LCAs (Ekvall & Weidema, 2004), would produce results that are much closer to real impacts. But there are many challenges to develop it and diffuse it within organisations, and these instruments are performative and are thus vectors of organisational change (Aggeri & Labatut, 2010). In this paper, we present a framework to analyse such change and answer the following research question: How can we study the organisational changes generated by the adoption of participatory instruments measuring ecological impacts?

Based on a knowledge-based view of organisations (Grant, 1996), we will design a framework to analyse the types of knowledge generated by the introduction of the instrument, as well as where and how has this knowledge been generated (Nonaka & von Krogh, 2009), for example by using the SECI model (Nonaka, 1994). Indeed, knowledge creation occurs in social spaces, communities of practice, epistemic communities, or communities of creation, which provide conversation spaces that promote trust and support the development of norms and values, as well as the sharing of locally anchored codes and conventions (Rutten, 2016).

In order to develop and test the new instrument measuring ecological impacts, an interdisciplinarity approach is required (Klein, 2017, p. 22), which implies blending knowledge coming from management sciences and computer sciences. The contribution of management sciences takes place at several levels: in the construction of the instrument (qualitative methods, knowledge-based approach…), in the analyses of the organisational changes incurred by the introduction of the instrument, and in the analysis of the obstacles to an efficient adoption of the instrument.

Besides the co-construction of an instrument to be used by actors, a foreseen theoretical contribution will derive from a critical assessment of existing organisational learning frameworks. They will be examined in the light of their capacity to analyse a new object of study (the aforementioned instruments that we termed IMIEN -Instruments de mesure des impacts environnementaux) and translate the knowledge related to instruments into new capabilities for the firm. We thus also plan to study the adoption and application of these instruments to different types of actors operating in both real and virtual worlds: digital service providers such as online platforms, telecommunication companies, users of digital products and services, etc. Beyond traditional qualitative methods for organisational studies (interviews, observation…), we intend to use newer methods to analyse the learning dynamics of these actors such as virtual ethnography (Hine, 2000).

REFERENCES :
Aggeri, F., & Labatut, J. (2010). La gestion au prisme de ses instruments : Une analyse généalogique des approches théoriques fondées sur les instruments de gestion. Finance Contrôle Stratégie, 13(3), 5-37.
Bresnahan, T. (2010). General Purpose Technologies. In H. H. Bronwyn & R. Nathan (Éds.), Handbook of the Economics of Innovation: Vol. Volume 2 (p. 761-791). North-Holland. https://doi.org/10.1016/S0169-7218(10)02002-2
Ekvall, T., & Weidema, B. P. (2004). System boundaries and input data in consequential life cycle inventory analysis. The International Journal of Life Cycle Assessment, 9(3), 161-171. https://doi.org/10.1007/BF02994190
Funtowicz, S., & Ravetz, J. (2018). Post-normal science. In Companion to Environmental Studies (Noel Castree, Mike Hulme, James D. Proctor). Routledge.
Gossart, C. (2015). Rebound Effects and ICT: A Review of the Literature. In L. M. Hilty & B. Aebischer (Éds.), ICT Innovations for Sustainability (Vol. 310, p. 435-448). Springer International Publishing. https://doi.org/10.1007/978-3-319-09228-7_26
Grant, R. M. (1996). Toward a knowledge-based theory of the firm. Strategic Management Journal, 17(S2), 109-122. https://doi.org/10.1002/smj.4250171110
Hilty, L. (2008). Information technology and sustainability: Essays on the relationships between information technology and sustainable development. Books on Demand.
Hine, C. (2000). Virtual Ethnography. Sage.
Klein, J. T. (2017). Typologies of Interdisciplinarity: The Boundary Work of Definition. In The Oxford Handbook of Interdisciplinarity (Robert Frodeman, Julie Thompson Klein, Roberto C. S. Pacheco). Oxford University Press.
Nonaka, I. (1994). A Dynamic Theory of Organizational Knowledge Creation. Organization Science, 5(1), 14-37. https://doi.org/10.1287/orsc.5.1.14
Nonaka, I., & von Krogh, G. (2009). Tacit Knowledge and Knowledge Conversion: Controversy and Advancement in Organizational Knowledge Creation Theory. Organization Science, 20(3), 635-652. https://doi.org/10.1287/orsc.1080.0412
Rutten, R. (2016). Beyond proximities: The socio-spatial dynamics of knowledge creation. Progress in Human Geography, 41(2), 159-177.

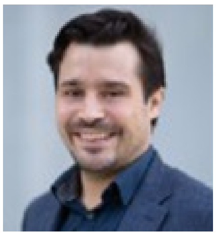
ORAL #16

BIOGRAPHY

David Ekchajzer

David is a PhD student. He works on the evaluation instruments of the environmental impacts of digital technologies (direct, positive, indirect) in an interdisciplinary approach. He explores the reciprocal links between the construction of these instruments and their integration within digital organizations. He conducts his research in an intervention research approach within the company Hubblo - that he co-founded - and the association Boavizta which both produce open tools, methods and data to assess the impacts of digital systems and services.

Benoit Tezenas-du-Montcel



Benoit is Assistant Professor in Strategy at Institut Mines-Télécom Business School since September 2020. He holds a Bachelor in management from the University Paris 1 Panthéon-Sorbonne (2013), a Master in Strategy from University Paris Dauphine (2015) and a PhD in Management from the Conservatoire National des Arts et Métiers (Cnam, 2019). His research focuses on Strategic Management of new technologies and innovation; he specifically investigates 3D printing and technologies of the industry 4.0. He teaches Strategic Management of innovation and technologies.

Cédric Gossart

Cédric is Professor in management sciences at Institut Mines-Télécom Business School. He holds a DPhil in Science and Technology Policy Studies from the University of Sussex (SPRU). His research focuses on digital social innovations, organisational learning, digital technologies and the third sector, and on the links between grand challenges and organisations. He lectures in both French and English on Grand challenges and organisations, Corporate Social Responsibility, and on the links between Digital technologies and sustainable development. He is Deputy director of LITEM, a research unit hosted by Université Paris-Saclay comprising 60 researchers and 22 PhD students, and founding member of the idea lab INESS (Innovations, Numérique, Économie Sociale et Solidaire). He also sits on the editorial board of the open access journal Terminal, and on the board of the nonprofit organisation Teragir.

ORAL #17

Testing the impacts of disaggregated renewable energy sources on economic growth: evidence of spatial spillover effects for developing countries

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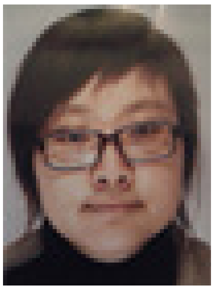
This study attempts to empirically investigate the validity of energy-led growth hypothesis for renewable energy sources for developing countries. To this end, this paper estimates the impacts of disaggregated renewable energy sources on economic growth within a multivariate framework including the disaggregated non-renewable energy sources, capital, labor, institutional quality and human capital by using panel data of 32 lower/upper middle income countries over the period 2009 to 2019 and applying spatial dynamic techniques. To investigate the impacts of renewable energy sources on economic growth, our study applies the multivariate framework for testing a production function. The individual fixed effect is included in the model to control for time-invariant regional characteristics. The time fixed effect is also incorporated into the model to account for time-dependent macro factors. We employ spatial dynamic panel models in order to simultaneously accommodate dynamic adjustments and spatial dependence and thus produce more accurate and reliable estimation results. For estimation methods, System Generalized Method of Moments (GMM) estimator is applied. To explore the existence of spatial autocorrelation in real GDP per capita, we adopt the global Moran's I index which has been widely used in the literature on spatial studies. Our results show the significantly positive impacts of individual renewable sources on economic growth. This study provides the first piece of evidence of spatial spillover effects from renewable energy on economic growth for developing countries. Our analysis reveals the significantly negative impacts of hydroelectricity on economic growth. Our analysis also confirms the importance of labor, institutional quality and human capital in driving economic growth.

Keywords: Renewable Energy, growth, Spatial effects JEL Classification: O13, O47

BIOGRAPHY

Dr. Yan



The research themes relate to energy intensity, household energy consumption, the determinants of CO_2 emissions, air pollution and water pollution, vulnerability to poverty, data econometrics panel, spatial econometrics and microeconometrics.
Dr. Yan defended a doctoral thesis in economics (Aix-Marseille University) in 2013, on "Challenges of China's sustainability: integrating energy, environment and health policies", Huijie Yan was a postdoctoral researcher for the ACE-ICSEN project "Adaptation to Environmental Changes: a multi-scale and transdisciplinary approach" funded by the University of Paris Saclay (CEARC, University of Versailles Saint Quentin-en-Yvelines) from 2018 to 2019 then Postdoctoral researcher for the MOMENTOM project (MOlecules and Materials for the ENergy of TOMorrow) funded by Paris Saclay University (CEARC, University of Versailles Saint Quentin-en-Yvelines). She was also a post-doctoral researcher at Gretha (University of Bordeaux). She is an associate researcher at the Institute of East Asia, Ecole Normale Supérieure de Lyon.

ORAL #17

BIOGRAPHY

Dr. Katia Radja

Dr. Katia Radja holds a PhD in Economics at UVSQ in December 2003 (thesis in microeconomics development: Household Economics: an application to marriage payments in India). In 2002, benefiting from a Research Grant from the Institute of Research for Development (IRD, France), in 2002 she was a visiting researcher at the National Council of Applied Economic Research (NCAER) in New Delhi (India).

Her current research activities deal with sustainable development, particularly in its human, social and ethical dimensions in interaction with environmental and climate issues. The work focuses on the one hand on the economics of well-being and quality of life; on the other hand, on the economic evaluation of the impacts of public policies in the context of environmental and climate change. This theoretical and empirical research concerns different fields of application: consumer microeconomics and ethics, health-environment; models of sustainable agriculture; lifelong work and training; child welfare; ethics - societal responsibility. She is currently participating in several projects in which CEARC is involved: IRS Paris-Saclay ACE-ICSEN Project Adaptation to environmental changes: a multi-scale and transdisciplinary approach (2017-2020), IRS Paris-Saclay MOMENTOM Project Molecules and Materials for the Energy of Tomorrow (2017-2020) and the European IMAGES Project, a comparative study on the resilience of young people (Greenland, France, Spain, Madagascar).

The theoretical framework is based on the resources allocation model and the capabilities approach. The research refers also to the measure issues: applied econometrics and empirical operationalization of capabilities

Dr Patrick Schembri

Dr Patrick Schembri, PhD in Economics (Univ. Paris 1 Panthéon-Sorbonne/Academic Tutor: Prof. Emeritus René Passet) is an Associate Professor in Economics at Versailles University and University of Paris-Saclay. Current member of the Observatory of Versailles Saint-Quentin-en-Yvelines, (CNRS-UVSQ), and research fellow at the Interdisciplinary Research Centre in Cultures Environments Arctic Representations Climate (CEARC-OVSQ). For his doctoral dissertation, he benefited from a Research Grant of Brown University (Providence, MA, USA). He has been a Postdoctoral fellow within the CRITINC European Research Project, making sustainability operational: CRITIcal Natural Capital and the implications of a strong sustainability criterion, funded by the DG XII of the European Commission and coordinated by the School of Politics, International Relations and the Environment, Keele University, U.K. He is member of the GDR AREES « ARctique: Enjeux pour l'Environnement et les Sociétés » (CNRS). Dr. Schembri published several articles and chapters on environmental policy, innovation & green technology transfers, natural capital assessment, indicators for sustainable development and economic modelling of sustainability. His research activities led him to take part in several national and European research programs concerning sustainable agriculture and water quality, greenhouse gas abatement through fiscal policy in the European Union, the economic and social aspects of environmental issues such as consumers lifestyles and pollutant emissions, the application of monetary and non-monetary procedures of economic valuation for managing sustainable development, the role of electricity grid and hydrogen in the energy transition, the modelling of socio-economic scenarios of climate change.

ORAL #18

The impacts of combining incentives on carpooling for commuting in Paris Metropolitan area

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Carpooling is one solution to help reduce the negative externalities of solo driving. Several studies have set out to encourage carpooling through either financial or nonfinancial incentives. However, there is little research on combining financial and nonfinancial incentives to shift commuter behavior from solo driving to carpooling (to work or school). Here, 1502 respondents, including 509 car drivers living in the Paris metropolitan area were surveyed by questionnaire, and econometric modeling was performed using multinomial logit (MNL) and binomial logit models. First, we analyzed the effect of non-financial incentives, such as nudges and trust in others, when carpooling is considered in isolation. Second, we analyzed the effect the combination of nudges with employer subsidies for sustainable mobility on intention to carpool as driver or passenger for the home-to-work (or home-to-school) commute. The results show that nudges are more effective among younger and more educated people as a way to encourage them to carpool more. Applying nudges in isolation appears to be more effective at encouraging carpooling for commuting than combining nudges with employer subsidies for sustainable mobility.

Keywords: Carpooling for commuting, Financial incentive, Non-financial incentive, Nudge, Sustainable mobility, Travel behavior, energy cost sharing

BIOGRAPHY

Mr Fawaz Salihou is a PhD student in economics applied to sustainable mobility. He holds a master's degree in eco-innovation, sustainable mobility and society from the University of Versailles Saint-Quentin-en Yvelines. He does his research at the VEDECOM Institute and is research associate to the Industrial Engineering Laboratory (CentraleSupélec, University of Paris Saclay) and CEARC(OVSQ). His research interests are in the field of sustainable mobility. His work focuses on the forms of economic and non-economic incentives for modal shift towards sustainable mobility solutions.

ORAL #19

Evaluation of industrial hubs designs to enable the infrastructure for a hydrogen market

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Hydrogen from renewable sources has been discussed worldwide as a crucial energy carrier for climate change mitigation. It has multiple possibilities of production routes, as well as many current and potential applications. In many sectors, the use of hydrogen is still frontier technology and/or is not yet fully consolidated, such as transportation and as energy storage for the electric power sector. On the other hand, hydrogen from fossil sources has been used for decades by industrial processes, mainly in petroleum refining (44.0%), ammonia (38.0%), methanol (12.5%) and steel production (5.5%) (IEA, 2021). Thus, the application of renewable hydrogen in these industrial facilities requires minimal adjustments and benefits from the already existing expertise for dealing with safety issues. The objective of this research is to evaluate industrial hubs designs that can be used as hydrogen anchor consumption sites to reduce the cost of infrastructure for the development of hydrogen markets. This subject deals with the dilemma of building a specific, intensive capital and long maturation time infrastructure in order to boost the H_2 demand; or wait for the emergence of a demand that remunerates the high investments in gas pipelines, compressors, processes units, also allowing gains of scale. This research aimed to address this dilemma, by evaluating hydrogen infrastructure designs, while assessing a way to remunerate them through industrial hubs. The methodology involved the development of an optimization model for expanding and operating the hydrogen infrastructure. The developed model can be applied for every location. It addresses the whole hydrogen value chain, from the H_2 production, including steam reform, electrolysis, pyrolysis and gasification, from different resources, up to the H_2 delivery to consumers. The model was developed in GAMS language using Mixed Integer Programming (MIP). Its objective function is to minimize the total cost of hydrogen supply, subject to demand, CO_2 emissions constraints, availability of resources and energy and mass balances of technologies. The objective is to find the optimal (least cost) configuration of the resources, technologies, sizes and location of process units to attend a given hydrogen demand vector. The model has an hourly discretization and includes options of hydrogen storage, electricity storage, grid electricity use, in addition to mixing different complementary resources and production technologies. This helps dealing with seasonal and/or variable resources. The model was applied for a case study in Brazil. Findings emphasize the impacts of inputs in hydrogen cost, such as natural gas prices, CO_2 prices and grid emission factors. They also highlight the importance of an already amortized infrastructure for the economic feasibility of low carbon technologies.

BIOGRAPHY

Gabriela is a PhD candidate at the Energy Planning Program, in Universidade Federal do Rio de Janeiro (COPPE/UFRJ) and is developing part of the studies at IFP School, in France. She holds a bachelor's degree in Chemical Engineering from Universidade Federal Fluminense (UFF) and a master's degree in Energy Planning from COPPE/UFRJ. Gabriela also develops research studies at Cenergia/COPPE/UFRJ in the energy area. Her M. Sc. dissertation theme addressed the production of renewable hydrogen to reduce CO_2 emissions from oil refineries and her main studies are related to: hydrogen, renewable energy, energy transition and GHG mitigation projects. She has also worked in the Chemical Industry, at Braskem and at Infineum (Shell-Exxon joint venture).

From energy technology complexity to socio-technical approach: the bioenergy example

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Energy production chains involve various conversion processes designed and implemented by different scientific and technical communities. These chains are implemented in variable social, political, economic and environmental contexts, conditioning their functioning. The technical structure of these chains and the contexts in which they are developed make them extraordinarily complex and at the crossroads of multiple disciplinary fields. In order to understand the structure of these energy supply chains as precisely as possible, and to organize their sustainable and equitable transition, they must be meticulously described with their complexity.

(1.) First, I will define epistemic complexity and show how complexity can be used to qualify energy supply chains and technological interactions in general (Hooker, 2011). I will argue that complexity is not an obstacle to be reduced but a valuable property of scientific and engineering representations. The concept of “system” is commonly used to represent complex objects without oversimplifying them (Holling, 2001). I am particularly interested in the concept of “socio-technical system” and its derivatives, which I will also describe, showing how it allows us to better understand the complexity and possible transitions of energy production chains (Smith, Stirling, Berkhout, 2005 ; Edomah, et al., 2020), without reducing them to technical structures.

(2.) Then, I wish to apply these conceptual clarifications to the case of bioenergy systems. Bioenergies have multiple forms (solid biofuels, liquid biofuels, biogas, electricity). Their production need to combine multiple technical stages: farming production, biomass management, conversion, network distribution (Ripa, Cadillo-Benalcazar, Gampietro, 2021). All these stages involve multiple interactions with ecological, social, political entities. Accordingly, they give interesting examples to deal with representations of technical complexity. I wish to propose concrete ways to adopt the above-mentioned “socio-technical system” approach to represent bioenergy.

ORAL #21

Use of reversible pump-turbines (RPT) as an alternative to expand "submotorized" hydropower plants (HPP) in Brazilian Electric System - Case Study of Foz do Areia

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The Brazilian Electric System (SEB, in Portuguese acronym) historically has been mostly supplied by hydropower plants (HPP) with large reservoirs, with capacity for long period. Following the global energy transition, a future scenario for SEB indicates a massive entry of Variable Renewable Electricity (VRE) sources, such as wind and solar, in the electric generation matrix of Brazil. The recent legislations hamper the commission of HPP with reservoirs, due to the great environmental impact. Nevertheless, the emerging scenario of SEB, with growing demand levels, reduced storage capacity, higher unpredictability both on the demand and on the generation side, requires the development of mechanisms to maintain the stability and reliability of the electric power grid, as well as providing energy security and flexibility to the system.

Brazil has large expertise in operating and generating energy with hydropower plants, but environmental constraints and expansion restrictions remain as a challenge for these plants. An alternative for this issue is to expand the storage capacity of already existing plants with reversible pump-turbines (RPT). RPT can take advantage of an existing reservoir and an idle transmission capacity by converting an existing HPP to a pump storage plant (PSP).

The modernization of existing Brazilian HPPs, including the possibility of converting existing plants to PSP, allows the expansion of the services' portfolio provided by HPPs, mainly the storage for energy balance, aiming to support VRE expansion and to promote the sustainability of the energy matrix. In Brazil, another important aspect for this application is the possibility of empowering by motorizing unused spots in "submotorized" plants, as it will be discussed in this study.

This study aims to analyze the economic feasibility of implementing RPTs in existing HPPs, especially "submotorized" HPPs, for SEB expansion. The methodology involves an evaluation of economical systemic benefits based on an integrated model for expansion and operation planning of the SEB and it will consider a case study for the Foz do Areia HPP. This study uses the software Plexos, an optimization model, with the solver Gurobi to represent SEB and to simulate its energy dispatch for 2040, considering investment decisions to expand the power system capacity by using a Mixed Integer Program (MIP) solution. The results using the software Plexos show that increasing storage capacity is more economically advantageous for the system than increasing power capacity. Storage capacity adds greater operational flexibility to the SEB, so it is possible to integrate even more low-cost renewable sources. Consequently, the promotion of storage technologies is important to drive the transition towards a net-zero path for energy systems.

BIOGRAPHY

Murilo de Miranda is PhD Candidate in Electrical Engineering (COPPE/UFRJ – Federal University of Rio de Janeiro), M.Sc. in Energy and Environmental Planning (PPE/COPPE/UFRJ) and in Renewable Energies at University of Jaén (UJA - Spain), B.Sc. in Water Resources and Environmental Engineer at Fluminense Federal University (UFF). He has 10 years of professional experience in the energy sector, focusing on research, development and innovation, having already worked with institutions such as Abeeólica, Light, CPFL, State Grid, EDP and Energisa. He is a specialist in technical-economic analysis of infrastructure projects and regulation of network industries. In addition, he works with the development of mathematical models for data analysis and system optimization. Author of books and articles published in Energy and Environment magazines and congresses. Throughout his career, he participated in several extension projects and scientific research groups, always focusing on the themes of integrated energy planning, environmental sustainability, alternative sources of energy production, energy storage technologies, hydrogen production chain, energy efficiency and regulatory analysis in the energy sector.

ORAL #22

Scalability of an Integrated-PEC for high efficiency H_2 production

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Photoelectrochemical (PEC) water splitting is an artificial photosynthetic process in which solar energy is stored in the chemical bonds of a clean and sustainable fuel1 such as H_2.
Our current communication focuses on the scalability of a 3D printed, integrated photoelectrochemical cell (IPEC2) that is the effective combination of a silicon/perovskite tandem solar cell3 and a PEM-type electrolyser4. Then, the fluid circuits, the stainless steel cathode plate, the robustness of the electrical contacts and the sealing have been optimized in order to build an IPEC module. The latter consists of a monoblock where 9 IPECs are electrically independent but connected in series as regards the water circuit.

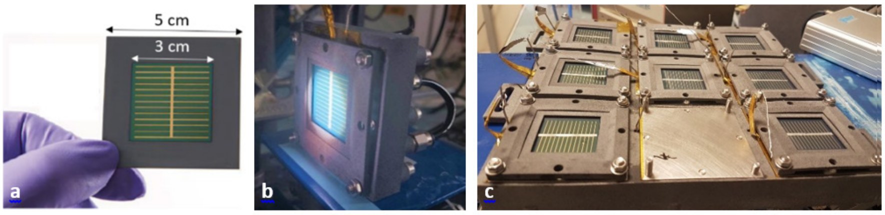

Fig. 1: Scalability of the device. (a) Silicon/perovskite tandem solar cell (b) IPEC (c) Module of 9 IPECs.

The presentation will focus on two key points: the role of electrical, fluidic and thermal integration that has the greatest impact at large scale, and the scientific and statistical analysis of the dispersion of photoelectrochemical results obtained by characterizing a large number of individual IPEC cells and modules.
Long-term experiments confirm the correct functioning of IPEC modules. In comparison to individual IPEC cells, the faradic and solar to H_2 efficiency is maintained. Such measurements also provide information about the stability of the device, which is a requisite for their integration in more complex and innovative systems, where, for instance, H_2 could be used as a clean and sustainable feedstock5 to produce green methane in a circular carbon economy.

1. A. C. Nielander et al., Energy Environ. Sci., 2014, 8, 16–25.
2. S. Tembhurne and S. Haussener, J. Electrochem. Soc., 2016, 163, H988–H998.
3. J. H. Kim, Y. K. Kim and J. S. Lee, Joule, 2019, 3, 2892–2894.
4. G. Chisholm et al., Energy Environ. Sci., 2014, 7, 3026–3032.
5. E. B. Agyekum, C. Nutakor, A. M. Agwa and S. Kamel, Membr., 2022, 12, 173.

ORAL #23

Bandgap tuning of Graphdiyne to promote photogenerated charge separation and Photocatalytic Hydrogen Production

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Solar water splitting into hydrogen is a promising means of dealing with energy shortages and environmental problems. In general, it is difficult to reach higher efficiency without using noble metal during the photocatalytic generation of H_2. In this presentation, a new material was used to tackle this issue and offer a novel carbon-based material for improved charge carriers separation and H_2 generation. H-substituted graphdiyne (H-GDY) is employed to fabricate a heterojunction with TiO_2P25 to improve the interfacial charge transfer and photocatalytic activity. The obtained TiO_2/H-GDY heterojunctions were characterized by XRD, EDX, TEM, XPS and UV-vis spectrums to ascertain the structure and electronic properties of the composites. Enhanced photocatalytic properties were demonstrated for the as-prepared samples. The influence of the H-GDY content on the photocatalytic activity was investigated and all the samples showed enhanced photocatalytic activity. The amount of hydrogen by the optimized heterojunctions was ~370 μmol (6200 μmol h−1 g−1) under UV-visible light and 40 μmol (670 μmol h−1 g−1) under visible excitation after 6 hours, much higher than that of pristine P25. Such enhancement was ascribed to the H-GDY/P25 heterojunction structure, which can simultaneously improve the interfacial charge transfer and injection during the photocatalytic process. This work opens new perspectives for the use of H-GDY in the photocatalytic field.

References:
Jian Li et al., Advanced Functional Materials 31 (29), 2021, 2100994

Jian Li et al., Angewandte Chemie 134 (43), 2022, e202210242

BIOGRAPHY

Ass. Prof. Dr. Ghazzal studied inorganic Chemistry at the Universtité Claude Benard de Lyon, France. He received his Ph.D. in 2008 at the “université Paul Verlaine de Metz”, France. After one year as an assistant professor, he went on a postdoctoral fellowship at the Institute of Condensed Matter and Nanosciences - Université catolique de Louvain”, Belgium. He moved as a researcher at the “Univeristé de Namur” and, then at the “Université de Mons” as a senior researcher in the Laboratory of Surface and Interfacial Physics, Belgium. In France, he obtained a permanent position as an Associate Professor at the Institut de chimie physique, Université Paris-Saclay. His research mainly focuses on elaborating nanostructured nanomaterial using cellulose nanocrystals as biotemplated and exploring different materials based on all-inorganic perovskites or graphdiyne for photocatalytic reactions.

ORAL #24

Highly Porous Iridium Oxides Electrocatalysts for Proton Exchange Membrane Water Electrolyzers

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Proton Exchange Membrane Water Electrolysis (PEMWE) is considered as the most promising technology for rapid and sustainable implementation of H_2 production at large scale. Nevertheless, some challenges still need to be tackled including decreasing the high overpotential towards the oxygen evolution reaction (OER) and the high noble metal loading at the anode.

We have recently extended the green, cheap and scalable aerosol synthesis technique to the preparation of highly porous iridium pure and mixed oxides. Beside beeing highly active towards the OER, the resulting porous structure is ideally suited for the preparation of highly porous catalyst layers.1 We are also taking advantage of the versatility of this process to prepare a large panel of iridium-based oxides with different crystallinity and surface states to provide a better understanding of structure-properties relationship of these highly active electrocatalysts. Indeed, despite extensive studies, the reason of the higher activity of amorphous materials compared to their crystalline counterpart is still the matter of a strong debate. By introducing molybdenum along with iridium into the structure, we are able to decouple the influence of the oxidation state from the structure of the material and provide unambiguous proof of the impact of the interatomic ordering onto the electrochemical activity of iridium based materials towards the OER.2 These findings are supported by a large set of techniques including SEM, XRD, XRF and STEM-EDX as well as surface (XPS) and bulk (XAS) characterizations, including operando XAS.

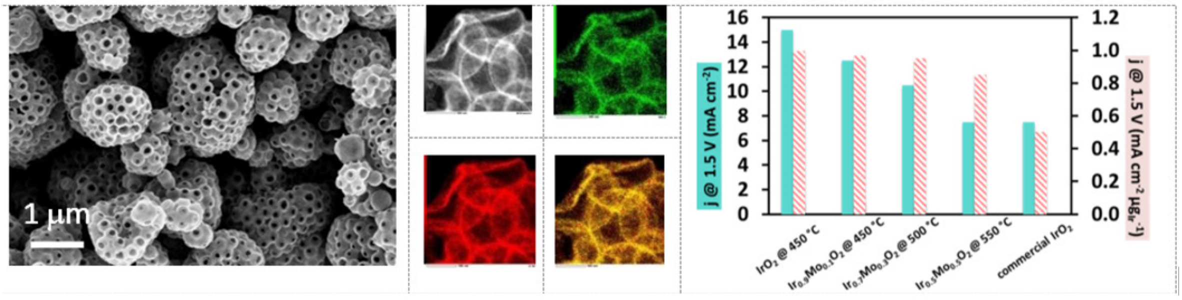

Figure 1: from left to right, SEM and STEM-EDX images of Ir0.7Mo0.3O_2 calcined at 550 °C, and histogram of activity at 1.5 V for different composition of mixed oxide refer to IrO_2

1. Faustini, M. et al., Advanced Energy Materials 2019, 9 (4), 1802136.
2. Elmaalouf, M. et al., Nature Commun. 2021, 12, 3935

ORAL #25

Ruthenium nanocatalysts for electrocatalytic hydrogen evolution reaction

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Replacing fossil fuels by clean energy vectors together with growing energy needs is one of the most challenging issues humanity is currently facing. Production of hydrogen from the catalytic water splitting process is an attractive solution to solve the energy problem. The use of metal nanoparticles (NPs) in electrocatalysis is advantageous in front of massive heterogeneous metal electrodes as the number of superficial active sites per volume of catalyst is increased, still keeping good robustness.[1] The organometallic method proved to be an efficient approach to access well-controlled NPs in terms of size, size dispersion, composition and surface-state.[2] Porous Ru-based nanoparticles synthesized following this method in the presence of an alcohol as the stabilizer provided an highly active electrocatalyst for the hydrogen evolution reaction (HER) in both acidic and neutral conditions.[3] The stabilization of Ru NPs by pyridine-based ligands led to the state-of-the-art electrocatalysts for HER in acidic and basic media.[4] Theoretical modelling of the Ru NPs by DFT, showed that the exchange current density obtained experimentally is related to the calculated Gibbs adsorption free energy of hydrogen atoms at the metal surface and changes in the electrocatalytic activity were found to be related to the capping ligand. Then, the deposition of Ru NPs onto carbon-type supports provided efficient nanomaterials when used as electrodes for HER. [5,6]

References
1- Ruthenium Nanoparticles for Catalytic Water Splitting, J. Creus, J. De Tovar, N. Romero, J. García-Antón, K. Philippot, R. Bofill, X. Sala, ChemSusChem, 2019, 12, 2493-2514.
2- Controlled metal nanostructures: Fertile ground for coordination chemists, C. Amiens, D. Ciuculescu-Pradines, K. Philippot, Coord. Chem. Rev., 2016, 38, 409-432.
3- A Porous Ru Nanomaterial as Efficient Electrocatalyst for the Hydrogen Evolution Reaction in Acidic and Neutral Conditions, S. Drouet, J. Creus, V. Collière, C. Amiens, J. García-Antón, X. Sala, K. Philippot, Chem. Commun., 2017, 53, 11713-11716.
4- Ligand-capped Ru nanoparticles as efficient electrocatalyst for the hydrogen evolution reaction, J. Creus, S. Drouet, S. Suriñach, P. Lecante, V. Collière, R. Poteau, K. Philippot, J. García-Antón, X. Sala, ACS Catalysis, 2018, 8, 11094-11102.
5- Ruthenium nanoparticles supported onto carbon microfibers for hydrogen evolution electrocatalysis, J. Creus, L Mallon, N. Romero, R. Bofill, R. Mas-Ballesté, X. Sala, K. Philippot, J. García-Antón, EurJIC, 2019, 2071-2077.
6- Ru nanoparticles supported on alginate-derived graphene as hybrid electrodes for the hydrogen evolution reaction, L. Mallón, C. Cerezo-Navarrete, N. Romero, M. Puche, J. García-Antón, R. Bofill, K. Philippot, L. M. Martínez-Prieto, X. Sala, New J Chem, 2022, 46, 49-56.

BIOGRAPHY

Dr Karine Philippot received her PhD degree in Molecular Chemistry and Catalysis in 1993 and her habilitation in 2007 from the University Paul Sabatier-Toulouse. She has been a CNRS Researcher at the LCC- Toulouse since 1996 where she has been the head of the group “Engineering of Metal Nanoparticles” since 2008. Her research interests concern the synthesis of metal nanoparticles and composite nanomaterials by using molecular chemistry concepts for their application in catalysis and energy. She is the co-author of ≈180 peer reviewed papers (including 8 reviews, 11 book chapters, 6 patents) and co-editor of 2 books “Nanomaterials in Catalysis” & “Nanoparticles in Catalysis: Advances in Synthesis and Applications” (2013 & 2021, Wiley-VCH).

ORAL #26

Challenge and prospects for the development of renewable Gases in France

Clothilde MARIUSSE, head of renewable gases – West Parisian Area, GRDF

As France's main natural gas distribution system operator, GRDF distributes natural gas to more than 11 million customers every day for heating, cooking, mobility and industrial processes, regardless of their supplier. Performing a public service mission, we build, operate, and maintain the largest gas distribution network in Europe (200,715 km) safely, with the highest standards of quality. We are committed to promoting the use of renewable gas as a crucial part of the energy transition.
We interact with players in the energy sector on a daily basis. First and foremost, we are in close contact with local and regional authorities, the owners of their networks. We also interact with natural gas suppliers who have signed a transmission contract with GRDF.
We are in regular contact with other stakeholders in the energy world, from public organizations to energy opinion leaders, including professional federations and consumer associations.

Under the terms of our public service mission, we guarantee that gas is supplied under the best conditions of quality, safety, performance and cost, and we give all gas suppliers access to the network with complete impartiality. We are also committed to ensuring that the environmental footprint of our installations is as low as possible, whether by reducing greenhouse gas emissions in the atmosphere or promoting technologies that produce renewable, carbon-neutral gas for uses ranging from heating to mobility.
Our aim is to build the gas distribution network of tomorrow :

- Maximizing the use of biomethane for injection into the distribution grid at regional level;
- production of gas through the anaerobic digestion of waste, pyro-gasification of biomass and energy production from micro-algae, representing 240 TWh of green gas by 2050;
- hydrogen produced from renewable electricity surpluses injected into the grid ready for use to supplement biomethane injections.
- Making gas a key driver in the energy transition, the GRDF future scenario will help meet France's commitment to divide its greenhouse gas emissions by four by 2050.

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BIOGRAPHY

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ORAL #27

Density Functional Studies on Photocatalytic Methane Coupling over Au/TiO_2

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Light is an ideal alternative energy source and is largely used in combination with semiconductors to drive chemical reactions, one of them being methane coupling. Methane activation by heterogeneous catalysis is of great importance to secure the future supply of energy, fuels, and chemicals for our modern society. Its high C-H bond energy (434 kJ mol-1), absence of functional groups and polarity result in a very low methane chemical reactivity and consequently harsh conditions of methane chemical transformations. High temperatures and high pressures at which industrial processes of direct conversion of methane into fuels and platform molecules are carried force researchers to look for new, alternative reaction paths and catalytic materials.
The experimental studies show that Au-TiO_2 catalyst under UV/VIS light irradiation is selective in the oxidative coupling of methane to ethane [1]. To understand the observed reactivity, we performed quantum-chemical calculations in the frame of Density Functional Theory (DFT) and Time-Dependent DFT (TD-DFT) with the B3LYP functional and the 6-31g(d p) basis set. The geometry and electronic structure of the catalytic system was characterized by computing selected bond lengths, Mayer bond indices, and the DOS plots. Then, methane interaction with Au6/TiO_2 (and the isolated Aun and TiO_2 fragments) was considered to find the most probable active site for the reaction. The C-H bond activation of methane requires 146 kJ/mol when occurring at the $TiO_2^{\delta+}$ phase. This energy, however, is lowered to 67 kJ/mol when occurring at the gold – titania interface. The reaction mechanism was elucidated and the reactivity under thermal and photocatalytic reaction conditions were compared.

Acknowledgements
This work was supported by the National Science Centre, Poland within Solar-Driven Chemistry project no 2019/01/Y/ST4/00024.

References
[1] Hu, D.; Ordomsky, V. V; Khodakov, A. Y. Appl. Catal. B Environ. 2021, 286, 119913.

BIOGRAPHY

Dorota Rutkowska-Zbik is currently employed as the Associate Professor at the Jerzy Haber Institute of Catalysis and Surface Chemistry, Polish Academy of Sciences (Krakow, Poland) where she leads "Heterogeneous catalysis: theory and experiment" group. She obtained PhD in physical and theoretical chemistry from the Institute of Catalysis and Surface Chemistry, Polish Academy of Sciences (Krakow, Poland) in 2005. After graduation, she held a visiting post-doctoral fellow position at the Theoretical Chemistry Department at the Lund University (Lund, Sweden).
Her research interests cover catalysis, bio-inorganic chemistry, photochemistry, and computational chemistry.

ORAL #28

Selective electrochemical reduction of CO to n-propanol and ethanol by nitride-derived bimetallic catalysts

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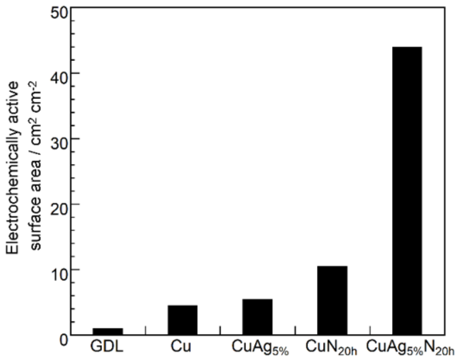
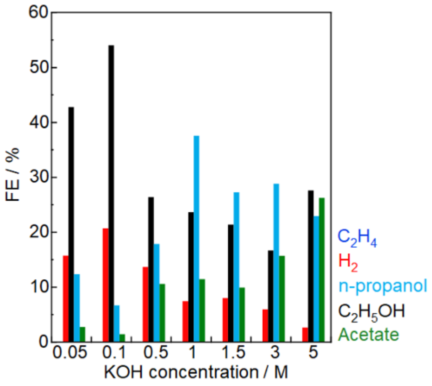
Electrocatalytic reduction of carbon dioxide (CO_2R) is known as one of the promising ways to produce high value chemicals from the greenhouse gas. In CO_2 reduction reaction, CO is the key intermediate for the formation of multi-carbon products, thus CO reduction (COR) is more thermodynamically feasible than CO_2R. Also, to minimize the competing hydrogen evolution reaction, CO_2R usually requires highly alkaline electrolyte, which causes the loss of CO_2 and poisoning effect on the cathode by the formation of carbonate. In contrast, CO does not react with alkaline electrolyte to form carbonate, thus COR to high value products has gained much attention lately (Nat Energy, 2022, 7, 170). In this work, a nitride-derived copper-silver bimetallic (CuAgN) catalyst exhibiting a high FE for COR to n-propanol of 40% at an applied current density of 150 mA cm-2 and 1 M of KOH electrolyte in a flow cell reactor will be presented. The synthetic process contained two consequent steps including a galvanic exchange reaction between copper and AgNO3, and a low temperature nitridation step using $NaNH_2$. Electrochemically active surface area measurement showed that the CuAgN had much larger number of active sites compared to Cu, CuAg and CuN samples (left figure). The content of Ag and the nitridation time were optimized as 5 atomic% in precursor compared to Cu and 20 h, respectively, to achieve the highest FEn-propanol. Regarding reaction conditions, the CO flow was optimized as 10 ml min-1. Interestingly, by varying the concentration of KOH electrolyte, the CuAgN electrocatalyst showed high FE for different C2+ liquid products. At KOH 1 M, CuAgN showed the highest FEn-propanol of 40%, while at KOH 0.1 M, the best value of FEethanol could reach approximately 55%, and at KOH 5 M, FEacetic acid was 25% (right figure). Further mechanistic studies such as DFT calculation and XAS measurements are on-going to clarify the mechanism of the high FE for ethanol and n-propanol of the CuAgN electrocatalyst.





BIOGRAPHY

I am interested in photo(electro)catalysts for production of sustainable energy. Since January 2021, I have been working with Prof. Marc Fontecave and Dr. Ngoc Huan Tran at Collège de France. In collaboration with TotalEnergies, the target of my research is to achieve efficient electrochemical CO and CO_2 reduction systems to produce high-value chemicals such as ethylene, n-propanol which are expected to show industrial scale application in the near future. From 2017 to 2020, I did my master's study under the supervision of Prof. Masato Kakihana and Prof. Hideki Kato at Tohoku University. I focused on a new spray drying synthesis and a surface modification method with two kinds of noble metal to enhance the activity of Rh-doped SrTiO3 photocatalysts for water splitting reaction. This project was aimed at achieving an economical and efficient system to produce hydrogen as a green fuel.

PUBLICATIONS

4. H.P. Duong, N.H. Tran, G. Rousse, S. Zanna, M.W. Schreiber, M. Fontecave, "Highly selective copper-based catalysts for electrochemical conversion of carbon monoxide to ethylene using a gas-fed flow electrolyzer", ACS Catal., 12, 10285-10293 (2022).

3. N.H. Tran, H.P. Duong, G. Rousse, S. Zanna, M.W. Schreiber, M. Fontecave, "Selective ethylene production from CO_2 and CO reduction via engineering membrane electrode assembly with porous dendritic copper oxide", ACS Appl. Mater. Interfaces, 14, 31933-31941 (2022).

2. D.N. Minh, H.P. Duong, L. Hoang, N.D. Phuc, P.D. Tran, P.N. Hong, "Plasma-assisted preparation of MoS2/graphene/MOF hybrid materials and their electrochemical behaviours", Materials Transactions, 61, 1535-1539 (2020).

1. H.P. Duong, T. Mashiyama, M. Kobayashi, A. Iwase, A. Kudo, Y. Asakura, S. Yin, M. Kakihana, H. Kato, "Z-scheme water splitting by microspherical Rh-doped SrTiO3 photocatalysts prepared by a spray drying method", Applied Catalysis B: Environmental, 252, 222-229 (2019).

ORAL #29

Shaping the Electrocatalytic Performance of Metal Complexes for Carbon Dioxide Reduction

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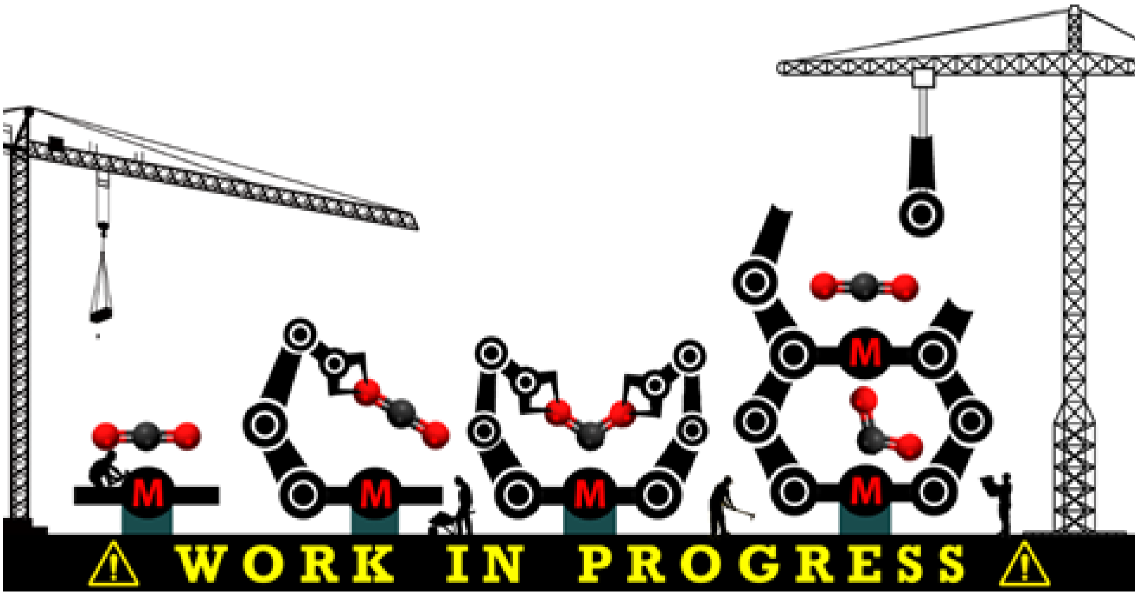
The mass scale catalytic transformation of carbon dioxide (CO_2) into reduced and value-added forms is an imperative to address the ever-increasing anthropogenic emission. Key to this challenge is the development of molecular catalysts for the selective transformation of CO_2. The catalyst design primarily hinges on the elaboration of ligand scaffolds to manipulate the electronic and structural properties for the fine tuning of the reactivity pattern.[1,2] Furthermore, understanding the mechanistic routes leading to the multi-electron-proton conversion of CO_2 provides guiding tools to overcome the kinetically and thermodynamically hard challenges. Herein, we present our efforts in the systematic advancement of the catalytic performance of the iron porphyrin molecular platform. By playing on electronic effects, proton delivery, hydrogen bonding and electrostatic interactions in the second coordination sphere of the catalyst,[3–6] we set forth important design guidelines to control the catalytic overpotential and improve the catalytic rates and product selectivity.



References:
[1] P. Gotico, Z. Halime, A. Aukauloo, Dalton Trans. 2020, 49, 2381–2396.
[2] P. Gotico, W. Leibl, Z. Halime, A. Aukauloo, ChemElectroChem 2021, 8, 3472–3481.
[3] A. Khadhraoui, P. Gotico, B. Boitrel, W. Leibl, Z. Halime, A. Aukauloo, Chem. Commun. 2018, 54, 11630–11633.
[4] P. Gotico, B. Boitrel, R. Guillot, M. Sircoglou, A. Quaranta, Z. Halime, W. Leibl, A. Aukauloo, Angew. Chem. Int. Ed 2019, 58, 4504–4509.
[5] P. Gotico, L. Roupnel, R. Guillot, M. Sircoglou, W. Leibl, Z. Halime, A. Aukauloo, Angew. Chem. Int. Ed 2020, 59, 22451–22455.
[6] A. Khadhraoui, P. Gotico, W. Leibl, Z. Halime, A. Aukauloo, ChemSusChem 2021, 14, 1308–1315.

ORAL #30

Forming multiple C – C bonds upon electrocatalytic reduction of CO_2 by molecular transition metal macrocycles

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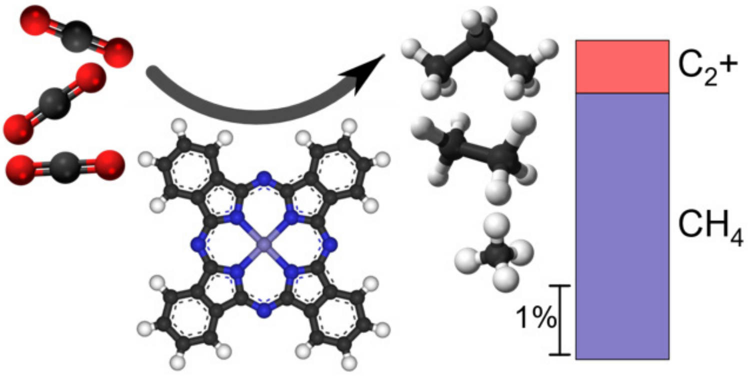
The generation and storage of renewable energy are crucial in combating climate change due to the high accumulation of atmospheric CO_2 by the extensive use of fossil fuels, which is threatening human life on Earth. The electrochemical reduction of CO_2 is a promising solution to produce fuels and chemicals using clean energy, turning CO_2 from a waste product into an economic opportunity. CO and HCOOH are the two most industrially-ready products of CO_2 reduction, while high-value products with C – C bonds, such as C2H4 and C2H5OH, present great potential. Due to the kinetic stability and thermodynamic inertness of CO_2, catalysts are required to lower the activation barrier, enhancing the reaction’s selectivity and efficiency. While copper-based catalysts remain the most popular choice for reducing CO_2 to C2+ products, the complicated nature of their active sites renders establishing detailed reaction mechanisms a challenging task. Molecular catalysts, having well-defined active sites, provide an excellent platform to study the involving catalytic cycles in depth. However, molecular catalysts are mostly limited to generating C1 products,1 with only a few examples where a small amount of C2 products were reported.2 Iron phthalocyanine (FePc), a molecular macrocycle made of Earth-abundant elements, can catalyze not only CO_2 to CO, but also further reduce CO_2 to methane in specific conditions.3 Here, we show the electrochemical reduction of CO_2 to light hydrocarbons, from CH4 to C5 products, using an iron phthalocyanine catalyst in a flowing system under mild conditions. 4 Operando X-ray absorption spectroscopy demonstrated the structural integrity of the catalyst during and after catalysis, as well as provided insights into the electronic structure of the catalyst under operating conditions. Using alternate reactants, we established a preliminary mechanism for the formation of C2+ products on iron phthalocyanine. Our results demonstrate, for the first time, the formation of multiple C – C bonds on a single-site molecular catalyst, which provides valuable insights into the development of catalysts for the CO_2 reduction reaction.

(1) Corbin et al., Nano Res. 2019
(2) Liang et al., ACIE 2022
(3) Li et al., Appl. Catal. B: Environmental 2020
(4) Dong et al., Chem. Sci., 2023



BIOGRAPHY

Mr. Si-Thanh DONG is a PhD student at University Paris Saclay, working with Dr. Benedikt Lassalle-Kaiser in the LUCIA beamline of Synchrotron SOLEIL. His research interests are renewable energy, energy storage, and artificial photosynthesis. In particular, he focuses on developing molecular electrocatalysts for CO_2 reduction. He obtained his Master degree from the SERP+ Erasmus Mundus program, focusing on physical chemistry and materials science. He had a Bachelor degree in Advanced Materials Science and Technology from the University of Science and Technology of Hanoi, Vietnam.

ORAL #31

Microbial electrochemical technologies for taking advantage of the energy and carbon content of organic waste to fuel the bioeconomy sector

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BioElectrochemical Systems (BES) can become a cornerstone technology of environmental biorefineries, where the energy and carbon content of mixed organic waste are converted to platform molecules, thus contributing to the development of the bioeconomy sector. The principle of the technology relies on coupling the oxidation of mixed organic waste in an anodic compartment to the reduction of carbon dioxide in a cathodic compartment (Figure 1)t. This disruptive technology has been matured from TRL1 to TRL4 in the framework of the French BIORARE “Investissement d’Avenir” program (ANR-10-BTBR-02).

The procedures for drawing electrons out of various residual organic feedstock (sludges, biowaste) at high current densities ranging from 7 to 30 A/m2 were established. At the cathode, the possibility of microbial electrosynthesis of multicarbon platform chemicals through CO_2 reduction by a mixed culture consortia was confirmed. Various procedures allowing the operation of BES comprising a bioanode oxidizing waste materials coupled to a cathode synthesizing platform organics were defined and patented. Stable operation of labscale BIORARE TRL3 (Technology Readiness Level) reactors was obtained during several months with good production yields. A several fold decrease in electric power consumption compared to competing technologies was especially documented. A larger and optimized TRL4 reactor was then designed with the help of an engineering company. Consistent performances were again obtained during several months with mixed biowaste as a feedstock.

In addition to the development of the technology, scenarios for the integration of BES into existing waste treatment facilities have been studied, including a scheme where the BES could be coupled to an anaerobic digestion line. Life Cycle Assessment confirmed the environmental benefits potentially associated to this new technology. Market and regulatory studies were also favorable. Even if numerous technological, environmental and socio economical hurdles still need to be overcome, the results of the BIORARE project highlight the great potential of BES to become a technological cornerstone of future environmental biorefineries. The further maturation of the technology to TRL6 is currently underway.

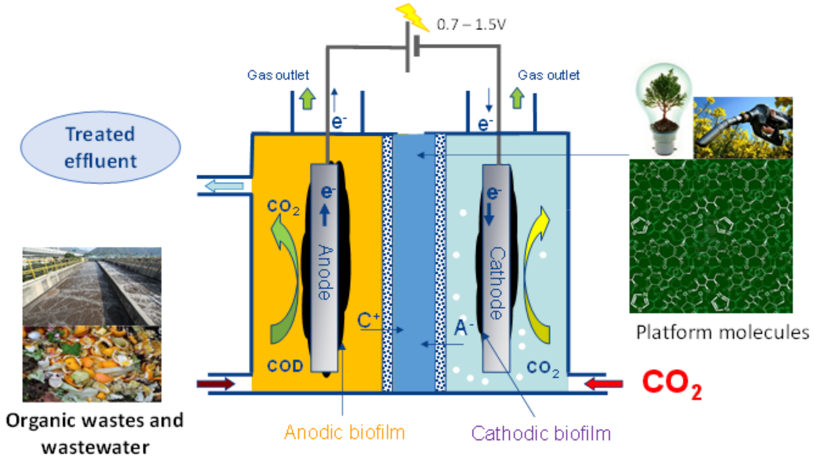

Figure 1: BIORARE technological principle.

ORAL #31

BIOGRAPHY

Currently Director of the INRAE-PROSE research unit in Antony (Procédés biOtechnologiques au Service de l'Environnement, https://www6.jouy.inrae.fr/prose/), Théodore Bouchez's career is at the interface between microbial ecology and bioprocess engineering. He obtained a PhD in 2000 on the study of the bioaugmentation of microbial cultures in activated sludge processes for wastewater treatment. Thereafter, he developed work on the understanding and exploitation of anaerobic microbial consortia for organic waste and wastewater valorization. He set up approaches combining isotopic analysis of material flows (isotopic tracing and fractionation studies) and molecular microbial ecology (Stable Isotope Probing and NanoSIMS) to understand the contribution of non-cultivable microbial groups to material transformation processes in bioprocesses. From the beginning of the 2010s, he then deployed high-throughput metaomic approaches with the aim of acquiring a holistic vision of the functioning of these microbial consortia. Then, particularly struck by the generic character of the energetic determinism of the functional assembly of microbial consortia, he has been working for several years on the development of the theory of the microbial transition state, a conceptual framework aiming to mathematically explain the role of energy in the growth and selection of microbial populations. Furthermore, driven throughout his career by the desire to explore the possible applications of his research, he proposes optimisations and innovations to better integrate environmental biotechnology processes into the bioeconomy. In particular, he coordinated the BIORARE project (AAP Bioressources et biotechnologies 2010) which aims to develop innovative electromicrobial technologies to produce multicarbon organic molecules from waste, using the properties of electroactive microbial communities (https://biorare.inrae.fr/). He is a consulting professor at Agroparistech, invited to give plenary lectures at international conferences (notably at FEMS2017), and is the author of more than 70 publications in international journals and the inventor of 7 patents.

Current research areas
Role of energy in microbial growth and selection of functional microbial assemblies, microbial thermodynamics, microbial transition state theory, mathematical modelling of microbial ecosystem dynamics of bioprocesses. Development of electromicrobial technologies for the bioeconomy, anodic biofilms, cathodic microbial communities, electrotrophic microorganisms, metaomic approaches, microbial electrolysers.
Key words activities: Environmental biotechnologies, microbial ecology, organic waste, anaerobic digestion, electromicrobial technologies, microbial consortia, exploitation of microbial functions, mixed culture bioprocesses, microbial thermodynamics.

ORAL #32

Microalgae for CO_2 capture

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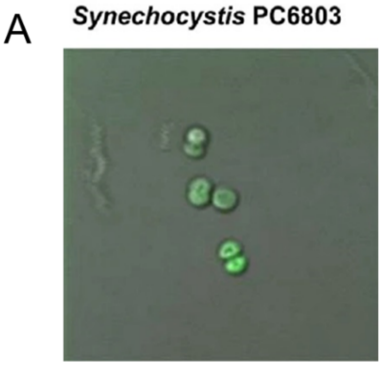
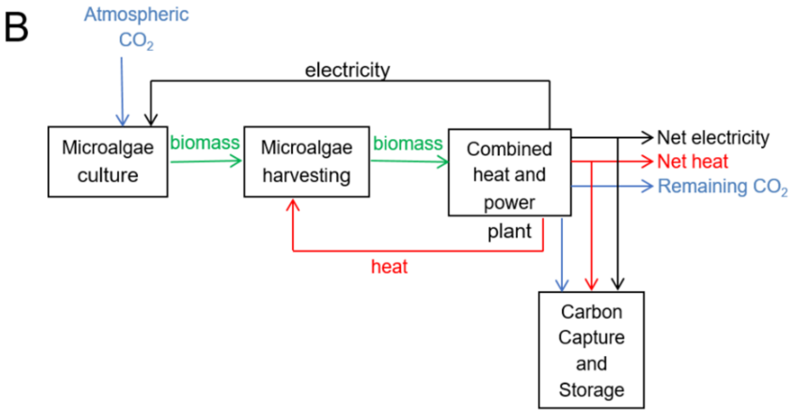
In the context of climate change, in order to reach carbon neutrality, it is necessary, not only to reduce anthropogenic CO_2 emissions, but also to realize “negative emissions” which means removing CO_2 from the atmosphere.
Bioenergy with Carbon Capture and Storage (BECCS) is a negative emissions process in which plants are grown, then fired in a power plant, which produces energy, and the emitted CO_2 is then captured and stored. BECCS is controversial since it requires large amounts of land, water and nutrients.
Microalgae are photosynthetic microorganisms (either prokaryotic or eukaryotic) that are responsible for half of global photosynthesis. The photosynthesis performed by microalgae is more efficient than that for plants, which implies that microalgae capture CO_2 in a more efficient way than plants.
In this work, microalgae instead of plants are considered for performing BECCS. Microalgae-based BECCS (MBECCS) is quantified for the first time, and compared to “classical” BECCS using plants. With the aim of removing 10 Gt per year of CO_2 from the atmosphere using MBECCS only, we show that: the needed area for cultivation is 4-8 times less than with BECCS, marine microalgae should be used, and nutrients remain an issue. We also studied the energy efficiency of the process and show that, depending on the areal productivity, MBECCS can be either energy producing or energy consuming.





Ref: C. Even, D. Hadroug, Y. Boumlaik, G. Simon, Microalgae-based Bioenergy with Carbon Capture and Storage, Energy Nexus 7, 100117 (2022).

BIOGRAPHY

I am an associate professor in physics at Paris-Saclay University.
After a PhD and a dozen years devoted to the physics of “soft matter”, I chose to focus on biophysics. In this field, I worked on three subjects: the first two being respectively on eukaryotic cells (muscle cells) and prokaryotes (bacterial biofilms). My current topic (microalgae) covers both types of cells. I came to this third topic because of my great concern about climate change. I also teach a course on climate physics and climate change at the university.

Development of the Biofuel industry in Europe: interactions with the oil industry and the agricultural supply through a modeling approach

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The development of the biofuel consumption aims to contribute to the reduction of the green gas emissions due to the petrol demand from the transportation sector. The biofuel demand grew rapidly over the last decades and represents around 4% of the Worldwide automotive fuel supply. Thus, biofuels are now the world's first alternative energy to fossil fuels in the transport sector, both globally and in Europe. Mainly used in the road transportation sector, their consumption amounts to about 16 million tons of oil equivalent (Mtoe) at European level. This stands to an incorporation rate of nearly 10% in energy term. As the world's leading agricultural sector, the European Union has historically positioned itself as a major player in the biofuels market. Over the past 20 years, the market has continued to grow, initially with very high growth dynamics and then slowed down by the questioning of the economic and environmental benefits of certain production sectors. Risks of competing uses with food and feed, risk of loss of biodiversity, reduction of limited GHGs.
In this context, the objective of this paper is to assess the potential development of biofuel supply in Europe taking into account the European environmental targets and the spatial distribution of biomass resources, processing units and demand. For this purpose, we use three optimization models which are combined to simulate the biofuel supply in Europe. Composed of three autonomous sectoral economic optimization models, the modelling chain aims to merge modeling tools of both the agricultural sector (AROPAj model, INRAE) and the oil refining sector (OURSE model, IFPEN). The biofuels industry model (GIRAF model) catches information from both agricultural and oil refining to simulate the biofuel supply which reach the demand in volume term and technical specification term.

We combined several scenarios for 2030: scenario with or without Russian oil, a REDII scenario without constraints on the choice of biofuel sectors, a REDII scenario with sustainability criteria binding the choice of biofuel sectors. The main issues from these analyses indicate that the RED sustainability criteria significantly increase the total annual cost of the sector in 2030 through the need to invest in new advanced biofuel production units. The sub-objective of minimum incorporation of advanced biofuels is also necessary to exceed consumption above 2 Mt/year and reach the expected level of 8 Mt/year. The expected production capacities for 2030 based on demonstrators and announcements of industrial projects are not enough to ensure local supply of advanced biofuels, the use of imports is necessary. From a geographical point of view, France appears to be the leading European producer of advanced biofuels in all sectors, and the countries of Eastern Europe are also showing a great deal of involvement in the deployment of the lignocellulosic ethanol sector.

Key words : Biofuel supply, European Environmental policy, optimization models

ORAL #34

Bio-Inspired Bimetallic Cooperativity Through a Hydrogen Bonding Spacer in CO_2 Reduction

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Inspired by the active site of carbon monoxide dehydrogenase (CODH) and its activity toward carbon dioxide (CO_2) reduction,[1] we studied a molecular catalyst implementing a synergistic effect of bimetallic iron center and second coordination sphere hydrogen-bonding interactions from a urea group, Fig. 1. We found that, when immobilized on carbon paper electrode, the dinuclear catalyst can perform the heterogeneous CO_2 reduction to CO in water with four times higher current density, improved selectivity (89 % instead of 72 %) and better stability compared to its mononuclear analogue at the same iron concentration. Interestingly, quasi-identical catalytic performances are obtained when one of the two iron centers is replaced by a catalytically inactive Zn metal, supporting a cooperative action of the two metals. X-ray structures show that the urea group used to link the two metalloporphyrin units is a good compromise between rigidity and flexibility to accommodate CO_2 capture, activation, and reduction.

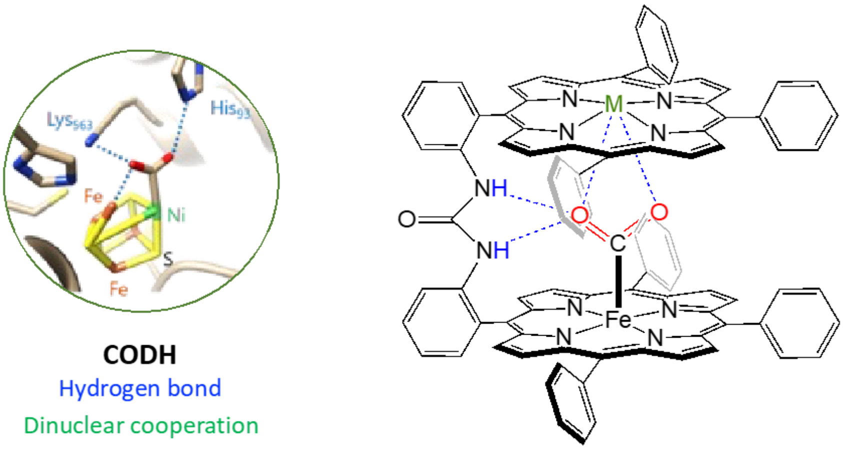

Figure 1: Schematic illustration of bimetallic porphyrins for CO_2 reduction inspired by CODH.

References
[1] J.-H. Jeoung, H. Dobbek, Science. 2007, 318, 1461-1464.

BIOGRAPHY

Chanjuan Zhang has obtained double master degrees of Chemical Engineering between Technical University of Denmark and University of Chinese Academy and Sciences in 2019. After that, she joined the inorganic group at ICMMO, University Pari-Saclay to continue her PhD study under the supervision of Prof. Ally Aukaoloo and Dr. Zakaria Halime. Her topics are focused on the heterogeneous CO_2 electroreduction and hydrogen evolution reaction by molecular catalysts. She is expected to defense in June, 2023.

ORAL #35

Solar to chemical energy conversion – what is the potential of photocatalysis?

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A fundamental difference between photocatalytic oxidation of pollutants and photocatalytic production of solar fuels should be perceived. Similarly to combustion, oxidation of pollutants is an exergonic process, while water splitting or carbon dioxide reduction are endergonic reactions. In energy downhill processes absorbed light is utilized to overcome the activation energy of elemental steps, e.g., activation of oxygen or C-H bond. The role of photons is therefore to “ignite” the energy downhill reaction. Production of hydrogen from water, or methanol from CO_2, are, however, highly endergonic reactions. Photocatalytic production of solar fuels is a process of solar quantum energy conversion to the energy of chemical bonds. In such processes photons can be considered as reagents. This differentiation is crucial to understand a theoretical limit of quantum efficiencies available in these types of processes. In the energy uphill reactions the energy gain (the energy of chemical bonds) originates from the energy of photons. One absorbed photon can generate one e−/h+ pair which can be used in single elemental reduction/oxidation reactions. Therefore, the limit of the overall quantum efficiency, defined as the number of e−/h+ redox steps divided by the number of absorbed photons, amounts 1. In the energy downhill reaction the energy evolved in the process can be dissipated as heat (and lost) or can be used to accelerate next elemental, catalytic steps. Taking this into account one can expect the overall quantum efficiency might exceed the unity. In order to facilitate it appropriate catalytic and redox conditions should be provided.

Solar to hydrogen conversion efficacy (STH) is the major descriptor of photoelectrochemical activity of electrodes in water splitting. The heterojunction architecture has been reported as the key design of enhancing STH, which has presented its own limitations. In this case, the reduced rate of charge transportation at the interface of semiconductors building the heterojunction architecture is the primary constraining factor. To address this issue, we have designed a double-oxide perovskite LaSrFe2−xCoxO6 (x = 0 (LSFF) and 1 (LSFC)). The presence of Sr2+ ions at the A-sites creates charge deficiency, which affects the B-sites and drive part of the iron/cobalt atoms at the B-sites to compensate it for by changing their oxidation number. This phenomenon alters the number of electrons holding by the B-sites, which results in a decrease in the work-function of the Co-containing perovskite, due to the increased ratio of Co4+/Co3+. The density of electronic states (DOS) reveals the presence of different states in LSFC compared to LSFF. Then a heterojunction of nanorod-Fe2O3@rGO@LaSrFe2−xCoxO6 system was constructed. The designed architecture based on nanorod iron oxide (absorber), reduced graphene oxide (hole transfer mediator) and double oxide perovskites (water oxidation catalysts) is a promising approach to efficient, cost-effective and durable PEC systems. In the presentation the role of all components of the system will be discussed. In addition, general differences between hydrogen generation and carbon dioxide reduction will be addressed.

The work was supported by the National Science Centre, Poland (NCN; 2019/01/Y/ST5/00027 and 2018/30/Q/ST5/00776).

BIOGRAPHY

Wojciech Macyk – graduated from the Jagiellonian University in Kraków (Poland), completed his PhD degree at the University of Erlangen-Nürnberg (Germany). In 2009 he completed his habilitation, since 2016 he is a full professor. Since 2013 until 2021 he was the head of the Department of Inorganic Chemistry at Jagiellonian University. Since 2020 he is the dean of the Faculty of Chemistry, JU. In 2014 and 2015 he was a visiting professor at the Catalysis Research Center, Hokkaido University, Sapporo, and at School of Computing, Engineering and Mathematics, Western Sydney University. His research interests include mechanisms of photocatalytic processes, redox properties of photocatalysts, photocatalytic detoxification and disinfection, photocatalytic carbon dioxide fixation, as well as photoelectrochemistry and spectroelectrochemistry of semiconductors. He is the author of >120 papers and book chapters (cited ca. 7100 times, h = 40), several patents and patent applications.

More info: www.photocatalysis.eu

ORAL #36

Sulfur-doped carbon nitride hybrid materials tested under green light for photoelectrocatalytic benzylamine oxidation and oxygen evolution reactions

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High-performing materials will dictate the pace of reinventing industrial chemical processes to achieve carbon neutrality [1]. Visible-light photoelectrocatalysts from abundant resources will play a key role in exploiting solar irradiation [2]. Anionic doping via pre-organization of precursors and further co-polymerization creates tuneable, extrinsic semiconductors. Triazole derivative-purpald, an unexplored precursor with sulfur (S) container, combined in different initial ratios with melamine during one solid-state polycondensation with two thermal steps yields hybrid S-doped carbon nitrides (C3N4). The series of S-doped/C3N4-based materials showed enhanced optical, electronic, structural, textural, and morphological properties and exhibited higher performance in organic benzylamine photooxidation, oxygen evolution, and similar energy storage (capacitor brief investigation) [3]. 50M-50P exhibited the highest photooxidation conversion yield (84±3%) of benzylamine to imine at 535 nm – green light for 48h (Figure 1), due to a discrete shoulder reaching ~700 nm, an unusual high sulfur content, preservation of crystal size, new intraband energy states, deep structural defects by layer distortion, low porosity, and 10-16 nm pores. An in-depth analysis of S doping was investigated coupling x-ray photoelectron spectroscopy, transmission electron microscope, and elemental analysis, providing insights on bonds, distribution, and surface/bulk content. This work contributes to the development of disordered photocatalysts with long-visible-light for solar energy conversion and storage.

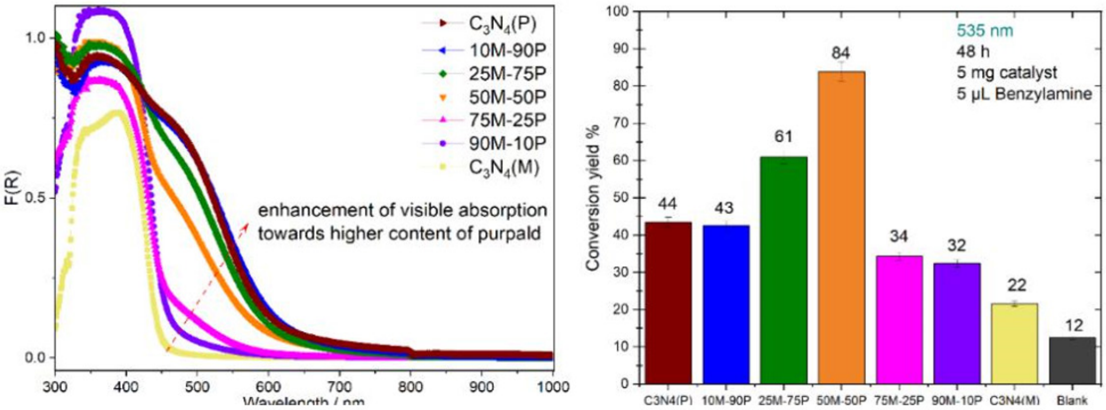

Figure 1. Left) Kubelka-Munk UV-vis spectra. Right) Photooxidation of benzylamine including the reaction conditions.

[1] Mark Isaacs, Julio Garcia-Navarro, Wee-Jun Ong, Pablo Jiménez-Calvo, Global Challenges, 2022, 7, 2200165.
[2] Pablo Jiménez-Calvo, Valérie Caps, Valérie Keller, Renewable and Sustainable Energy Reviews, 2021, 149, 111095
[3] Maria Jerigova, Yevheniia Markushyna, Ivo F. Texeira, Bolortuya Badamdorj, Mark Isaacs, Daniel Cruz, Iver Lauerman, Miguel Ángel Muñoz-Márquez, Nadezda V. Tarakina, Nieves Lopez Salas, Aleksandr Savateev, Pablo Jimenéz-Calvo, ChemRxiv Cambridge Open Engage, 2022

Synthesis and performances of non-noble metal ORR electrocatalysts by ammonia induced CO_2 laser pyrolysis of liquid droplet aerosol

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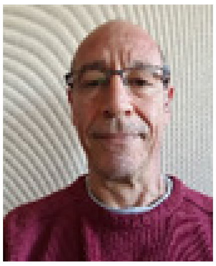
Proton-exchange membrane fuel cells use platinum-based electrocatalysts in particular at the cathode where the sluggish Oxygen Reduction Reaction (ORR) occurs. The long-term development of these devices motivates the research for non-noble metal-based electrocatalysts. The so-called M/C/N electrocatalysts where M is a transition metal (mainly iron or cobalt) are with that respect extensively studied over the world. Different processes are used to produce these electrocatalysts, which involves several steps including ball milling, multiple high temperature thermal treatments under inert or reactive atmosphere [1]. More recently, the use of tailored precursors such as metal organic framework led to performing materials through the formation of so-called single-atom catalysts and reduced synthesis steps [2]. Our laboratory develops an original approach for the synthesis of M/N/C ORR electrocatalysts, which consists in a CO_2 laser pyrolysis of liquid droplet aerosol precursors promoted by ammonia. The latter is used as both, a nitrogen source to incorporate nitrogen in the carbon based catalysts and as an energy transfer agent thanks to its ability to slightly absorbs the CO_2 laser radiation at 10.6 µm wavelength. Our first paper on this topic [3] showed that ORR electrocatalysts with significant ORR activity in acid media is obtainable in a single step and safe-by-design process. Then, a two steps approach consisting in the synthesis of ORR catalysts by CO_2 laser pyrolysis followed by a high temperature treatment under ammonia provided a highly active ORR catalyst with an ORR onset potential of ≈ 930 mV vs SHE [4]. Here, we report on these results and our more recent research aiming at the synthesis of highly active ORR M/C/N catalysts in single step process including two approaches. The first one involves a two-stage ammonia induced pyrolysis [5] in a classical configuration in which the overlap between the CO_2 laser beam and the aerosol (at the first stage) and then the catalyst (at the second stage) is orthogonal. The second original approach consists in a collinear overlap between the laser and the aerosol liquid droplet precursor. This opens new perspectives to our research for the synthesis of M/C/N non-noble electrocatalysts.

[1] L. Osmieri, Chem. Engin. 2019, 3(1), 16; doi.org/10.3390/chemengineering3010016
[2] H. Zhang, S. Hwang, M. Wang, Z. Feng, S. Karakalos, L. Luo, Z. Qiao, X. Xie, C. Wang, D. Su, Y. Shao, G. Wu, J. Am. Chem. Soc. 2017, 139, 14143–14149; doi.org/10.1021/jacs.7b06514
[3] H. Perez, V. Jorda, P. Bonville, J. Vigneron, M. Frégnaux, A. Etcheberry, A. Quinsac, A. Habert, Y. Leconte, C 2018, 4, 43; doi:10.3390/c4030043
[4] H. Perez,V. Jorda, J. Vigneron, M. Frégnaux, A. Etcheberry, A. Quinsac, Y. Leconte, O. Sublemontie,r C 2019, 5, 26; doi:10.3390/c5020026
[5] H. Perez, M. Frégnaux, E. Charon, A. Etcheberry, O. Sublemontier, C 2020, 6, 63; doi:10.3390/c6040063

BIOGRAPHY



Henri Perez obtained a research permanent position at CEA by the end of 1990 and received his Ph.D. in material science from Paris-Sud Orsay University in 1991. After a post-doctoral research at York University (Canada) in 1995, his interests focused on nanomaterials synthesis, and nanoparticle functionalization, especially on platinum. This led to the development of Langmuir-Blodgett nanostructures for bio detection and the study of the Oxygen Reduction Reaction. Further development involved model porous electrodes devoted to the Oxygen Reduction Reaction for proton exchange membranes fuel cells. His current research focus on non-noble metal based catalysts synthesized by laser pyrolysis.

Olivier Sublemontier has been a research engineer at the CEA since 1998. His research activities include the synthesis, characterization and applications of gas-phase nanoparticles. Since 2006, he has been in charge of the silicon nanocrystal synthesis process by laser pyrolysis at Saclay, as well as calculations and experiments on aerodynamic lenses. He has developed the characterization of isolated nanoparticles by X-ray photoelectron spectroscopy (XPS) using aerodynamic lenses. He was coordinator of the HYMALAYAN Project (ANR, 2014-2018) dedicated to the production of nanostructured composite materials by coupling several jets of nanoparticles with physical vapor deposition (PVD).

ORAL #38

Tuning the syngas composition obtained via electrochemical reduction of CO_2 by in situ potential cycling

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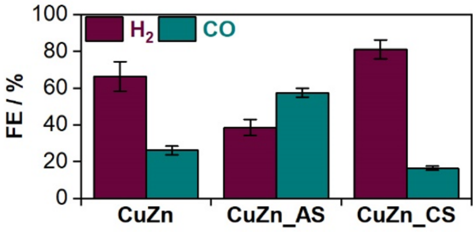
Electrochemical reduction of carbon dioxide ($ERCO_2$) is considered a promising approach for producing value added chemicals, energy storage, and carbon recycling. The $ERCO_2$ is inevitably accompanied by the hydrogen evolution reaction (HER), leading to H_2 production. Thus, among the products that can be obtained from $ERCO_2$, syngas (mixture of CO and H_2) is a very valuable and versatile energy vector. In turn, the H_2/CO ratio is critical for meeting the requirements of downstream processes [1]. Thus, previous works have shown that it is possible to tune the syngas composition obtained via $ERCO_2$. However, this fine-tuning has mainly been achieved by changing the catalyst properties during synthesis stage [2].

The present work proposes a disruptive and straightforward new strategy for tuning the syngas composition. In particular, this work demonstrates that the H_2/CO production ratio obtained using a bimetallic CuZn catalyst can be tuned by applying in situ potential cycling treatments (AS and CS, Fig. 1) immediately before the electrochemical measurements. Thus, for an applied potential of -1.0 VRHE, an H_2/CO ratio value of 2.5, 5, and 0.7 was obtained using the CuZn catalyst. Detailed physicochemical characterization suggests that in situ treatment AS strengthens the CuZn interaction and increases the number of oxygen defects on the catalyst surface, improving the CO_2 binding strength and adsorption capacity, ultimately promoting CO production. On the other hand, in situ treatment CS decreases the number of surface oxygen defects, hindering charge transport phenomena and hampering CO_2 activation, which enhances the H_2 evolution.

The present results open new perspectives for tuning the syngas composition produced via $ERCO_2$ by highlighting the importance of post-synthesis procedures.



Sample	H_2/CO ratio	Potential Application
CuZn	2.5	Methanol: $CO + 2H_2 \rightarrow CH_3OH$
		Fischer-Tropsch: $nCO + (2n+1)H_2 \rightarrow C_nH_{2n+1} + nH_2O$
CuZn_AS	5	Methane: $CO + 3H_2 \rightarrow CH_4 + H_2O$
CuZn_CS	0.7	Hydroformylation: $CO + H_2 + R \rightarrow R'\text{-}CHO$

Fig.1. Faradaic efficiency before (CuZn) and after in situ potential cycling (AS and CS) at 1.0 VRHE. H_2/CO ratio obtained and corresponding possible industrial application.

References
[1] Y. Hua, J. Wang, T. Min, Z. Gao, J. Power Sources 2022, 535, 231453.
[2] Y. Chen, M. Li, Z. Li, F. Liu, G. Song, S. Kawi, Energy Convers. Manag. 2022, 265, 115744.

ORAL #39

Conducting Polymer-Based Heterojunction for Photocatalytic Hydrogen Generation

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Photocatalytic hydrogen production offers a potential avenue for the production of clean and storable energy in the form of hydrogen [1]. Traditionally, Inorganic semiconductors can be used as photocatalysts that facilitate the production of hydrogen and oxygen from water via water splitting and recently conjugated polymer nanostructures (CPNs) has received extensive consideration as potential alternative due to its low-cost synthesis, superior redox chemical properties, and facile functionalization [2-4]. However, the pure CPNs shows unsatisfactory photocatalytic activity due to high binding energy of charge species and the limited separation efficiency of photogenerated charge carriers. Notably, introducing semiconductors or co-catalysts to construct CP–based heterojunction photocatalysts is an effective approach to improve the catalytic activity [5]. The presence of oxides-based semiconductors (ZnO, Cu2O, TiO_2 etc.) in polypyrrole (PPy) nanofibers shows higher catalytic efficiency, charge carrier density, low resistivity and greater photocurrent density compared to bare PPy nanofibers. A p-n junction has been formed between polymer and metal oxide interfaces which further improve the catalytic activity by creating an internal electric field. CP–based heterojunction has great potential as an abundant, cheap, and environmentally benign solar-energy conversion catalyst. The emerging understanding of the photoelectrochemical processes, materials fabrication, mechanisms, as well as challenges may helpful in designing future solar conversion devices.

Keywords: Conducting polymer nanostructures, metal oxides, water splitting, H_2 generation, photoelectrochemical properties

References
[1] Q. Wang, T. Hisatomi, Q. Jia, H. Tokudome, M. Zhong, C. Wang, Z. Pan, T. Takata, M. Nakabayashi, N. Shibata, Y. Li, I. D. Sharp, A. Kudo, T. Yamada and K. Domen, Nat. Mater., 2016, 15, 611–615.
[2] S. Ghosh, K. A. Natalie, L. Ramos, S. Remita, A. Dazzi, A. D. -Besseau, F. Goubard, P.-H. Aubert and H. Remita, Nat. Mater., 2015, 14, 505–511.
[3] S. Ghosh, M. Thandavarayan and R. N. Basu, Nanoscale, 2016, 8, 6921–6947.
[4] S. Sardar, P. Kar, H. Remita, B. Liu, P. Lemmens, S. K. Pal and S. Ghosh, Sci. Rep., 2015, 5, 17313.
[5] S. Ghosh, H. Remita and R. N. Basu, Appl.Catal. B Environmental, 2018, 239, 362–372.

Corrosion of metallic bipolar plates and porous transport layers in proton exchange membrane water electrolyzer anodes

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Proton exchange membrane water electrolysis (PEMWE) is one of the low temperature processes for producing hydrogen at industrial scale. However, the high capital expenditures (capex) due to the use of expensive corrosion-resistant materials limit the economic competitiveness of this technology compared to the well-established fossil fuel-based hydrogen production, like steam reforming, that generates intensive CO_2 emissions. In particular, on the anode side, porous transports layers (PTL) and bipolar plates (BPP), that constitute more than half of the PEMWE stack costs, are currently made of titanium protected by coatings of precious metals in order to withstand the harsh oxidizing and corrosive conditions. The presentation will review the early investigations and the recent developments of BPP and PTL corrosion protection driven by capex reduction, notably the replacement of titanium by stainless steels and the application of novel, more cost-effective anti-corrosion coatings.

Keywords: proton exchange membrane water electrolysis, porous transport layers, bipolar plates, corrosion, coatings.

ORAL #41

Development of a High-Throughput Approach for the Research of Materials for Protonic Ceramic Cells

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The research of efficient and innovative materials for protonic ceramic cells requires the characterization of countless compositions. A high-throughput approach was chosen to initially evaluate the electrochemical performance of hundreds of compositions as electrolyte materials inside the ternary system Ba(Ce,Sn,Zr)0.8Y0.1Yb0.1O3-δ (BCSZYY). The thin film combinatorial library was produced by pulsed laser deposition on top of Si(100) single crystal substrate with a 100 mm diameter (Fig.1A). The composition gradient is obtained through alternate depositions of BaCe0.8Y0.1Yb0.1O3-δ (BCYY), BaSn0.8Y0.1Yb0.1O3-δ (BSYY) and BaZr0.8Y0.1Yb0.1O3-δ (BZYY) centered on the edges of the substrate. The thickness of thin film deposition was characterized by XY-resolved spectroscopic. The deposition centers correspond to the maximum values, i.e., 220 nm for BCYY and BSYY and 200 nm for BZYY (Fig.1B). XY-resolved X-ray diffraction was performed to study the deposition structure. A Matlab code was developed to analyze all the XRD patterns and calculate the cell parameters of the thin film using a pseudocubic structure. The resulting values of the a cell parameters range from 4.176 Å for the BSYY rich part, to 4.251 Å for the BZYY area, up to 4.418 Å for the BCYY one (Fig.1C), in good accordance with the values obtained by Rietveld refinement for reference powders of single materials. A custom-made furnace was developed and calibrated for the compositional and structural analysis in dry and wet conditions at high temperature. This characterization was performed at the Soleil synchrotron through the simultaneous acquisition of XY-resolved XRD and XRF signals. A custom-made setup for electrochemical impedance spectroscopy is under development to measure the electrochemical performance.

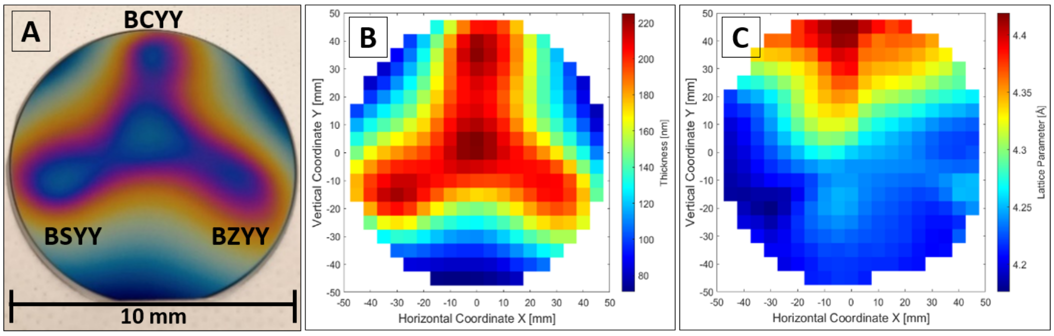

Figure 1. A: Photo of the BCSYY thin film library.
B: Map of the deposition thickness measured with Spectroscopic Ellipsometry.
C: Map of the pseudocubic a cell parameters.

ORAL #42

Hydrogen Storage and Dynamics in Clay Materials

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Hydrogen storage technologies play an important and crucial role in the so-called “hydrogen economy”. However, clay minerals have poorly been studied for this purpose, while they possess valuable properties (stability, low cost, green material) to be exploited in this domain

We have recently studied H_2 adsorption on a synthetic clay, laponite and on gel-laponite, obtained at an intermediate step of the synthesis; nickel ions are inserted into the structure (Fig.1(a)). Obtained X-ray scattering (Fig. 1(b)), the local structure of the gel-laponite sample, noted gel-Ni-laponite, is shown to be similar to that of Ni-laponite, while long-distance order is significantly reduced. The adsorption isotherms (Fig.1(c)) reveal a higher hydrogen sorption for gel-laponite than that for laponite.

Inelastic neutron scattering (INS) is extremely useful at probing locally the direct vicinity of adsorbed molecular H_2. The INS spectrum of a free H_2 molecule is characterized at low temperature by a sharp and well-defined rotational feature at an energy of 14.7 meV corresponding to the transition of H_2 from a para- (molecular spin S = 0, angular momentum J = 0) state to an ortho- (S = 1, J = 1) state. The para-to-ortho transition line J01 has a three-fold degeneracy which is lifted as a function of the local symmetry of the adsorption site, with line-shifts that are dependent on the interaction between the H_2 molecule and the host surface. We will present here the results obtained on gel-Ni-laponite using the spectrometer PANTHER at the ILL. At 41K, well above the solidification temperature of bulk H_2, the J01 peak exhibits a fine structure which can be can fitted by two gaussian lines with an intensity ratio of 2:1 (low energy component: high energy component, fig. 1(d)). The splitting is the one of a 2D rotor (H_2 axis lying parallel to a surface) with an attractive potential wall equal to ~ 27 K. The evolution of the J01 fine structure down to 5K will be discussed.

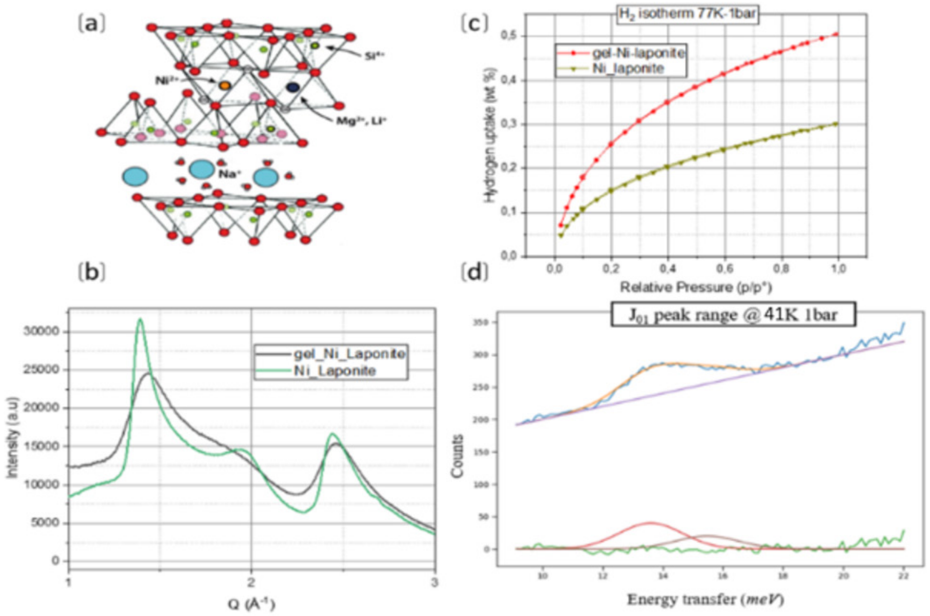

Figure 1. (a) Atomic structure of Ni_Laponite, (b) X-ray scattering of Ni_Laponite & gel_Ni_Laponite, (c) Hydrogen adsorption isotherm, (d) INS spectra in the region of the J_{01} transition (blue: data, orange: fit results, green: difference between data and fit, red & brown: splitted components, violet: slopping background)

ORAL #43

Analysis of Low Temperature Combustion (LTC) process in internal combustion engines

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Low Temperature Combustion (LTC) is a promising process for internal combustion engine (ICE). This combustion mode is based on premixed fuel/air and fuel lean in-cylinder charge. These operating conditions allow low NOx and PM emissions due mostly to the low local combustion temperature, without penalizing the performances. LTC process can be achieved by various modes like: Homogeneous Charge Compression ignition (HCCI), Premixed Charge Compression Ignition (PCCI), Reactivity Controlled Compression Ignition (RCCI), etc. The present study focuses on HCCI process which is one of the advanced low temperature combustion (LTC) concepts. In theory, in the LTC and/or HCCI processes the ignition occurs in perfectly homogeneous conditions without a significant influence of turbulence. However, as shown experimentally, the completely homogeneous charge is not reached and inhomogeneities of temperature and fuel concentration are observed in the combustion chamber. In this case, the turbulence mixing has a large impact on ignition timing, combustion duration and pollutant formation processes. Therefore, the modeling of turbulence mixing and the interaction of turbulence with chemistry constitute a great modeling challenge for new alternative combustion modes for internal combustion engine.

An IEM (Interaction by Exchange with the Mean) model has been used to describe the micromixing. This deterministic model is easy to implement, and gives reliable results with a short computational time. The fluid within the combustion chamber is represented by a certain number of computational particles. The evolution of each particle is determined by the rate of change due to the chemical reaction term and the mixing term. The chemical reaction term has been calculated using a reduced mechanism of n-heptane oxidation with 25 species and 26 elementary chemical reactions developed previously. In this study, the turbulent time scale included in the IEM model is modeled through the turbulent kinetic energy and its dissipation. Hence, a (k-ε) turbulence model based on zero-dimensional energy cascade applied during the compression and the expansion cycle is used. On another hand, the confidence interval introduced in this approach related to the initial heterogeneities amplitude of temperature and species mass has been described as a function of the turbulent Reynolds number.

The in-cylinder pressure predicted by the model was validated against the experimental results. On the optical engine different injection pressures were analyzed. This step points out that they present the same behavior in terms of homogenous combustion. At varying turbulent time scale the comparison has shown an excellent agreement in terms of in-cylinder pressure traces. When the time scale was fixed constant, the ignition delay times were advanced, and the peak pressure was higher. This study points out that the turbulent time scale coefficient must be correctly estimated in order to implement reliable and autonomous models.

BIOGRAPHY

After an engineer and PhD degrees in 1989, Fadila Maroteaux has been a Research Scientist at the M.I.T (USA) at the Sloan Automotive Laboratory for 2 years. She joined the Paris 6 University from 1992 to 2003 as associate Professor and she graduated as Research Director in 2002. From 2003 to 2006 she was a research scientist at INRIA Rocquencourt and since 2007 she is University Professor at the University of Versailles Saint Quentin en Yvelines.

She was responsible for the energetics option from 1995 to 2002 at Paris 6 University. She was the head of chemical engineering department from 2007 to 2011 at IUT of Rambouillet-UVSQ.

Fadila Maroteaux is expert in internal combustion engines. Her research work in the fields of combustion, propulsion and energy has been the subject of numerous articles in peer-reviewed journals. She is member of Society of Automotive Engineers (SAE) USA since 1991. She is member of numerous scientific committees of international conferences.

ORAL #44

Analysis of Low Temperature Combustion (LTC) process in internal combustion engines

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Solar energy can be converted into chemical energy by an appropriate combination of solar cells coupled with efficient catalysts, splitting water into H_2 and O_2. Performance optimization includes matching the voltage and current of the solar cells to the precise requirements of the catalytic reaction, which vary according to the catalysts used, the pH and the electrolytes.

In this work, we present the fabrication of bifunctional oxygen evolution catalysts (OEC) and hydrogen evolution catalysts (HEC) based on earth abundant NiMoFe, , materials for electrochemical water splitting, synthesized by physical vapor deposition (PVD). In alkaline water electrolysis, the HER and OEC of MoNi, NiFe, MoFe, and NiMoFe intermetallic compounds supported on different current collectors were investigated and compared. The effect of composition and deposition conditions materials properties was studied using AFM, Raman, XPS, CA and SEM. Our results show that bifunctional bimetallic and trimetallic water splitting catalysts can significantly reduce the overpotential required to drive a 10 mA cm2 current density with nonprecious and commercially available materials. The work also emphasized the importance of a prolonged testing time to ensure the capability of an electrocatalyst. For solar to hydrogen generation, various modules and tandem solar cells, such as CIGS, c-Si, or cSi/Perovskite developed at our institute, were used showing the dependence of solar to hydrogen efficiency on the characteristics of solar cells. The operational stability of the coupled PV–EC system during a week have been assessed.

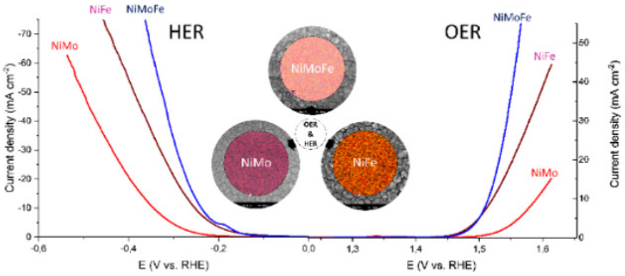

Figure 1: Bifunctionality of bi and tri metallic alloys based on NiMoFe

1 Lee, M.; Turan, B.; Becker, J.-P.; Welter, K.; Klingebiel, B.; Neumann, E.; Sohn, Y. J.; Merdzhanova, T.; Kirchartz, T.; Finger, F.; Rau, U.; Haas, S. arXiv, 2019.

2 Badrnezhad, R.; Nasri, F.; Pourfarzad, H.; Jafari, S. K. Int. J. Hydrog. Energy, 2021, 46, 3821.

BIOGRAPHY

My name is Maria Mendez. I did a joint PhD, between Mexico and France and got a double degree, a PhD in Nanosciences and Materials (IPICYT, Mexico) and a PhD in Chemistry (Université Paris-Saclay, France). During my PhD, I received the Eiffel Excellence Scholarship. I developed new plasmonic active photocatalytic materials for hydrogen production and water treatment under visible light. After my PhD, I continued to work as a postdoctoral researcher at the l'nstitut de Chimie Physique. (ICP, C'Nano IdF) and studied bismuth-based catalysts and obtained promising results for hydrogen production. Interested in the production of green solar fuel, I joined the MOMETOM project, as a postdoctoral researcher at the Laboratoire de Physique des Interfaces et des Couches Minces (LPICM, Ecole Polytechnique). I worked on the development of photoelectrodes based on silicon nanowires impregnated with NiFe co-catalysts to generate hydrogen under sunlight in a photoelectrochemical cell (PEC). And I am currently working on the development of a solar fuel laboratory at the Institut Photovoltaïque d'Ile de France (IPVF) and on the development of bifunctional catalysts by physical vapor deposition (PVD) for the alkaline water electrolyser (AWE) and coupled to photovoltaics (PV) in a PV-EC system.

ORAL #45

Unveiling the Mechanism of the Photocatalytic Reduction of CO_2 to Formate Promoted by Porphyrinic Zr-Based Metal-Organic Frameworks

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Among the many strategies to mitigate the amount of CO_2 in the atmosphere is the transformation of CO_2 to give more complex synthetic compounds, typically using artificial photosynthesis. In this context, our group targets Zr-based porphyrinic metal-organic frameworks (MOFs) as fully noble-metal free heterogeneous catalysts that are able to photo-catalytically reduce CO_2 to formic acid in acetonitrile/triethanolamine (TEOA) solutions (Figure 1, left).

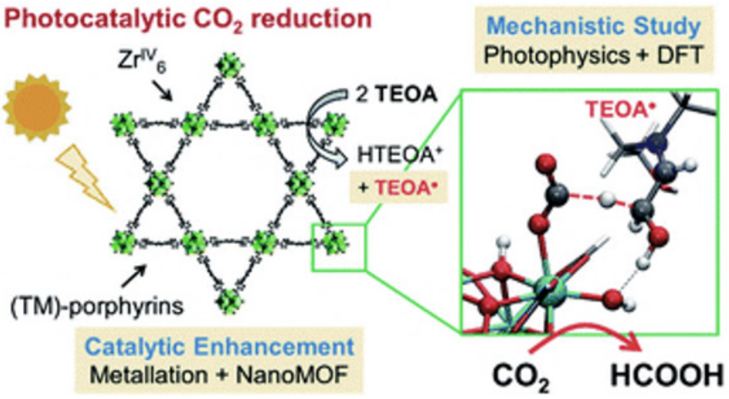

Figure 1: Structure of the (TM)-porphyrin MOFs (left) used in this study with a proposed intermediate determined by the DFT study (right).

In this work,[1] we explored the effect of metalation (MnIII, FeIII, CoII, CuII, ZnII) of the porphyrin linkers in MOF-545(TM) (TM = transition metal) on the CO_2 reduction and production of formate. Of note, we developed a method to synthesize nano-sized MOF-545(Fe) materials (150-200 nm) that yielded one of the highest CO_2RR activities under visible light irradiation reported thus far (6000 µmol.g-1 of formate after 4h) for MOF-based materials. The experimental work was coupled with a thorough DFT study of the mechanism, revealing the respective roles of TEOA, the porphyrin linkers, and the Zr6-nodes. Specifically, this study revealed that TEOA• radicals generated photochemically at the porphyrin linkers play a crucial role in the formal hydride transfer to CO_2 at the ZrIV center (Figure 1, right).

References
[1] Y. Benseghir, A. Solé-Daura, D. R. Cairnie, A. L. Robinson, M. Duguet, P. Mialane, P. Gairola, M. Gomez-Mingot, M. Fontecave, D. Iovan, B. Bonnett, A. J. Morris, A. Dolbecq, and C. Mellot-Draznieks, J. Mater. Chem. A., 2022, 10, 18103-18115.

ORAL #46

Synthesis of p-Silicon/AgxCu100-x photocathodes applied to light-assisted CO_2 reduction

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Reducing anthropogenic CO_2 emissions is a major scientific and socio-political challenge. Among the different ways of transforming CO_2, the photoelectrochemical reduction (PEC-CO_2RR) using semiconductors can be considered a pragmatic solution since it addresses simultaneously the problems of CO_2 emissions and solar energy storage [1].

In the present work, we report on the synthesis of bimetallic AgxCu100-x nanoparticles (NPs) directly on p-type Silicon (Si) supports (specifically flat Si and Si MicroWires (MWs) arrays) and their application as photocathodes for PEC-CO_2RR. A one-step electroless deposition has been developed, based on Si metal assisted chemical etching [2]. We have selected the bimetallic system AgCu by virtue of its high performance for electrocatalytic CO_2RR [3]. As far as we know this system has not been exploited on the illuminated side of a Si photocathode yet.

With its absorption in the Vis-NIR region and mature processing Si constitutes a photoelectrode material of choice. An extra advantage is the possibility to elaborate well-defined 3D microstructure networks (e.g. SiMWs) that allows: (i) enhanced contact area with the electrolyte vs. flat electrodes, (ii) improved carrier separation and collection and (iii) reduced surface defects vs Si nanostructures [4]. Despite their interest, only one work has dealt with the PEC-CO_2RR on metal decorated SiMWs so far [5].

The synthetized AgxCu100-x/Si photocathodes were characterized by SEM-EDX, XRD, TEM and XPS. A phase-separated Ag/Cu crystalline structure was observed, with a very high dispersion of Ag and Cu atoms. The shape of the bimetallic NPs ranges from spherical to worm-like as the Ag fraction increases. PEC experiments in CO_2-saturated 0.5 M NaHCO3 display photocurrent densities of c.a. 10 and 17 mA/cm2 for flat p-Si/Ag50Cu50 and p-SiMWs/Ag50Cu50, respectively (MP dimensions: 50 x 5 x 60 µm pitch/side/height), with a shift in onset potential of +0.5 V vs n+-Si/Ag50Cu50 (non-photoactive electrode). CH4 and CO are identified as main CO_2 conversion gas products. An important Cu loss is however observed after photoelectrolysis. Current studies are oriented to minimize this problem.

[1] P. Chen et al., Nano Materials Science 2021, 3, 344.
[2] E. Torralba et al, ACS Appl. Mater. Interfaces 2016, 8, 45, 31375
[3] W. J. Dong et al., ACS Appl. Mater. Interfaces 2021, 13, 18905.
[4] E. L. Warren, J. Phys. Chem. C 2014, 118, 747.
[5] N. S. Lewis, ACS Energy Lett. 2020, 5, 2528.

BIOGRAPHY

Encarnación TORRALBA-PEÑALVER – Chargée de Recherche CNRS since Oct. 2017
I have a degree in Chemistry from the University of Murcia in Spain (2008) and a master's degree in advanced chemistry (2009). I obtained my PhD in Electrochemistry in December 2013, with the group Theoretical and Applied Electrochemistry of the University of Murcia, under the direction of Profs. Angela Molina and Carmen Serna. My PhD research was focused on the theoretical modelling and experimental application of charge transfer processes through liquid/liquid interfaces (extraordinary Thesis Prize awarded in 2014). After my PhD I moved to France where I work as a postdoctoral researcher on the subjects of CO_2 photoelectroreduction on Si nanowires using molecular catalysts (Institut de Sciences Chimiques de Rennes, 2014 - 2015, with Bruno Fabre) and on the nano and microstructuring of Si surfaces by metal-assisted chemical etching (Institute de Chimie et des Materiaux Paris-Est, ICMPE, 2015-2017, with Stéphane Bastide). In October 2017, I was recruited as a CNRS researcher at ICMPE. My research here is mainly focused on the development of new photo/cathode materials for the photo-electrochemical reduction of CO_2, a new research line at my institution.

ORAL #47

Diamond semiconductor: its challenging n-type doping

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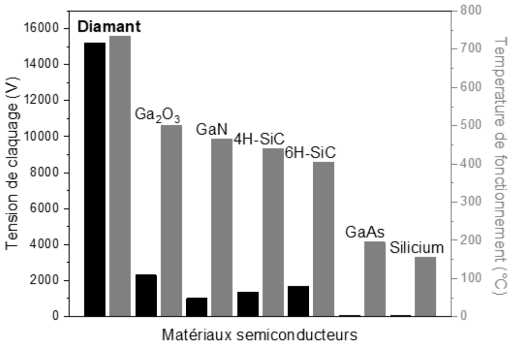
Semiconductors are materials whose electrical conductivity lies between that of a metal and an insulator. To modulate their electrical properties, they must be doped by introducing a small amount of foreign atoms into their crystal structure. The foreign atoms provide charge carriers which carry electric current through the crystal. Semiconductors make up a lot of electrical equipment. The most common electronic component is the diode which allows current to flow in only one direction. It generally consists of a junction between two layers of the same semiconductor, doped in different ways: one p-type, with electron acceptors, and the other n-type, with electron donors.

Power electronics semiconductor components are essential throughout the electrical network. However, due to materials unsuitable for high powers, significant losses of electrical energy occur between each transformation point. To increase the efficiency of electricity production and management, it is necessary to increase the performance of electronic devices. As shown by the comparison of the expected performances of semiconductors (see figure), diamond is the most promising material to fulfill this mission.



Diamond is a rare natural mineral. It was formed under conditions of very high temperatures and pressures (1100 - 1400°C, 4.5 - 6 GPa) in the Earth's mantle after 1 to 3.3 billion years of growth. It is made up of carbon atoms: each carbon atom is surrounded by, and connected to, four other carbon atoms. Since the 1960s, it can be synthesized in a few months at low temperature and pressure (~900°C, 10-5 GPa), thanks to chemical vapor deposition (CVD). Nowadays, the CVD diamond is produced in a reproducible way while controlling its chemical purity. Its p-type doping is easily obtained with the substitution of carbon atoms by boron atoms. But diamond suffers from a doping asymmetry making its n-type doping very difficult.
GEMaC is one of the very few laboratories worldwide that master the n-type doping of CVD diamond. A selection of work from the last 20 years will be presented and will highlight the challenges faced and still to overcome for n-type doping of diamond.

BIOGRAPHY

Dr. Marie-Amandine Pinault-Thaury is a researcher of the French National Center for Scientific Research (CNRS), working at the "Groupe d'Etude de la Matière Condensée" (GEMaC) laboratory. The GEMaC lab is a joint research unit (UMR) between CNRS and the University of Versailles Saint-Quentin-en-Yvelines (UVSQ). It is located in Versailles, close to Paris (France), on the site of the Faculty of Sciences of the UVSQ. Dr. Marie-Amandine Pinault-Thaury co-heads the Semiconductors Axis. She is also in charge of the diamond synthesis and of the ion analysis of materials (through an open facility focused on secondary ion mass spectrometry, SIMS). She is an expert in epitaxy and physical study of semiconductors. Since more than 15 years, she studies diamond, especially its doping and the influence of the impurities/defects on its physical properties. Ten years ago, she has discovered a new growth window allowing the full incorporation of phosphorus in donor sites in (100) oriented diamond. More recently, in 2019, she evidences a breakthrough towards bipolar diamond devices with phosphorus n-type doping on (113) oriented diamond.

ORAL #48

Influence of GaN NW diameter on their piezo-conversion properties: Effect of the surface charges

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The III–N semiconductor nanowires (NWs) are potential candidates for lead-free piezoelectric materials. At nanoscale, the piezoelectric properties of NWs can be significantly enhanced compared to their bulk counterpart due to the existence of novel phenomena, such as the modulation of the free carrier concentration thanks to the surface charge effects which are strongly pronounced in sub-100 nm wide GaN NWs. However, the effect of NW geometry on their piezoelectric properties is still not completely explored due to the difficulties of performing characterizations at this nanoscale.

In this work, we investigate the effect of dimension on the piezoelectric properties of Gallium Nitride (GaN) NWs grown by plasma-assisted molecular beam epitaxy (PA-MBE). By using an atomic force microscopy (AFM) equipped with a home-made modified Resiscope module, we directly measure the piezoelectric conversion capacity (direct piezoelectric effect) of GaN NWs with different diameters ranging from 20 to 100 nm. We establish an increase of the output voltages by decreasing the NW diameter. Especially, by quantifying the electromechanical coupling coefficient of our GaN NWs, we demonstrate a large increase of piezoelectric efficiency from 5.9 up to 43.4% when the NW diameter is lower than 60 nm. This enhancement of the electromechanical coupling coefficient is attributed to the strong influence of the surface charge effects, which for smaller diameters, lead to reduced screening effect of the piezoelectric charges by the free carriers. In consequence, the internal piezoelectric field is enhanced, resulting in an exalted piezoelectric response of the GaN NWs.

These results demonstrate the strong influence of GaN NW dimension on its piezoelectric properties as well as establish new perspective to further improve the GaN NW-based piezoelectric devices.

BIOGRAPHY

Dr. Quang Chieu Bui received his Ph.D. degree in 2022 at Université Grenoble Alpes for his work on developing ZnO nanostructures by Metal-Organic Chemical Vapor Deposition (MOCVD) for piezoelectric applications. From November 2022, he is postdoctoral researcher at Centre de Nanosciences et de Nanotechnologies (C2N) and Laboratoire Génie électrique et électronique de Paris (GeePs). His research activity is focused on investigating the piezoelectric conversion properties of GaN nanowires.

ORAL #49

Micro-device optimization for energy harvesting applications

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With a number of connected objects constantly on rise, the question of their energetic autonomy becomes a key worldwide challenge with strong economic and environmental repercussions. The recent miniaturization of electronic devices, resulting in the reduction of their energy consumption to mW or even µW open today new perspectives to develop autonomous power systems based on the renewable energy harvesting. Energy harvesting, i.e. direct conversion, without any external voltage source, of the ambient energy into usable electrical energy appears as a promising approach to power wireless micro-devices (microsensors, medical implants…). Among the alternative sustainable energy resources, the mechanical deformations and vibrations have the advantages of being ubiquitous, permanently available, and potentially harvested through piezoelectric materials.

These last years, a new generation of nanogenerators, based on materials structured on a nanometer scale has appeared. Due to their specific characteristics, the nanomaterials, when compared with their 2D-film and bulk material counterparts, present higher mechanical properties, flexibility, or electromechanical coupling. These improved properties give undeniable advantages to significantly enhance the transducer conversion efficiency, as demonstrated with nanowire-based piezo-transducers, and generate an output power density reaching up to several µW/cm3 -> mW/cm3.

However, the transducers which are developed are only the active part of the generator ensuring the electromechanical conversion. Complete harvesters, i.e. nanomaterial-based transducers combined with mechanical and electrical module, and integrated to micro-devices, are yet to be developed.

We aim at developing first prototypes of nanomaterial-based piezoelectric generators. Such a goal requires that we optimize the transfer of the environmental input towards the transducer in order to maximize its electromechanical response. This transfer is ensured through a seismic mass encased through various types of nano-beams in a mechanical module which integrates the transducer and processes the frequencies of the input signal in order to extract the maximum of conversion efficiency. We study here the case of a direct integration of the transducer on the vibrating beams which can be bistable pre-buckled beams as previously demonstrated for interdigitated electrostatic combs [1].

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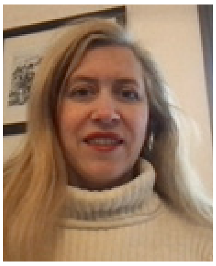
[1] Vysotskyi B., Parrain F., Aubry D., Gaucher P., Le Roux X., Lefeuvre É. Engineering the structural non linearity using multimodal-shaped springs in MEMS, J. of microelectromecha¬nical systems 27(1): 40–46, 2018.

BIOGRAPHY



Ann-Lenaig Hamon is an associate professor working at CentraleSupélec and a member of the newly formed LMPS. Her first research topics were on materials physics and the study of carbonaceous materials (carbon nanotubes, amorphous carbon films, nanocomposites with carbonaceous fillers and a polymer matrix), with the principal use of electron microscopy. She teaches Continuum mechanics, Nanomechanics, or Multiphysics couplings. She is a co-author of “Mécanique pour l’ingénieur”, edited by Dunod (2021).

ORAL #50

Unlocking the photophysics of mesoporous graphitic-carbon nitride (mpg-CN)

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The future application of solar energy depends largely on affordable and efficient solutions for solar-to-chemical energy conversion.[1,2] An interesting method of solar energy storage is through chemical bonds via solar fuels using for example, photo-active semiconductors. These materials utilize photoelectrochemical (PEC) and photocatalytic (PC) processes to produce affordable solar fuels such as ammonia, hydrogen, or methanol. Graphitic carbon nitride (mpg-CN) and their tailored derivatives (through chemical functionalization, and heterojunctions) [3,4] are sustainable, stable, and cost-effective compared to other materials for solar-to-chemical energy conversion. Despite the potentially low costs of these processes; their applicability so far has been limited by their low conversion efficiencies.[5] Thus studying the process dynamics is essential to isolate any reaction bottlenecks and thus improve their efficiencies. The photophysics of mpg-CN under different conditions was studied using transient absorption and time-resolved photoluminescence spectroscopy. These spectroscopic studies revealed the presence of radiative and non-radiative intermediates involved in the photocatalysis at early (100 fs) to intermediate (few ns) timescales. These results in combination with molecular simulations and photocatalytic studies from our collaborators, were used to propose a mechanism for the photoactivation process of mpg-CN.

(1) PNAS 2006, 103 (43), 15729–15735. (2) Chem. Commun. 2018, 54 (50), 6662–6680.
(3) Chem. Mater. 2019, 31 (18), 7478–7486. (4) Materials & Design 2021, 210, 110040.
(5) Nano Futures 2017, 1 (2), 022001.

BIOGRAPHY

Jokotadeola Odutola currently works at Tampere University as a doctoral student on the Solar2Chem Project. Within this project, her role is to determine rates, mechanisms, and efficiencies of charge carriers within photoelectrodes and/or photocatalysts using time resolved laser technologies such as pump-probe spectroscopy and flash photolysis.

On robust optimization, blackouts and the law

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Vehicle-to-grid is the idea of meeting the growing demand of electricity storage, e.g., for frequency regulation with batteries of parked electric vehicles. Frequency regulation providers promise to charge or discharge their batteries whenever the grid frequency deviates from its nominal value. They must honor their promises for all frequency deviation trajectories that satisfy certain properties prescribed by EU law. We encode the law in a robust optimization model and find that the penalties for non-compliance with market rules are currently too low. This suggests that "crime pays".

Topics: Energy storage and conversion

Keywords: Robust Optimization; Vehicle-to-Grid, Frequency Regulation

Predator-Prey model of a technological renewable-based energy transition

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The energy transition is a pathway toward transformation of the global energy sector from fossil-based to zero-carbon technologies, in order to cut energy-related CO_2 emissions to limit climate change. Since provision of energy is one of the main ingredient in the economy, transition scenarios must be assessed by a thorough modelling activity.

We use Lotka-Volterra ecological modelling to study the introduction of a new energy technology, able to mitigate the limits and pollutions of energy provision from natural capital. This well-known dynamical system of differential equations is interpreted in terms of energy investment, related to the notion of Energy Return on (Energy) Invested [EROI], an important question that stays for the moment outside the scope of mainstream economical modelling. Human beings, and their social buildings, are treated as one predator species, preying energy from the stock of natural capital, in the form of wood from a forest, the lowest level prey. A new species is introduced, first acting as a predator when energy must be invested in industry and devices [e.g. solar panels], later working as a prey when energy streams are harvested by the devices and distributed to humans.

We study the case where a traditional agrarian society, initially preying solely on wood, could avoid collapse and reach steady state thanks to the advent of renewables, while preserving natural capital. Depending on system parameters, a stable fixed point exists where natural forests, renewable energy technologies and humans coexist, but a narrow path links it to a previously collapsing situation. The level of human population at the start of the transition is a key parameter, a minimum number of humans (i.e. energy invested in humans) being necessary to trigger a successful transition.

A meta-analysis of the concept of “green jobs” : the search for sustainable development paths in developing countries

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The last decade has been characterized by an accumulation of shocks: economic, pandemic, climate and environmental. This concentration of cumulative crises reinforces the need for a combined response. The issue of employment is central because it cuts across the activity of a country and its people. It is notably through the concept of “green employment” that a possible response to these crises has taken shape. But the literature on Green Jobs, which has been developing rapidly for more than ten years, still lacks consensus. Around this question of the opportunities offered by these jobs, debates on the definition of the concept still persist today. Moreover, developing countries are excluded from the analyses. While this question of “green” is mainly debated in the countries of the North, the context of the countries of the South goes further: it is both the question of “green” and “job” that is being asked. What activity are we talking about? Is it a formal or informal job? Does the notion of employment remain coherent? A major challenge for these territories is to take into account the market/non-market, private/customary, and formal/informal characteristics of activities, even before asking more specific questions such as the “greening” of work tasks.

Based on a database of 416 scientific articles dealing with green jobs, the objective of this paper is to provide answers to two main questions:
1°) On what conceptual pillars is this concept based? Does it relate to an economy in search of market growth or one that is both sustainable and resilient?
2°) Can we speak, and under what conditions, of “Green Jobs” in the context of Southern countries?

Methodology and analysis

The collection of scientific references is based on the PRISMA (Preferred Reporting Items for Systematic Reviews and Meta-Analysis) approach (Moher et al. 2009). This selection work was carried out on Web of Science and SCOPUS using keywords close or similar to “Green Jobs” in the title, abstract or keywords of the articles. After a careful selection, and by merging the two databases Web of Science and SCOPUS (Caputo and Kargina 2022), 416 articles were selected.

Different analyses are carried out, firstly bibliometric approaches such as citation analysis, co-citations, or co-occurrences of keywords to identify the most influential articles, authors and journals; but also thematic clusters behind the use of the concept of “Green Jobs” are identified. For each cluster, we present the most important contributions in the more or less generalized, and/or contextualized, definition of this concept.

Finally, we look at the place of Southern countries in the literature and reflect on how the particular context of these countries can be taken into account in the study of Green Jobs.

ORAL #54

Damping analysis of Floating Offshore Wind Turbine (FOWT): a new control strategy reducing the platform vibrations

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In this work, the coupled dynamics of the floating platform and the wind turbine rotor is analyzed. Firstly, it analyzes the NMPZ related to the system of equations describing the dynamics of a floating offshore wind turbine (FOWT). The equation of the rotor dynamics and the one of the platform dynamics are analyzed in the complex domain to explicit the conditions leading to their respective NMPZs.
The damping analysis is further investigated proposing a new strategy control for Floating Offshore Wind Turbine (FOWT), named ζ_plt-fixed. This strategy is based on a compensation parameter k_β proportional to the platform pitch velocity. It considers the coupling between the rotor dynamics and the floating platform dynamics. The idea behind this control strategy is to activate the blade pitch to damp the platform motions. An explicit expression linking k_β to ζ_plt (damping ratio imposed to the platform) is obtained by deriving a second order filter from the equation of the platform dynamics.
This is different with respect to already existing strategies based on platform pitch compensation which aims at decoupling rotor and platform dynamics [1].
ζ_plt-fixed strategy is tested analytically and numerically by considering an OpenFAST numerical twin of the Umaine IEA15MW FOWT [2] (Figure 1). For a test representative of the DLC1.2, the ζ_plt-fixed strategy allows to reduce the loads at the tower foundation interface for all the considered wind speeds, without significant losses in terms of power production.
The damage analysis shows a remarkable gain in terms of fatigue lifetime (Figure 1). This work highlights the importance of defining proper controller strategies for FOWT to reduce loads on the structure and, it aims at helping the industry to reduce LCOE.

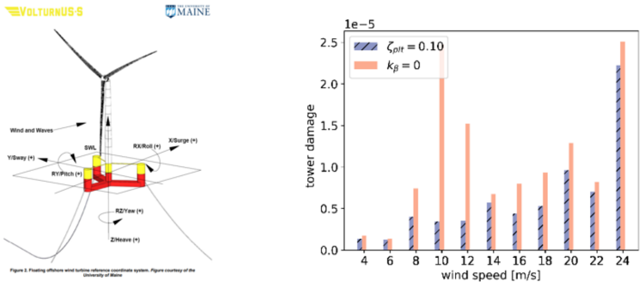

Figure 1 : On left, Umaine IEA15MW Floating Offshore Wind Turbine [2].
New control strategy improvements on fatigue cumulative damage at tower bottom by using rainflow counting and linear Miner's rule

[1] Abbas, N., Zalkind, D., Pao, L. & A., W.: A Reference open-source controller for fixed and floating offshore wind turbines, Wind Energy Science, 7, 53–73, https://doi.org/10.5194/wes-7-53-2022, 2021
[2] Allen, C., Viscelli, A., Dagher, H., Goupee, A., Gaertner, E., Abbas, N., Hall, M. & Barter, G.: Definition of the UMaine VolturnUS-S Reference Platform Developed for the IEA Wind 15-Megawatt Offshore Reference Wind Turbine, Golden, CO: National Renewable Energy Laboratory. NREL/TP-5000-76773.

BIOGRAPHY

Dr. Matteo Capaldo started his education at "Scuola politecnica e delle scienze di base" in Univ. Federico II of Naples, where he studied as Aerospace Engineer.
After a master focus on structure mechanics and fluid-structure interaction, he was awarded of a scholarship for a PhD thesis at Ecole Normale Supérieure de Cachan. He investigated about model order reduction technics for solid mechanics, publishing a hyper-reduction method under the supervision of Prof. Pierre Ladevèze.
Since 2015, he has been involved in industrial and R&D project for offshore and onshore wind energy.
He co-supervised some PhD students on topics such as Digital Image Correlation, Digital Twin for Offshore structures and probabilistic approaches in offshore structural design. During 2020 and 2021 he participated to the Hiperwind European project.
He currently works as research engineer for Wind Energy dealing with wind turbine design, fluid-structure interaction, control and fatigue of structures.
He is also lecture of Wind Power in the Master 2 Sciences and Technology for Energy and assistant lecture of "fatigue of structures" at ENSTA ParisTech, Institut Polytechnique.

INNOVATION SESSION

Airthium, an engine to decarbonize the planet

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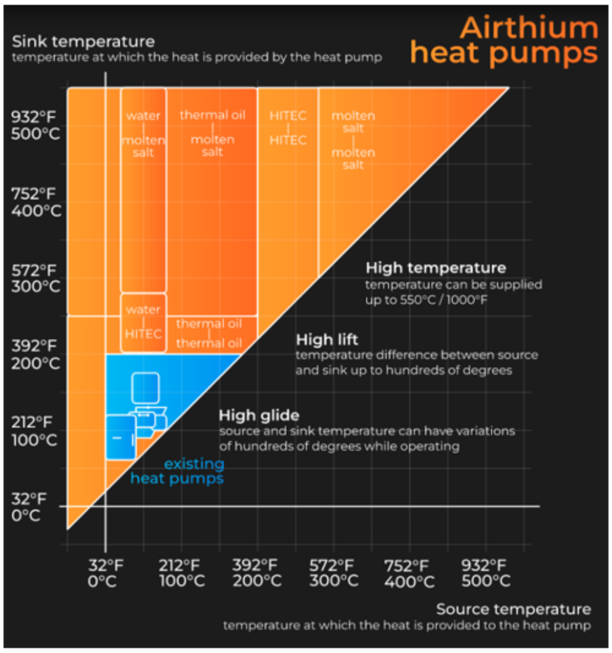
Our mission

We build heat engines that allow the industry and the electrical grid to stop polluting at scale in a cost-effective way.
Our engine is built to replace fossil-fired industrial steam boilers and dryers by a low-cost, fully electric alternative, in the form of high temperature heat pumps.
Long-term, we plan to replace gas-fired peaker power plants, which provide backup power when there is no sun or wind, by a hybrid daily and seasonal renewable energy storage system, powered by the same engine as the heat pumps.
Combined, those two market opportunities can prevent one third of worldwide direct CO_2 emissions, or more than 12 Gt/year. Enough to change the fate of our climate.

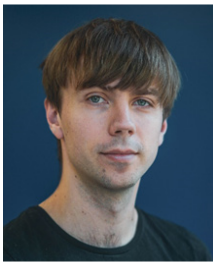
Our Engine

Our heat pump harvests available waste heat at any temperature from 210°F/100°C to 930°F/500°C, or atmospheric heat down to -60°F/-50°C, and runs a near-ideal Stirling-like thermodynamic cycle to upgrade this heat to the desired process temperature.
Our heat pump uses Helium (R704) as the working gas, and various heat transfer fluids depending on the source and sink temperatures. It even works with intermittent processes requiring heat in bursts/duty cycles, or heat at temperatures that strongly vary in time (high glide). Its extremely simple mechanical design allows very low maintenance and downtime.
Depending on the set of temperatures, the Carnot efficiency can reach up to 86%, compared to about 60% for best-in-class high temperature heat pumps today.



2016	2017	2019	2021
Founded	Y Combinator Pre-seed round	Hosted by Air liquide	Seed round $1.3M raised

BIOGRAPHY



Andreï Klochko (X 2007), founder and CEO of Airthium.
Ph. D. Plasma Physics, École Polytechnique.

Innovation across organizational and disciplinary boundaries at Lemon Energy: enhancing industrial energy performance based on data analysis

Ana Rocha
Technical expert at Lemon Energy

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Born in the incubator of CentraleSupelec, a member of FrenchTech Paris-Saclay, Lemon Energy develops innovative solutions for industrial energy efficiency.
Lemon Energy has been recognized as an innovative startup by the French Ministry of Higher Education, Research and Innovation. Our research projects focus on developing digital twins based on Industry 4.0 technologies to improve energy efficiency and rely on predictive analytics for optimizing energy consumption in industrial processes.

Throughout its development as a company, Lemon Energy has benefited from strong relationships with academia. During its early incubation days at CentraleSupelec, Lemon Energy developed projects with the help of students on site through the Industrial Study Convention Program and worked in partnership with CentraleSupelec's Industrial Engineering Laboratory (LGI). Lemon Energy also leveraged the institution's documentation resources to back industrial data analysis and propose efficient solutions.

At the core of the growth and success of Lemon Energy is the use of real-life industrial data collected on the field, that is used to build models and predictions of energy consumption. Lemon Energy takes it to heart to carry out their R&D projects independently from private funding. Projects are therefore financed through regional and state loans as well as the company's own funds. This independence provides a sound ground for academic partnerships. Currently, there are teams working on research activities for a variety of installations, such as chillers, heat pumps, air handling units (with and without humidity control), cleaning in place (CIP) installations, air compressors, boilers, and associated equipment.

The challenge of academic collaboration is two-fold: first, Lemon Energy as a private company works directly on client projects and needs to connect theoretical research with practical benefits for its customers; second, Lemon Energy innovates by bringing together existing models and techniques into a service, across disciplines such as machine learning, thermodynamics, and industrial engineering.

BIOGRAPHY

Ana Rocha is a technical expert in energy efficiency at Lemon Energy. She supervises research activities within the Operations team of engineers and project managers.

She is a chemical engineer with 8 years of experience in process and energy efficiency. Ana has a master's degree on Energy and Environment from IMT Atlantique (ex-Mines Nantes) and Politécnica de Madrid. She also has a master's degree on climate change adaptation from the University of Paris-Saclay.

Low-electricity Hydrogen Production with Methane Pyrolysis Catalyzed by NanoPulsed Plasma

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Today, more than 90% of hydrogen is produced using Steam Methane Reforming, which emits about 11 tons of CO_2 per ton of hydrogen produced [1]. The main clean alternative, water electrolysis, requires a large electricity input 40 kWh/kg H_2. Methane pyrolysis is a third way that is both CO_2-neutral and requires much less electricity.

In methane pyrolysis, methane is directly converted to hydrogen H_2 and unoxidized solid carbon C(s) by-products. In theory, methane pyrolysis requires an energy input of as little as 5 kWh/kg H_2. However, kinetics of the methane pyrolysis reaction are slow.

Therefore, methane pyrolysis today is mostly developed in high temperatures processes such as thermal plasma [2], which induce large heating losses and material constraints. Low-temperature methane pyrolysis approaches using solid catalysts are limited because the solid carbon rapidly deactivates the catalyst [3].
The startup SPARK Cleantech has developed a novel approach using non-thermal PMP, which relies on nanosecond pulses to accelerate the chemical conversion to H_2 and C(s) at lower temperatures. The activation of chemical reactions occurs via electrons that are accelerated by the electric field and collide with neutrals to create radical species that subsequently initiate a chain of chemical reactions.

Today, SPARK has two working low-temperature plasma reactor prototypes and is working on scale-up with a first industrial pilot plant planned for the end of 2023.

[1] Hydrogen strategy : enabling a low-carbon economy, U.S.D.o. Energy, Editor. 2020
[2] Gautier, M. et al, Direct decarbonization of methane by thermal plasma for the production of hydrogen and high value-added carbon black. Int. Jour. Hyd. En., 2017. 42(47): p. 28140-28156
[3] Parkinson, B., et al., Hydrogen production using methane: Techno-economics of decarbonizing fuels and chemicals. Int. Jour. Hyd. En., 2018. 43(5): p. 2540-2555

BIOGRAPHY

Erwan Pannier graduated from Ecole Centrale Paris in 2013. He holds a Ph.D in Plasma Physics from Université Paris Saclay where he worked on CO_2 splitting by non-thermal plasma generated by nanosecond pulses

He co-founded Spark Cleantech in 2021 to work on Hydrogen production and is now the CTO of the company.

SoY PV: the photovoltaic innovation in action

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Photovoltaic conversion of solar energy is becoming one of the pillars of the energy transition. Installed capacity has just crossed the symbolic threshold of one terawatt (TW) and is expected to increase rapidly, particularly in a context where the war in Ukraine is bringing the issue of energy independence to the forefront. The entire value chain of the photovoltaic industry, from research and development to production and distribution, must be ready to face this challenge, given that almost all module production is still imported.

Today, the dominant technology is that of crystalline silicon (95% of the market) in constant evolution. Thin-film technologies (CdTe, CIGS, etc.) account for only about 5% of the market, even though they offer significant development potential in terms of flexibility, lightness and performance, and open the way to new applications not covered by the rigid and heavy solar panels currently on the market. SOYPV’s flexible and high efficiency solar cells can be integrated into a wide variety of supports (canvas, plastic, fabric...), opening up new uses in the building industry, for light roofs or awnings, transport, nomadism, boating, agrivoltaism, events, autonomous objects, dirigibles or stationary balloons... SOYPV is also now involved in the race for very high conversion efficiencies (> 30%) thanks to tandem configurations in thin films (CIGS-perovskite).

Combustion engines, the only viable and scalable means of decarbonizing maritime mobility immediately.

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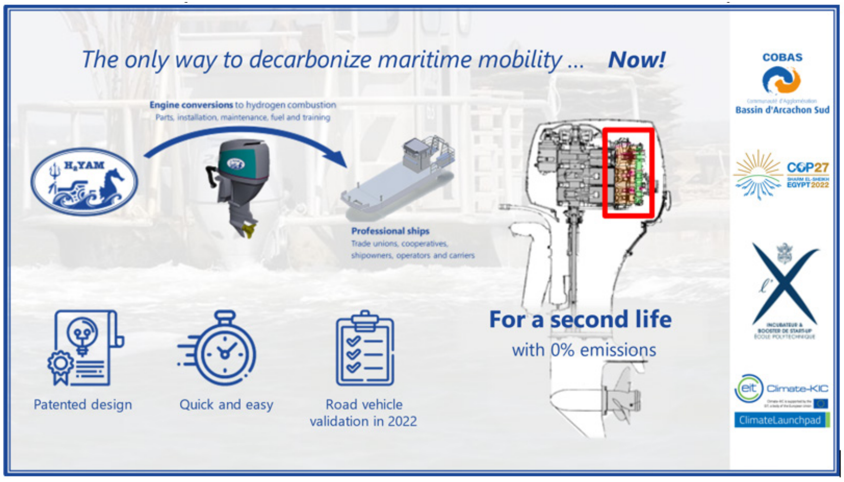
Climate change is accelerating, and all the current indicators suggest society will fail to stay within 1.5°C above pre-industrial levels. According to the Intergovernmental Panel on Climate Change (IPCC), exceeding this limit by any margin substantially amplifies the likelihood of food and water scarcities, conflicts, fatal severe weather events, and other emergencies. This is expected to push the world beyond hazardous thresholds, from which there is no hope for reversal.

Despite the urgent need for action, policy and financing focus heavily on favoring innovative technologies that lack the maturity and economies of scale to enter the market quickly and affordably. This is particularly true for the mobility space with electric solutions powered by lithium batteries or hydrogen fuel cells becoming increasingly prevalent.

At H_2YAM, we subscribe to a tried and tested design principle: Keep It Simple, Stupid (KISS). Across the world, communities are already equipped with the assets, skillsets, and resources needed to decarbonize their mobility operations. Our mission is to demonstrate this fact, limiting the impacts of human activity on the environment and thereby contributing to the protection of marine and river ecosystems.

Based on a patented internal combustion engine design, we are commercializing a simple and quick retrofit procedure to enable marine engines to run on hydrogen or biogas. By replacing a limited number of parts, we enable an immediate, affordable, accessible, and thus smooth transition to a blue and circular economy. Together, let's make maritime mobility sustainable not in 2050, not in 2030, but today.



*The only way to decarbonize maritime mobility … **Now!***

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with 0% emissions

POSTERS

POSTER #1

Acidic Electroreduction of CO_2 to Multi-Carbon Products with Continuous CO_2 Recovery from Carbonate

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Electrochemical CO_2 reduction (CO_2R) can be operated in gas-fed flow cells to enhance conversion at high reaction rates. In addition, a flowing acidic catholyte is an attractive option as it allows regeneration of gaseous CO_2 from the (bi)carbonate that forms close to the electrode from the feed CO_2 due to the locally alkaline pH at the cathode. This avoids massive loss of CO_2 usually encountered under standard neutral/alkaline conditions. However, current systems have solely employed proton exchange membranes with acidic anolyte solutions that require precious-metal anode catalysts. Here, we present an acidic CO_2R electrolyser using a copper catalyst and a bipolar membrane in reverse bias (Figure 1), which enable simultaneous high Faradaic efficiency for C_{2+} products (> 60%), whilst maintaining a constant pH gradient and preventing product and contaminant crossover, when a Ni-foam anode is used in an alkaline anolyte. Through analysis of the gas compositions of the two reactor outlets, we show that the regenerated CO_2 output from the cell is almost product-free under low-flow, high conversion conditions, enabling straightforward recycling of unreacted CO_2.

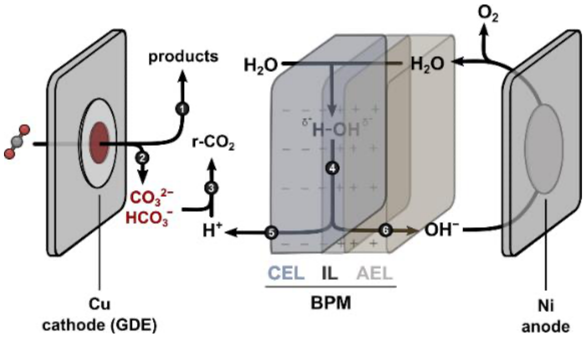

Figure 1: Representation of the electrocatalytic setup.

POSTER #2

Strain and Optoelectronic tuning in Mixed Halide Perovskites with Ion Irradiation

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We are showing how to control in a new way the hybrid perovskite optoelectronic properties with ion irradiation and defect engineering.The role of defects in hybrid perovskite is deeply related to the success of these materials for making solar cell devices. We show here that ion irradiation can be used to modify thin film strain, optoelectronic properties, and phase segregation dynamics [1,2]. We performed proton irradiation at 1 MeV and different fluences in triple-cation mixed halide perovskites. Moderate irradiation allows for improving the lifetime as measured with PL, as a consequence of initial stress release from about 450 ns to 1 μs. In contrast, high irradiation fluence is shown to restore compressive strain leading to sample degradation, with lower lifetimes values (200 ns). Also, the phase segregation occurring under light illumination between bromine-rich and iodine-rich regions is shown to be defects-mediated as the segregation rate increases by a factor of five for high proton irradiation fluence. The irradiation defects are also revealed with low-temperature photoluminescence (PL) through bound exciton radiative recombination mechanisms. This detailed investigation will open new perspectives for optimizing mixed-halide perovskite properties using ion irradiation techniques.

[1] S. K. Gautam, et al., *Reversible Photo-Induced Phase Segregation and Origin of Long Carrier Lifetime in Mixed-Halide Perovskite Films*, Advanced Functional Materials (2020) 2002622.
[2] S. K. Gautam, et al., *Strain and Optoelectronic tuning in Mixed Halide Perovskites with Ion Irradiation*, under submission Advanced Functional Materials (2023).

POSTER #3

Characterization of molecular catalysts by Atomic Force Microscopy combined to Scanning Electrochemical Microscopy for the Hydrogen Evolution Reaction

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Emmanuel Cadot[2], Loïc Assaud[1]
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Nowadays, Energy is considered as a global environmental concern. The increase in the world population, the decrease in fossil fuel and the anthropogenic release of CO_2 have led to the need of the implementation of "clean" energy sources. At this point, hydrogen is considered the most suitable energy vector, if obtained from a renewable source. Among several hydrogen production methods, water electrolysis, namely Proton Exchange Membrane (PEM) technology, is one of the most promising technologies for massive H_2 production from renewables. However, PEM electrolysis faces some limitations due to its high cost because of the use of Platinum Group Metals (PGMs) catalysts. In recent years, our research team developed innovative non-PGM Transition Metal-based molecular complexes for the Hydrogen Evolution Reaction (HER) electrocatalysts as an alternative to Pt [1,2].

The electrochemical activity of these nanomaterials can be locally analyzed using Scanning Electrochemical Microscopy (SECM) (see Figure 1). SECM measurements can be operated in different modes (*e.g.* Feedback Mode, Generation-Collection Mode and Redox Competition Mode) [3]. For HER, Generation-Collection Mode is commonly adopted since the produced H_2 on the substrate can be collected (oxidized) on the tip of the SECM probe. One major update of this characterization technic is the fact that SECM can be combined with Atomic Force Microscopy to reach higher resolution and correlate the topological, the mechanical (using Quantitative nanomechanical microscopy (QNM) mode) properties to the electrocatalytic activities (using SECM mode) [4,5]. In fact, AFM-SECM delivers electrochemical properties using an innovative probe design with nanoscale resolution (*i.e.* 25 nm) whereas classical SECM measures electrochemical properties with an ultramicroelectrode (UME) size ranging from 5 to 25 µm. The AFM-SECM platform as well as preliminary results will be presented.

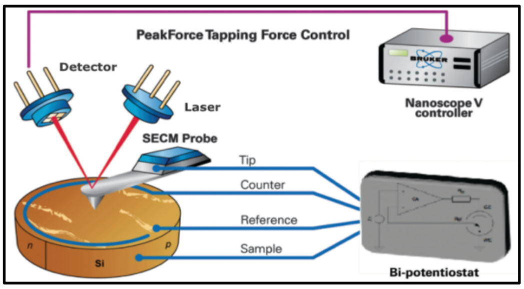

Figure 1: Schematic illustration of a the AFM-SECM platform available at ICMMO [5].

[1] M. Antuch *et al.*, *Electrochim. Acta*, **2017**, 245, 1065.
[2] J. Al Cheikh *et al.*, *Mater. Adv.*, **2020**, 1, 430.
[3] D. Polcari *et al.*, *Chem. Rev.*, **2016**, 116, 13234.
[4] Z. Huang *et al.*, *Micros. Today*, **2016**, 24, 18.
[5] Z. Huang *et al.*, Bruker Application Note 147, **2017**.

POSTER #4

Compositional, structural, and surface Characterization of Titanium doped Imogolite Clay Nanotubes: Implications for Photocatalytic Hydrogen Production

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In the last decades, great attention has been devoted to hydrogen production from water splitting by photocatalysis. Imogolite is a natural clay mineral nanotube that can easily be synthesized under hydrothermal conditions. The fine control of structural properties during the synthesis make these nanotubes potential candidates in many applications including photocatalysis.

In this work, we synthesized for the first time a novel titanium-doped alumino-germanate imogolite nanotubes (Ti@GDWINT) catalysts using a single-step hydrothermal procedure. Microstructures, morphologies, compositions, optical and electrochemical properties of the as-prepared catalysts were characterized by a multiscale approach coupling TEM, FT-IR, SAXS, DRS, XPS, RAMAN, PL, EIS and PEC experiments. Compared with pristine Imogolite (GDWINT) sample, the as-prepared titanium doped imogolite (Ti@GDWINT) catalysts showed a narrower optical band gap energy and capability to absorb light in the UV range. Ti@GDWINT catalysts exhibited promising photocatalytic activity compared to pristine imogolite, demonstrating that Ti@GDWINT material is promising photocatalyst for hydrogen generation.

The present work not only provides new insights into the structure of doped-imogolite but also demonstrates a low-cost and eco-friendly photocatalyst for solar-to-chemical energy conversion.

Acknowledgements:

This work is supported by Investissement d'avenir LabEx PALM (ANR-10-LABX-0039-PALM, project SP3).

POSTER #5

Copper based nanoparticles for CO_2 electroreduction

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The electrochemical reduction of CO_2 (CO2RR) supported by electrocatalysts is an alternative for the valorization of CO_2 into products of added value. Copper-based materials exhibit good performance during the electrochemical conversion of CO_2 into different by-products such as carbon monoxide, methanol, methane, formaldehyde, and formic acid. However, a problem of selectivity remains during this reaction. The combination and cooperation of metals have shown to increase the selectivity, activity, and stability of electrocatalysts, especially when they are presented in the form of nanomaterials. Some of the advantages that such materials present, are the need for fewer electrocatalysts due to the increase of the surface area. In this work nanoparticles (NPs) synthesized via radiolysis were evaluated as electrocatalysts for the CO_2RR. The physicochemical characterization of the products was done via UV-Vis spectroscopy, XRD and SEM/EDS, while the electrochemical properties were characterized using cyclic voltammetry and EIS techniques. The products of the CO2RR were identified using micro-GC and UV-Vis spectroscopy for the gas and liquid phases, respectively. Among the different compositions, CuPd NPs exhibited the best performance for the conversion of CO_2 into formic acid (HCOOH) in the liquid phase. Therefore, the use of bimetallic NPs led to an enhancement of the selectivity and activity of the electrochemical reaction since Pd increases the production of HCOOH and Cu decreases the production of H_{2n}. Results shed light on the synergetic effects of bimetallic catalysts for the valorization of CO_2

POSTER #6

Decentralized Control of EVs in Smart Grid using Multi-Agent Multi-Armed Bandits

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High penetration of solar photovoltaics (PVs) and the influx of electric vehicles (EVs) may introduce new challenges such as network congestion and peak load demand on the existing electrical distribution networks, which were not designed for this purpose. This may lead to an increase in network investments to tackle these challenges. EVs smart charging is one of the elegant solutions that could reduce network investments. However, the complexity of this smart charging optimization problem is increased when multi-level constraints local constraints of the prosumers and global constraints of the distribution network s stability are considered.

Based on the system s architecture, existing smart charging solutions can be classified as centralized, hierarchical, or decentralized. Centralized and hierarchical systems could suffer from drawbacks such as scalability, potential single point of failure, and privacy breaches. These problems can be solved by decentralizing the system. In recent years, decentralized smart charging solutions using standard reinforcement learning (RL) algorithms have been proposed in the literature. While these algorithms work well to optimize the studied objective cost, the inclusion of multi-level constraints is still a difficult task as unlike computer games there is no pre-defined reward signal in smart-grid applications. Moreover, no, or weaker theoretical guarantees (regret bounds) of RL algorithms with deep learning exist due to the complex nature of these algorithms.

We propose a decentralized smart charging algorithm designed as a multi-agent system using combinatorial 2-armed bandits with Thompson Sampling. The algorithm minimizes the total charging cost of the prosumers EVs (based on the dynamic electricity price signal and under uncertainty of PV production) while keeping the fairness of each prosumer into account. The constraints of the prosumers and the distribution system operator are taken care of in the algorithm itself rather than modeling through the reward function, which would lead to lesser convergence time. It is shown that the proposed algorithm is scalable. The performance of the proposed system is evaluated against other solutions through a large-scale case study (more than 10,000 EVs & PVs each).

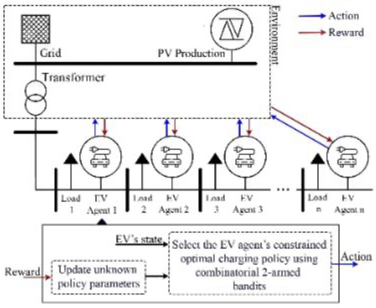

Figure 1: Proposed framework for decentralized smart charging using multi-armed bandits

POSTER #7

Direct Synthesis and Electrochemical Characterization of Nasicon-Type $Li_2NaV_2(PO_4)_3$ Cathode

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NASICON are a family of materials known for their high lithium ion mobility and the stability of their three-dimensional structure. The general formula of Nasicon is $A_3M_2(XO_4)_3$, with A a monovalent cation, M a transition metal, and X a small cation. The compounds crystallize in two different structures: monoclinic and rhombohedral. Monoclinic $Li_3V_2(PO_4)_3$ has three plateaus in its galvanostatic profile, which is not interesting for practical applications. On the contrary, $Li_2NaV_2(PO_4)_3$ rhombohedral structures have a high voltage plateau with a well-defined discharge voltage near 3.7 V and are generally synthesized by the ion exchange of $Na_3V_2(PO_4)_3$ precursor. In this communication, we report the direct synthesis of the cathode active material $Li_2NaV_2(PO_4)_3$ with a rhombohedral symmetry by a modified Pechini method (LNVP-direct). Its crystallographic structure is a three-dimensional sequence of PO_4 tetrahedra linked to VO_6 octahedra, favoring the migration of Na^+ and Li^+ ions through the crystal lattice. The alkaline ions (Na^+ and Li^+) are distributed randomly according to two crystallographic sites A1 and A2 (respectively in 6b (0,0,0) and 18e (x, 0, ¼)). For comparison, the material was also prepared by a conventional ion-exchange preparation using the intermediate material $Na_3V_2(PO_4)_3$ (LNVP-ions). Then, the electrochemical properties of LNVP-ions and LNVP-direct were compared by means of impedance spectroscopy (EIS), cyclic voltammetry (CV), and galvanostatic cycling measurements in liquid electrolyte. The results obtained showed better cycling performance for the direct synthesis (LNVP-direct) (Figure 1) than for the ion-exchange method (LNVP-ion) with a discharge capacity of around 97 mAh/g and a coulombic efficiency of 98 %.

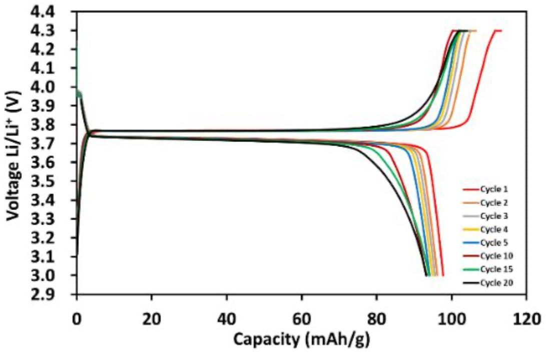

Figure 1: Galvanostatic cycling curve over 20 cycles for the LNVP-direct cathode

Doping influence on g-C_3N_4 based heterojunction for hydrogen production by water splitting under solar irradiation

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Photocatalysis is one of the promising technologies for clean and environmentally friendly hydrogen production, providing a way to use sunlight for generating hydrogen as a renewable green fuel. The concept of direct solar energy conversion through water splitting (water photoelectrolysis) has already been validated on numerous semiconducting materials [1]. A lot of work has already been done on titanium dioxide (TiO_2) to improve efficiency under visible light illumination [2] and graphitic carbon nitride, with a lower band gap, appears as a good candidate to produce H_2 from water under visible light irradiation [3].

The strategy of this work consists in comparing the impact of different doping (boron or iron) strategies on heterojunctions between TiO_2 (obtained via Sol-Gel process) and g-C_3N_4 (obtained from different precursors) for increased visible light absorption and/or to induce beneficial charge separation and electronic properties in order to enhance the overall photocatalytic activity.

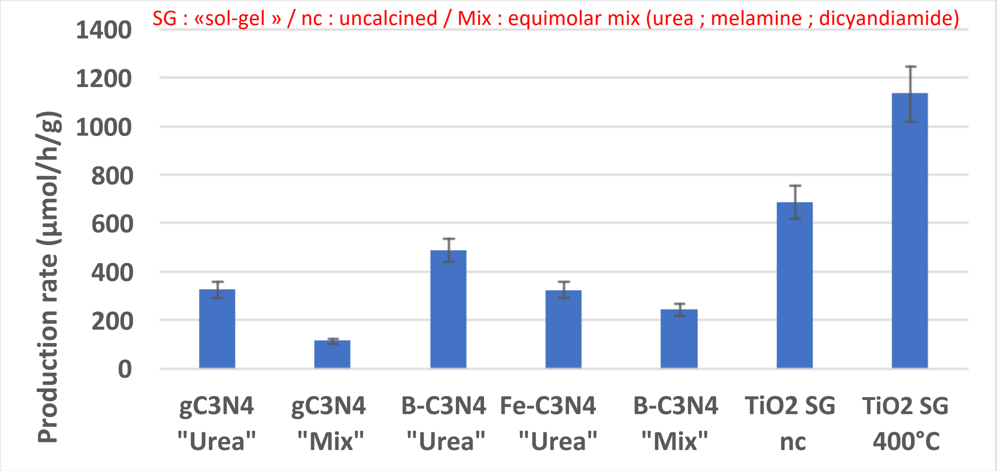

Figure 1: Hydrogen production yield for 1wt.% Au/bare materials before heterojunction design (TEOA 1 vol.%, 100 mg of photocatalysts).

This study will show that, amongst all the synthetized heterojunctions, Au/B-doped g-C_3N_4/TiO_2 material present a higher activity compared to its counterpart without doping. The best heterojunction is obtained via Au (1%) - g-C_3N_4 "equimolar mix"+ 2 g TiO_2 SG uncalcined + 10 mg B with a hydrogen production of 1425 µmol/h/g_{cata}. The main objective of this work is to find the best doping element between B or Fe based heterojunctions in order to study their influence on the photocatalytic activity.

[1] A. Fujishima, K. Honda, Nature, **1972**, *238*, 37.
[2] P Dhanasekaran, N. M. Gupta, Int. J. Hydrogen Energy, **2012**, 37, 4897.
[3] J. Wen, J. Xie, X. Chen, X. Li, Appl. Surf. Sci., **2017**, *391*, 72.

POSTER #9

Effect of hydration on the properties of a superionic conductor $M_2Ti_2O_5.(H_2O)_x$

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The search for new materials containing non-critical mineral resources with remarkable physical properties for numerous applications for example energy storage is one of todays major goals.

In addition to the safety aspect, the solid electrolyte which constitutes the supercapacitor, is a crucial element whose main requirement is a high ionic conductivity and a dielectric equivalent permittivity at room temperature. The family of compounds $M_2Ti_2O_5.nH_2O$ (MTO) with M an alkaline element is a solid electrolyte, which presents interesting electrical and electrochemical properties that can be controlled by tuning the hydration rate. For instance, a very promising ionic conductivity of 10^{-3} S/cm and a colossal permittivity of 10^9 have been measured for $Rb_2Ti_2O_5{\cdot}nH_2O$, which are not observed for the dehydrated compound.

The mechanism of the transport properties of the ionic species present in these compounds remains unknown to date. Therefore, it is of primary importance to focus on the study of the formation and conduction of the mobile ion(s) and to identify their nature.

In this study, the crystallographic structure and chemical stability of RTO and KTO have been characterized with X-ray diffraction (XRD), TGA and FT-IR. Furthermore, new compound containing both potassium and rubidium (RKTO) have been investigated.

At this conference, the hygroscopic character of the compound and the chemical stability will be focused on, by presenting the different results of FT-IR and XRD measurements. Finally, the link between these chemical properties and the ionic conductivity of the compound will be presented.

POSTER #10

Electrical behavior and stability under real outdoor working conditions of triple-mesoscopic perovskite solar cells

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At the beginning of the 21st century, carbon neutral and sustainable energy sources need to be considered instead of exhaustible fossil fuels to meet the growing energy demand and combat global warming. Within this very challenging race for alternative energy sources, metal halide perovskite solar cells (PSCs) have undergone unprecedented progress with efficiencies reaching now 25.7% and even 29.8% in tandem configuration. These remarkable performances result from the exceptional optoelectrical properties of hybrid perovskite materials such as wide and efficient absorption up to 800 nm, high charge carrier mobility (66 cm^2/Vs), low exciton energy (<10 meV) and long electron- and hole diffusion length (up to 1 µm).[ii] Coupled with their potential for low fabrication cost, perovskite solar cells are very promising especially incorporated in tandem device. However, since hybrid halide perovskites have a highly ionic character, they can decompose under external stresses such as moisture, solvents and heating cycles. Reducing environmental stresses imposed by moisture or oxygen for example, in order to improve the long-term stability of perovskite solar cells, is critical to the deployment of this technology.

In 2017, we published a structure proven to be stable for more than 10,000 h, measured under controlled standard conditions, by engineering an ultra-stable 2D/3D perovskite junction. This structure is based on a fully printable architecture made of three mesoporous layers in which the perovskite is embed.

In this communication, we will disclose preliminary results on triple-mesoscopic perovskite solar cells in real outdoor working conditions. The experiment was designed and implemented on a new SIRTA test bench that will be presented. Based on the first results, perovskite fabrication and measurement processes will be optimized.

Estimation d'état des réseaux basse tension par des techniques d'apprentissage automatique

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Les réseaux de distribution basse tension (BT) sont confrontés à une transition majeure en raison de la forte pénétration de la production d'énergie décentralisée et de l'introduction de nouveaux types de consommateurs tels que les véhicules électriques. Par conséquent, les gestionnaires de réseaux de distribution (GRD) pourraient utiliser un estimateur d'état pour évaluer en temps réel l'état du réseau de distribution (notamment l'amplitude de la tension). Bien que les estimateurs d'état soient déjà appliqués avec succès aux réseaux haute et moyenne tension [1], leur application aux réseaux BT fait face à de nombreux défis [2]. Parmi ces défis, on peut noter le déséquilibre des réseaux BT et le manque de mesures transmises en temps réel en raison des contraintes de communication qui limitent l'utilisation des données des compteurs intelligents.

Cependant, la disponibilité des données historiques des compteurs intelligents donne l'opportunité d'entraîner les estimateurs d'état de l'apprentissage automatique et ensuite d'exécuter le modèle entraîné en temps réel, même dans le cas d'un nombre limité de mesures remontées des compteurs intelligents.

Dans le travail proposé, nous nous concentrons sur le développement et le test d'un estimateur d'état basé sur des techniques d'apprentissage automatique et en particulier sur des auto-encodeurs [3]. Afin d'étudier les performances de l'estimateur d'état considéré dans des conditions proches de la réalité, nous nous intéressons à la reconstruction des réseaux BT à partir de l'Open Data des GRD.

L'estimateur d'état développé est testé sur un réseau généré par la technique de modélisation de réseau BT proposée. Les scénarios de test visent principalement à tester la robustesse de l'estimateur dans des conditions de déséquilibre du réseau, d'absence de mesures en temps réel et d'intégration de production d'énergie renouvelable distribuée.

Les résultats obtenus pour les scénarios proposés sont analysés et évalués. Des améliorations et des modifications sont proposées selon les limitations identifiées.

[1] D. Croteau et O. Carre, « Distribution state estimation: outcomes from a field implementation aimed at tackling MV mastering in the presence of distributed energy resources (DER) », CIRED - Open Access Proceedings Jounal, vol. 2017, no 1, p. 1715-1717, 2017.

[2] K. Dehghanpour, Z. Wang, J. Wang, Y. Yuan and F. Bu, "A Survey on State Estimation Techniques and Challenges in Smart Distribution Systems," in IEEE Transactions on Smart Grid, vol. 10, no. 2, pp. 2312-2322, March 2019.

[3] P. N. Pereira Barbeiro; H. Teixeira; Jorge Pereira; R. Bessa, "An ELM-AE State Estimator for real-time monitoring in poorly characterized distribution networks", IEEE PowerTech, Eindhoven Conference, 2015.

Experimental investigations on atmospheric water harvesting using composite desiccant-based solar collector

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During the last years, freshwater scarcity has become a major worldwide issue. There are three main ways for providing arid areas with fresh water. Unfortunately, these methods require heavy investments are very energy intensive. Some unconventional solutions are being tested to make water available to the population in remote areas. Ambient air is a renewable source of water and is available everywhere on the Earth. In this investigation, a bed containing a composite desiccant made of river sand impregnated with calcium chloride solution ($CaCl_2$) has been used to absorb water vapour from ambient air. The experiments occurred under the climatic conditions of Agadir city, Morocco (latitude 30.406° N and longitude 9.544° W). The system collects water from atmospheric air through two steps; the first step involves water vapour absorption during the night by subjecting the composite desiccant material to surroundings air, and the second step involves regeneration and water vapour condensation during the day by using a solar collector. The sun rays increased bed temperature, evaporation occurred, and the vapour condensates on the internal surface of the glass cover. Then, water was collected in a graduated flask through a collecting pipe attached to the device. Many parameters were measured during the tests to evaluate the influence of atmospheric conditions on water productivity during regeneration. The amount of water produced from the system was 180 ml per kg of calcium chloride and the maximum efficiency during the experiments was 13 %.

Keywords: Water harvesting; Ambient air; Absorption; Solar energy; Desiccant;

POSTER #13

Fault location on MV distribution grids with distributed measurements

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With the increase of distributed generation (DG) penetration level, distribution system operators (DSO) need faster while accurate location of faults on medium voltage (MV) feeders. Usually, the only instrumented node in a MV distribution feeder is located at the busbar in the primary substation, thus only single-ended impedance-based fault location methods (FLMs) can be deployed. To overcome the multiple estimation problem faced by such methods, transient-based methods have been proposed in the literature. However, the need for very high sampling frequency and the damping of travelling waves in the distribution grids limit the implementation of such methods.

This poster presents an impedance-based FLM designed for MV grids leveraging distributed measurements on some secondary substations to overcome the multiple estimation problem. By comparison of two zero-sequence voltage estimate sets (*Figure 1*), the algorithm can locate any type of earth fault into a location area whose size depends only on the number and location of the additional voltage measurements. To ensure that the best locating performance is reached, an optimal placement algorithm has been developed for the additional measurements (*Figure 2*).

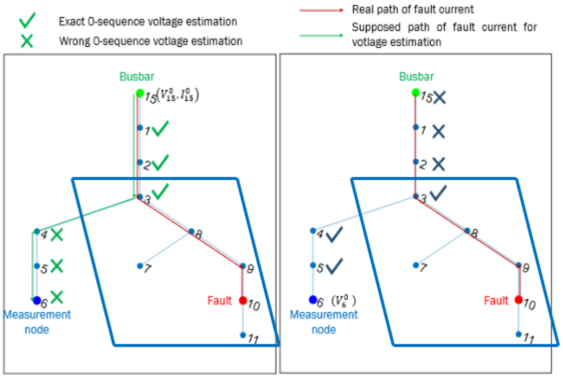

Figure 1

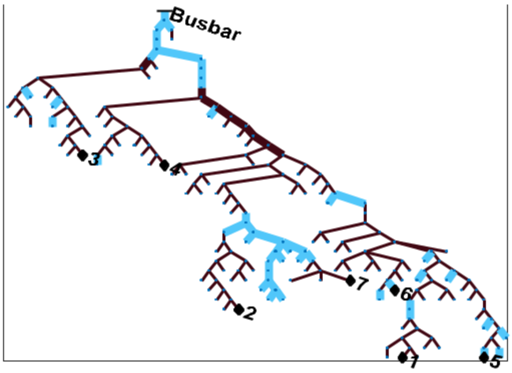

Figure 2

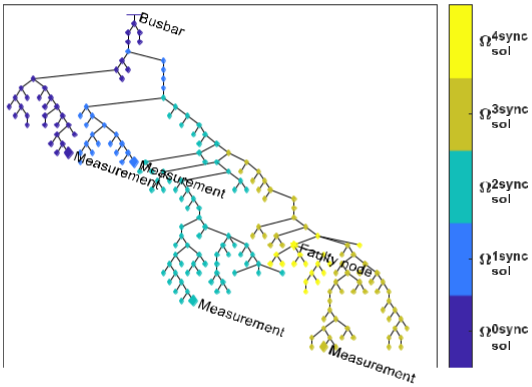

Figure 3

We used twenty reconstructed realistic feeders from E edi Opendata. The set of realistic feeders includes more complex and ramified grids than most of the benchmark ones usually used in the literature. Thus, the performance of the proposed FLM has been verified in the worst-case scenario. In Figure 3, we observe a 211-node feeder with a high number of ramifications. In this case, with only four optimally placed additional synchronized (using phasor measurement units) measurements, the location area Ω contains 7.379.8% of the feeder lines. This exemplifies the locating potential of the method, which gives a convex set of nodes as the solution area, meaning that it is not subject to multiple estimations being far away from each other. A sensitivity analysis shows that the method is not sensitive to the fault resistance value and to the presence of DG, which confirms that it is well suited for the MV distribution grids.

POSTER #14

Graphdiyne quantum dots: new metal free co-catalyst for efficient photocatalytic hydrogen generation

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Graphdiyne (GDY) is an emerging two-dimensional carbon material with unique configurations comprising of both sp and sp^2-hybridized carbon atoms that form an extensive network of benzene rings interconnected by diacetylenic linkages.[1] The GDY structure is chemically stable and offers uniform pore size and distribution, rich in π-conjugated electrons, superior electronic properties, tunable band gap and electron donor/acceptor properties enabling applications ranging from energy harvesting and storage to sensing, medical uses or water purification.[2] Titanium dioxide (TiO_2) is one of the earliest known and most studied photocatalyst used for photocatalytic degradation of pollutants and photocatalytic water splitting.[3] TiO_2 is low cost, non-toxic and shows good photostability but its efficiency is relatively low due to its large band gap of about 3.18 eV and fast electron-hole pair recombination, which hampered its ability to photocatalytic activity. To reduce the band gap energy and prolong the electron-hole recombination life, TiO_2 is usually reacted with other metals, metals oxide, organic compounds, and carbon materials.[4] Nevertheless, the high cost of metallic based materials limits their use in commercial applications while the coupling to novel carbon materials seems a more promising path.

In this work, graphdiyne quantum dots (QDs-GDY) were coupled to commercial TiO_2-P25 as a co-catalyst for photocatalytic H_2 generation. Different ratios were tested, and optimal conditions were determined to obtain very high amount of H_2 (ca. 2240 Pmol/g for TiO_2 with 1% GDY-QDs compared to 98 Pmol/g for TiO_2 alone) under UV-visible light. More importantly, the hybridization of QDs-GDY demonstrated good activity and stability under visible light. The hybrid photocatalyst was characterized by variable technics, such as TEM, UV-vis spectroscopy, time resolved photoluminescence spectroscopy to shed light on the synergetic effect and role of QDs-GDY as metal-free co-catalyst.

1 B. Liu, L. Xu, Y. Zhao, J. Du, N. Yang and D. Wang, *J. Mater. Chem. A*, 2021, **9**, 19298–19316.
2 Y. Fang, Y. Liu, L. Qi, Y. Xue and Y. Li, *Chem. Soc. Rev.*, 2022, **51**, 2681–2709.
3 A. Brindha and T. Sivakumar, *J. Photochem. Photobiol. A Chem.*, 2017, **340**, 146–156.
4 P. S. Basavarajappa, S. B. Patil, N. Ganganagappa, K. R. Reddy, A. V Raghu and C. V. Reddy, *Int. J. Hydrogen Energy*, 2020, **45**, 7764–7778.

POSTER #15

Investigations of Diffusion and NMR properties in LLAZO through a Multiscale Simulations approach linked to Experimental data

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Designing solid-state batteries (SSBs) requires the design of highly efficient solid electrolytes (SSEs) that exhibit high ionic conduction properties. Though they have numerous draw-backs, liquid organic-based electrolytes are the ones most commonly used in the commercial batteries. They are not only dangerous and less efficient but also degrade faster which decreases its life time for long-term applications. Hence the necessity for a safer and longer lived alternative for batteries is a must. To this end, SSEs are now in the forefront of all the materials, as they combine factors of safety (non-flammable), efficiency, lower cost and ease of fabrications. Among them, doped – LLZO[1] ($Li_7La_3Zr_2O_{12}$) is considered of the most promising ceramics serving this purpose. Herein, we aim to model Li diffusion mechanisms and its respective spectroscopic properties (NMR and EIS[2]) using multi-scale simulations approaches by harnessing both (i) short time and length scales (from DFT and AIMD[3]) and (ii) long time and length scales (from classical MD and KMC[4]) to define multi-scale methodology for understanding the impact of doping have on Li mobility in the material in question by linking the simulations data to the microscopic diffusion measurements (NMR and EIS). Our aim is to develop a Kinetic Monte Carlo model, parameter-ized with inputs from MD simulations (both classical and ab-initio) capable of predicting NMR properties such as ^{7}Li NMR lineshapes and nuclear relaxation times. Density based clustering approaches are employed to analyze Li -trajectories. Additionally, standard DFT-GIPAW calculations are performed for predictions of MAS-NMR[5] spectra of ^{27}Al in Al – doped LLZO (LLAZO). By adapting the same methodology, Na diffusion in NASICON[6] and Sc^{+3} – doped NASICON have been investigated and analyzed.

~~ACKNOWLEDGEMENTS: ATTIA, M. is supported by the CEA NUMERICS program, which has~~ received funding from the European Union's Horizon 2020 research and innovation program under the Marie Sklodowska-Curie grant agreement No 800945.

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[1] Lithium Lanthanum Zirconium Oxide
[2] Electrochemical Impedance Spectroscopy
[3] ab-initio Molecular Dynamics
[4] Kinetic Monte Carlo
[5] Magic-Angle Spinning Nuclear Magnetic Resonance
[6] Na Super Ionic CONductors

POSTER #16

Innovation across organizational and disciplinary boundaries at Lemon Energy: enhancing industrial energy performance based on data analysis

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Born in the incubator of CentraleSupelec, a member of FrenchTech Paris-Saclay, Lemon Energy develops innovative solutions for industrial energy efficiency.

Lemon Energy has been recognized as an innovative startup by the French Ministry of Higher Education, Research and Innovation. Our research projects focus on developing digital twins based on Industry 4.0 technologies to improve energy efficiency and rely on predictive analytics for optimizing energy consumption in industrial processes.

Throughout its development as a company, Lemon Energy has benefited from strong relationships with academia. During its early incubation days at CentraleSupelec, Lemon Energy developed projects with the help of students on site through the Industrial Study Convention Program and worked in partnership with CentraleSupelec’s Industrial Engineering Laboratory (LGI). Lemon Energy also leveraged the institution’s documentation resources to back industrial data analysis and propose efficient solutions.

At the core of the growth and success of Lemon Energy is the use of real-life industrial data collected on the field, that is used to build models and predictions of energy consumption. Lemon Energy takes it to heart to carry out their R&D projects independently from private funding. Projects are therefore financed through regional and state loans as well as the company’s own funds. This independence provides a sound ground for academic partnerships. Currently, there are teams working on research activities for a variety of installations, such as chillers, heat pumps, air handling units (with and without humidity control), cleaning in place (CIP) installations, air compressors, boilers, and associated equipment.

The challenge of academic collaboration is two-fold: first, Lemon Energy as a private company works directly on client projects and needs to connect theoretical research with practical benefits for its customers; second, Lemon Energy innovates by bringing together existing models and techniques into a service, across disciplines such as machine learning, thermodynamics, and industrial engineering.

Metalloporphyrins bearing imidazolium groups for CO_2 reduction

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Transforming CO_2 into valuable reduced forms of carbon is a strategy that is currently attracting the interest of the scientific community. Converting and not only capturing CO_2 can be an efficient way to recycle this greenhouse gas by introducing non-fossil fuel based C1 building blocks back into the carbon cycle. The design of new molecular catalysts for the reduction of CO_2 is therefore essential to better understand how to activate and reduce efficiently this unreactive molecule. Metalloporphyrins have been shown to be good catalysts for CO_2 reduction. When trying to optimize the performances of iron tetra-arylporphyrins, electron-withdrawing groups were introduced to lower the overpotential of CO_2 reduction, but at the expense of a lower turnover frequency. Looking at the structure of the Ni-Fe active site of Carbon Monoxide Dehydrogenase (CODH), several positively charged groups appear to have an important role in the interconversion of CO_2 to CO. For this reason, our group and others introduced cationic functions in the second coordination sphere of tetra-arylporphyrins with the objective to stabilize the Fe^{I}-CO_2 reactive intermediate that is formed during CO_2 reduction. The benefits of these cationic groups were an important lowering of the overpotential and a higher catalytic rate. In this study, different iron porphyrins were synthetized with an imidazolium group at various distances from the metal center in order to better understand the effect of the positively charged moieties on the different steps of the reaction mechanism (Figure 1). The goal of this study was to establish a Hammett s parameters like correlation for through space interactions that can guide the design of more efficient catalysts for CO_2 reduction. After electrochemical investigations, the imidazolium moieties were found to be electrochemically active and to have a strong impact on the catalytic performances of the porphyrin.

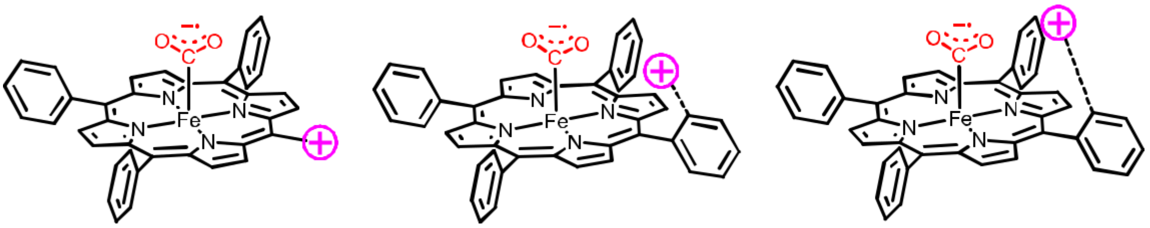

Figure 1: Simplified structures of targeted cationic porphyrin catalysts with various distances between the cationic group and the Fe^{I}-CO_2 intermediate.

POSTER #18

Nb, N co-doped TiO_2 nanoparticles for broad spectrum solar light activation photocatalysis

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TiO_2 photocatalyst co-doped with Nb and N (Nb,N:TiO_2) were synthesized via a sol-gel method followed by a post thermal nitridation in ammonia atmosphere. The photocatalytic performance of Nb,N:TiO_2 was evaluated by conducting the photo-degradation of methylene blue (MB) solution under the irradiation of UV light or visible light and compared with TiO_2 and N doped TiO_2. Specific thermal condition of nitridation was found to significantly differentiate the photocatalytic activity of Nb,N:TiO_2. By using XPS, EPR and photoacoustic spectroscopy, we demonstrated that proper thermal condition for N incorporation can elevate the level of charge compensation between Nb^{5+} and N^{3-}, leading to negligible formation of bulk defects and therefore strongly enhance the photocatalytic activity (Figure 1) in the visible. However, over-intensive thermal condition of nitridation caused the generation of Ti^{3+} and oxygen vacancy in the bulk acting as charge recombination centre, resulting in the significant deterioration of photocatalytic performance. This study has emphasized the importance of understanding the complexity of the charge compensation scheme in the co-doped system, and that various defects can be introduced depending on the synthesis conditions. The photocatalytic performances in the UV and visible solar region then depend not only on the amount of cation and anion introduced, but also from the crystallographic nature of these introduced dopant in the lattice.

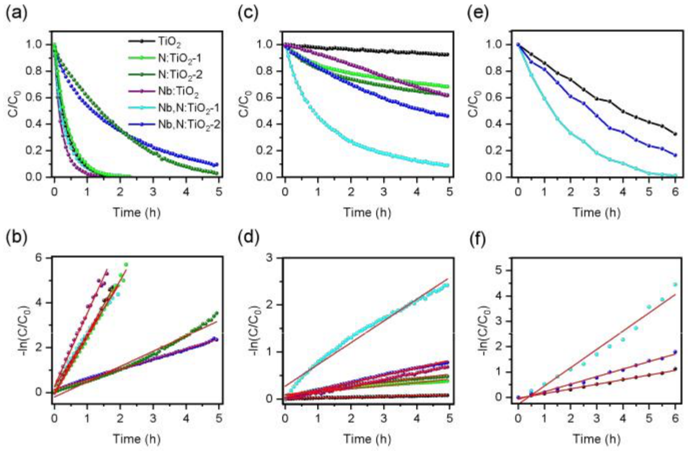

Figure 1. Photocatalytic activities of MB degradation and the corresponding pseudo-first-order kinetics for TiO_2, N:TiO_2, Nb:TiO_2 and Nb,N:TiO_2 under the irradiation using UV LED (365 nm) (a and b), visible LED (450 nm) (c and d) and AM 1.5 simulated solar light (e and f).

Photocatalytic Oxygen Reduction to Hydrogen Peroxide from Oxygen and Water by Metal- free Nano-Polypyrrole

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Photocatalytic hydrogen peroxide (H_2O_2) generation from oxygen via a $2e^-$ reduction reaction is an emerging concept for solar-to-fuel conversion. Benefitting from its high energy density comparable to H_2, H_2O_2 is a highly sought-after alternative fuel to H_2 in fuel cells[1]. In addition, H_2O_2 is one of the most important chemicals in the industry because of its wide application in many fields, such as a green oxidant for many chemical syntheses and advanced oxidation processes for environmental remediation. Graphitic carbon nitride (g-C_3N_4) has been the most studied polymeric photocatalyst for H_2O_2 production. Although it has excellent stability, unmodified g-C_3N_4 was shown to have low photocatalytic H_2O_2 formation in pure water. Our work has proven that PPy is a promising visible light photocatalyst for oxygen reduction to H_2O_2 in pure water. The photocatalytic reaction was carried out using Oriel 300 W Xenon lamp. The photogenerated H_2O_2 was quantified using the KI method using a UV Visible Spectrophotometer (HP 8543). Under O_2 atmosphere, nano-PPy (1 mg/mL) produces around 2.18 μM H_2O_2 /min under visible light irradiation ($\lambda \geq 420$ nm) and in the absence of sacrificial agents. The H_2O_2 generation is also conducted at a pH range of 2- 7, with different light intensities and PPy concentrations. The results of this experiment can be a potential avenue for other catalytic applications, for instance, as a catalyst for Photo-Fenton reactions or in the transformation of important organic compounds via oxidation reaction.

Polymeric porphyrin-based material for the activation and reduction of CO_2

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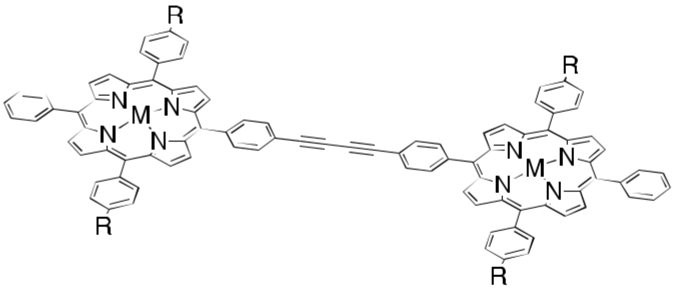
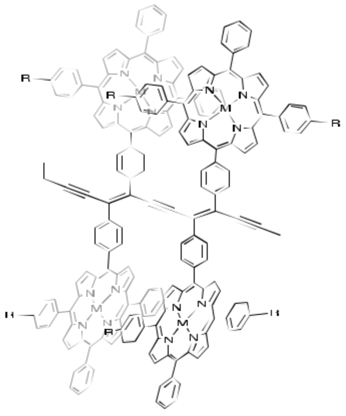
The capture and storage of renewable energy is a crucial step in combating climate change caused by the accumulation of atmospheric CO_2 from the extensive use of fossil fuels, which is threatening human life on Earth. One route towards the generation of green fuels and chemicals is the electrochemical reduction of CO_2 towards carbon-containing chemical building blocks, such as CO, CH_4, or C_2H_4. Due to the kinetic inertness and thermodynamic stability of CO_2, catalysts are required for the reactions to be carried out efficiently. Catalytic materials that are under scrutiny come from different approaches: i) molecular catalysts are being transferred on carbonaceous electrodes ii) Single-site catalysis is a very hot topic where chemists are generating graphitic type materials with inserted metal ions surrounded by a well-defined coordinating environment iii) designing polymeric catalysts at the surface of electrodes has already proven to form stable and cost-effective catalytic material for CO2 reduction. However, there are still many issues to be solved to understand and optimize such materials.

Herein, we report on our ongoing efforts to develop polymers of porphyrins for multiple-electron and multiple-proton CO_2 reduction to higher reduced forms than CO with C-C bond containing products such as ethene or ethanol. The idea is to obtain a topochemical organization with a face-to-face disposition between two catalytic units to favor synergy between two metal centers. The monomer has been synthesized by Ellington coupling. The polymers are obtained by irradiation of the diacetylene function in the monomer.



Monomer



Target Polymer

POSTER #21

Porous Composite Nanomaterials For Green Hydrogen Production

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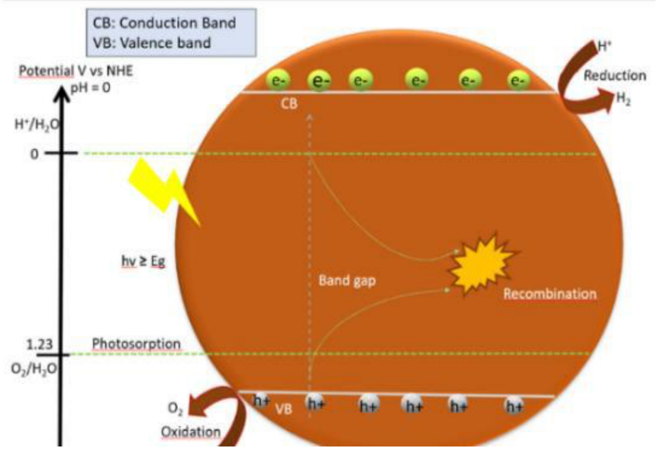
The excessive consumption of fossil fuels (to produce energy) results in harmful pollution and climate change. The focus is shifted towards consuming renewable sources to produce energy. Hydrogen is a rising star that serves as a great solution to lessen our dependence on fossil fuels as it is a clean energy vector that resolves problems related to energy crises and environmental pollution. However, it must be produced from green resources! Photocatalysis is a promising way to produce green hydrogen from water and sunlight. The ICP team developed highly active photocatalysts based on conjugated polymer nanostructures or TiO_2 (including composite nanomaterials) as well as metal cocatalysts for hydrogen generation and water treatment [1,2]. Also, it has been reported by ICP team that composite TiO_2/HKUST-1 shows good photocatalytic activity for generation of hydrogen by photo-reforming of a glycerol-water mixture under artificial sun light [3]. Encouraged by these observations, herein we developed composite nanomaterials based TiO_2 coupled with Cu-MOFs (different mass ratios) for application in hydrogen generation by photocatalysis. We modified these nanomaterials with metal nanoparticles used as cocatalyst (Pt, Cu induced by radiolysis). The photoactive composite materials obtained were further characterized by transmission electron microscopy (TEM), UV-Vis spectroscopy, time resolved microwave conductivity (TRMC), X-ray Photoelectron spectroscopy (XPS) and photoelectrochemical studies. Finally, the photocatalytic activity of these nanocomposites was studied for hydrogen generation under UV-visible light by using Micro Gas Chromatography (MicroGC).



[1] Ghosh, S. et al. Conducting polymer nanostructures for photocatalysis under visible light. Nat. Mater. 14, 505–511 (2015).

[2] Yuan, X. et al. Photocatalytic degradation of organic pollutant with polypyrrole nanostructures under UV and visible light.Appl. Catal. B Environ. 242, 284–292 (2019)

[3] Martínez, F. M. et al. Hydrogen Production from Glycerol Photoreforming on TiO_2/HKUST-1 Composites: Effect of Preparation Method. Catalysts 9, 338 (2019)

POSTER #22

Power Grid Structure for the Energy Transition

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The worldwide process of replacing fossil fuels with low carbon energy source is underway. During this transition, energy networks are expected to be deeply modified in nature and structure.

One of the novelty aspects of our project is the merge of graph-theoretical statistical physics tools and the key concept of Energy Return On [Energy] Invested [EROI] in transition scenarios. Which power grid topology is possible to enable the energy transition?

What is the economic impact of the energy and matter investment needed to deploy a new multi-energy network? Our first milestone work is to model the French electric transmission network as a weighted network of coupled dynamical systems and to study its geometrical properties. The weights will encode the information contained in the spatial part of the Real-World graph. The model shall take into account the energy and matter investment in the evolution of the high voltage lines and associated devices.

POSTER #23

Surface Modification of TiO_2 with bimetallic Au-Pd Nanoparticles for Photocatalytic Hydrogen Generation

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Green hydrogen production by photocatalytic water splitting offers a promising way to solve environmental and energy issues. Over the past decades, oxide-based semiconductors, particularly TiO_2 has been recognized as an efficient photocatalyst due to its excellent properties such as low toxicity, cheap, high reactivity, environmental friendly, photochemical and biological stability. However, its practical applications are limited by high charge carriers recombination and can be only excited under UV irradiation due to its large band gap (~3.2 eV). Surface modification of TiO_2 with metal nanoparticles (NPs) reduce charge carriers recombination increasing the photocatalytic activity for hydrogen generation. Gold nanoparticles (Au-NPs) have attracted much attention due to their localized surface plasmon resonance (LSPR), and their plasmonic properties can be used to induce the photocatalytic activity of the semiconductor material under visible light. In this work, commercial titania (TiO_2-P25) was modified with mono- and bimetallic (Au, Pd Au-Pd) NPs synthesized by chemical reduction method using $NaBH_4$ as a strong reducing agent at room temperature. Bimetallic Au-Pd nanoalloys homogeneous in size and well dispersed on the TiO_2 surface are obtained. Alloying Au-Pd with low Pd content presents synergetic effects for hydrogen generation under UV-visible light. The charge carrier dynamics, which is a key factor in photocatalysis was studied by Time Resolved Microwave Conductivity (TRMC). The AuPd/TiO_2 photocatalysts are stable with cycling.

POSTER #24

Thermogalvanic Energy Conversion improvement in Ionic Liquids redox solvation and coordination chemistry

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Room temperature ionic liquids (RTILs) are molten salts that are liquid below 100 °C and up to 200-400°C. Compared to classical liquids, they exhibit many favorable features such as high boiling points, low vapour pressure, high ionic conductivity and low thermal conductivity accompanied by higher Seebeck coefficient (Se) values. The latter is believed to stem from a complex and strong ionic environment in the solvation/complexation layer surrounding the redox species unique to ionic liquids. A clear understanding and the precise control of the speciation of metal ions and their impact on the structural entropy change of the solvation layer is a key to the rational design of future thermoelectric liquids. In this work, we first investigate the relationship between the ionic constituents of the liquid (various RTIL/solvent mixtures) and the thermogalvanic effect of commercially available redox salts (Co(bpy)$^{3+/2+}$) via the Seebeck coefficient (open-circuit voltage), impedance and power measurements. The solvation shell surrounding the redox couple molecules and the overall solvent viscosity are found to play an important role in both the Seebeck coefficient and the power output from the thermocell, which is analyzed in terms of the Reichardt polarity scale. The study is then extended to the coordination chemistry of transition metal redox ions made with commonly available metal, Ce, involving metal complexation studies and spectral & electrochemical characterization methodologies. Our long-term goal is to deepen the understanding of the complex thermogalvanic phenomena in RTILs, and to demonstrate the application potential of liquid thermoelectrics based on affordable, abundant and safe materials for thermal energy harvesting as an energy efficiency tool.

POSTER #25

Towards the Electrolysis of Seawater by Iridium and Iridium Mixed Based Oxide Nanoclusters for the Generation of the Hydrogen Energy Carrier

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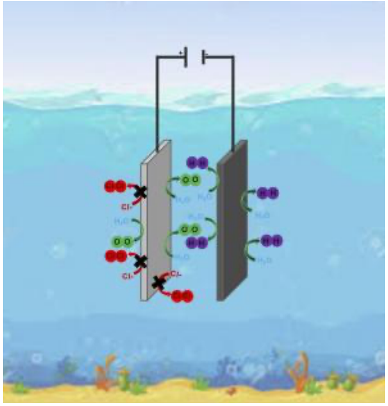

Provisioning seawater sources for the electrolysis of water and the production of the hydrogen energy carrier would provide an economic and environmentally conscious technological solution to secure the greater demands for energy across our globally increscent societies. Though fulfilling the high purity requirements of current water electrolyser technologies contributes to the curtailment of freshwater sources and the amplification of carbon emissions through the significant energ needs demanded to desalinate of Earth s ater sources. The direct electrolytic production of hydrogen from an abundant, impure water sources such as seawater would alleviate this curtailment and elicit a sustainable and renewable water source that could be electrolytically harnessed to produce a hydrogen energy vector to meet the global energy demands. However, the more kinetically favorable oxidation of the chloride ion, present in seawater at concentrations of 3.5 wt. %, at the anode impedes the selectivity for the oxygen evolution reaction. The selectivity is hypothesized to be controllable through mitigation of the species transport toward the anode through the deposition of a synthetized silica layer with a thickness greater than the concentration gradient interval of the chloride ion. The silica precursor is hydrolyzed and condensed onto a commercially available Vulcan carbon material interdispersed with iridium nanoclusters. Aliquots are taken during the silica encapsulation and compared to aliquots taken during a silica encapsulation of a similar Vulcan carbon material interdispersed with platinum nanoclusters and analyzed through infrared Spectroscopy, thermogravimetric analysis, transmission electron microscopy, and linear sweep voltammetry to elucidate a mechanistic interpretation for the high overpotentials measured to elicit electrocatalytic activity towards the oxygen evolution reaction by the synthesized materials. Results indicate that precise control of the shell thickness is a crucial parameter to selectively arrest the transport of the chloride ion while permitting OER reactant and product diffusion to and from the electrocatalytic material. Further studies with X-ray photoelectron spectroscopy will enable a mechanistic understanding of the molecular interaction between the silica overlayer and the catalytic nanoclusters to conceive a potent overlayer selectively tuned to improve the selectivity and activity of the electrocatalysis for the direct electrolysis of seawater.

POSTER #26

Interfacial properties of a ZnO-polymer nanocomposite for PENG applications

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Performances of piezoelectric nano-generator for energy harvesting mainly relies on the capability of nano-object to generate charge from mechanical deformation. In practise, making most of efficient conversion requires optimized devices. A key parameter for this is the polymer matrix whithin which the nano-objects are embedded.

In this work, the properties of the interface between ZnO nanowires and various polymers were investigated. Not only the size of nanoscaled piezoelectric structures makes them suitable for miniaturized devices, but it enhances the piezoelectric properties through a favorable aspect ratio and a low defect density as well. For the nanostructures to bend, the external strain has to be transferred by the polymer matrix which implies a strong coupling between the two materials. Both mechanical adhesion is determined by the nature and the strenght of the chemical bonds the polymer forms at the ZnO surface. Given they can induce electronic transfer too, those interfacial chemical bonds turn out to be crucial for applications.

We report here preliminary results on the adhesion of commercial polymers on ZnO nanowire assemblies. Several ways were used to tune the polymer properties such as the molecular mass, the termination chemical function and the energy input to form chemical bounds. The polymers are characterized on their own as well as coated on ZnO nano-objects assemblies, using contact angles measurements, surface roughness, mechanical properties mapping and nano-indentation. The adhesion was estimated by peeling the coating polymer layer off the nanowire assembly and observing the amount of nanowires left on the substrate.

[1] D. Ponnamma *et al.*, Materials Science & Engineering C 98 (2019) 1210–1240
[2] G. Sengupta *et* al., J. Solloid and Interface Science 69 (1979) 2

POSTER #27

Intrinsic photoanode band engineering: surface segregation mediated enhanced solar water splitting efficiency in Ti-doped hematite nanorods

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Hydrogen production by splitting water molecules into H2 and O2 using sunlight is a very attractive idea because it allows storing solar energy in the H2 molecules using a clean method. First demonstration of water splitting was reported 50 years ago using TiO2 as photoanode[1]. Since then, plethora of studies were reported, owing to materials chemists' infinite imagination, addressing different classes of photosensitive materials including semiconducting oxides, III-V semiconductors[2], MOF (metal-organic framework) architectures[3], ferroelectric materials[4], etc. Band engineering is additionally often employed targeting each time the same single aim: enhance the efficiency of the photoelectrochemical (PEC) process, increasing thus H2 production efficiency.

We report here a simple band engineering approach applied to one of the most Earth abundant materials, the hematite, using Ti doping[3-5] and tuning annealing conditions: temperature and atmosphere. Enhanced PEC activity was obtained, mediated by surface states, as evidenced using electrochemical impedance spectroscopy. Annealing atmosphere components (N2 and O2) were varied between 100% N2 – 0% O2 to 0% N2 – 100% O2, allowing to determine the optimum O2/N2 ratio. The nanoscale origin of the increased PEC activity was addressed using combined XPEEM, STXM, X-rays spectro-ptychography and STEM. Shadow XPEEM alone can be used to discriminate surface and bulk contributions of the chemistry and chemical coordination. STXM complement successfully these results evidencing formation of Ti-rich clusters in the Ti-doped hematite nanostructures annealed in O2-free atmosphere. Spectro-ptychography allows to better identify and isolate both spatially and chemically Ti-rich clusters. X-ray spectromicroscopies altogether were confronted with STEM measurements and DFT calculations, the results suggesting formation of pseudo-brookite clusters at the surface of the Ti-doped hematite.

2) Fujishima, A. & Honda, K. Nature 238, 37–38 (1972)
3) Van De Krol, R. & Gratzel, M. International Journal of Renewable Energy Research vol. 2 (Springer, 2012)
4) Wang et al., Chem. Cat. Chem. 13, 5058–5072 (2021)
5) Rioult et al., Appl. Phys. Lett. 107, 103901 (2015)
6) D. Stanescu et al., J. Mater. Chem. A 8, 20513 (2020)

POSTER #28

A multiscale study of the electronic and ionic transport processes influencing the performance of Lithium-ion batteries

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The use of low-cost and highly efficient lithium-ion batteries in electric vehicles is critical to enabling the essential transition to carbon-free energy systems in the transportation sector. As a result, several research projects are focusing on the optimization of existing materials as well as the search for novel materials and elaboration methods. However, an all-inclusive challenge is the several kinetic setbacks that limit rate processes in advanced lithium-ion batteries. These multiscale interfacial barriers exponentially affect the optimum electronic and ionic transfers in conducting networks of the composite electrode. Several studies have used electrochemical impedance spectroscopy and *dc* conductivity measurements to access the variations of the charge transport across model electrodes, but these low-frequency methods only provide macroscopic interfacial information and overall conductivity measurements. By using broadband dielectric spectroscopy (BDS) over a wide frequency range from 10^2 Hz to 10^{10} Hz, we are able to characterize the influence of the different interfaces on the frequency-dependent charge transfers in two active materials used in the composite positive electrode of electric vehicle grade battery[1,2]: NMC532 ($LiNi_{0.5}Mn_{0.3}Co_{0.2}O_2$) and NMC811 ($LiNi_{0.8}Mn_{0.1}Co_{0.1}O_2$) using multiple electrode models, both in the dry (ex-situ) and wet states (with electrolyte). The Nyquist fittings of the obtained dielectric permittivity and conductivity data provided a multiscale description of the electronic and ionic transport across the composite electrode and the influence of material variations. The initial results reveal a higher frequency and lower interfacial activation barrier for the nickel-rich electrode NMC811, projecting the material to have a better rate performance.

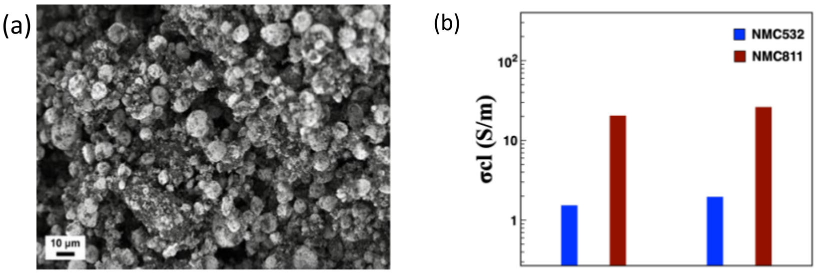

Fig. 1. (a) SEM image of NMC811 electrode mix with 5% carbon black. (b) Cluster conductivity cl in dry and wet electrodes at room temperature.

1. K.-A. Seid, J.-C. Badot, C. Perca, O. Dubrunfaut, P. Soudan, D. Guyomard, B. Lestriez, *Adv. Energy Mater.* **2015**, *5*, 1400903.

2. A. Agrawal, O. Dubrunfaut, L. Assaud, S. Franger, B. Lestriez, J. C. Badot, *J. Phys. Chem. C* **2021**, *125*, 17629.

Routes for low cost III-V solar cells

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Solar cells based on III-V materials have reached the highest efficiency of any technology available today, i.e. up to 47% under concentration. Nevertheless, their cost is a hundred times higher than that of c-Si solar cells. Most of this cost difference comes from i) the III-V or Ge substrate required to grow a single crystal layer and ii) the growth process.

In a previous study we have shown how the use of a virtual substrate can tackle the first part of the challenge. This innovative substrate is composed of a crystalline silicon wafer coated with an ultrathin (20 nm) epitaxial layer of germanium. Thus, costs can be drastically reduced as Si wafers are much more affordable than those made of III-V or Ge semiconductors, mainly due to the greater abundance of Si in the earth's crust. In addition, the silicon can be used directly as a bottom cell in a tandem architecture, further increasing the efficiency/cost ratio.

In this work we focus on the development of a new strategy for the epitaxial growth of III-V materials by using Plasma-Enhanced Chemical Vapor Deposition (PECVD) technique, with the aim of drastically reducing the processing costs in comparison with usual semiconductor deposition techniques such as Molecular Beam Epitaxy (MBE) and Metal Organic Chemical Vapor Deposition (MOCVD). Indeed, plasma assistance allows us to work at lower temperatures, thus reducing thermal stresses and hopefully defects but also the well-known issue of gallium mixing with silicon at high temperature (*meltback etching* in litterature). Moreover, PECVD enables low pressure operation, which reduces drastically the precursor consumption i.e. the main source of cost in a deposition process. Some works showing the feasibility of such an approach were published in the 1980s and the subject is again attracting interest due to the strong growth of the photovoltaic market. Here we will present the results of the GaN thin films grown by PECVD in terms of deposition conditions (temperature, pressure, plasma power, precursor flow rate and the crystalline (Fig. 1), morphological and compositional properties of the films obtained. Finally, we will show that the so-called *meltback etching* effect is reduced by the low temperature used in PECVD (inset Fig. 1).

In sum, these results open the prospect of a more affordable method for the production of III-V materials, thus addressing the important issue of costs for III-V photovoltaic industry with the possibility of obtaining large-scale epitaxial films, thanks to a low-cost substrate and deposition process.

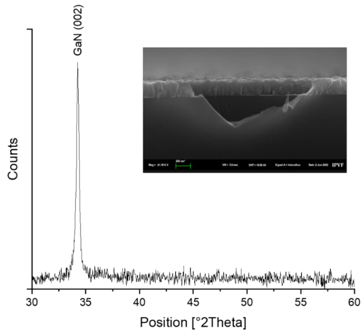

Figure - 1 XRD spectrum of a GaN thin film grown by PECVD
(inset shows a SEM cross section image of a hole in the c-Si substrate resulting from Ga diffusion)

POSTER #30

3 generations of green gas: from the circular economy of the territory to the resilience of gas networks

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As France’s main natural gas distribution system operator, GRDF distributes natural gas to more than 11 million customers every day for heating, cooking, mobility and industrial processes, regardless of their supplier. Performing a public service mission, we build, operate, and maintain the largest gas distribution network in Europe (200,715 km) safely, with the highest standards of quality. We are committed to promoting the use of renewable gas as a crucial part of the energy transition.

By 2050, 100% of the gas consumed in France could be renewable thanks to 3 generations of renewable gas:

- Methanization (of agricultural residues, biowaste, sewage sludge), regulated in France since 2010 and which is experiencing significant growth
- Pyrogasification and hydrothermal gasification (from industrial waste, solid recovered fuel, wood, plastic, etc.)
- Methanation, with a CO_2 recovery issue

The local production of green gas is fully integrated into a circular economy logic at the mesh of a territory and is a pillar of energy resilience. The gas infrastructure developed has the capacity to accommodate these new renewable gases. Also, the development of hydrogen will also be addressed, in a more prospective way.

As a public service actor, GRDF proposes to give its testimony on the challenges and perspectives in the development of green gases with the participants, during a poster session.

Artificial strong metal- support interaction on plasmonic core-shell nanostructures for photo(electro)catalytic reactions

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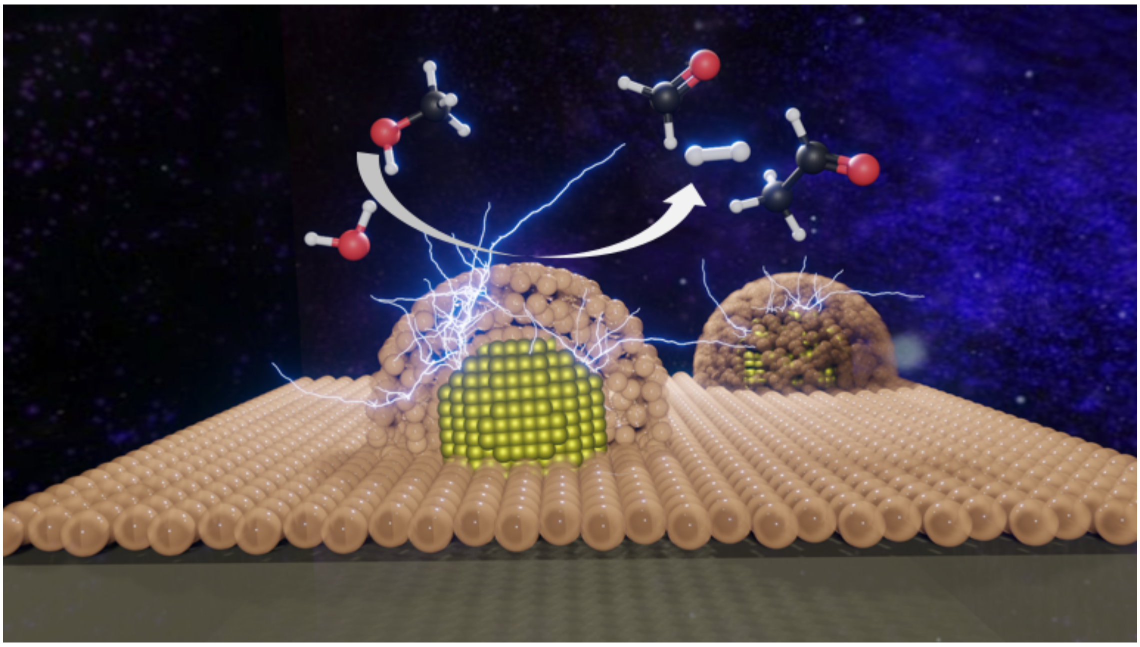
Photocatalysts mediated by metal nanoparticles have offered a huge contribution to photon-to-hydrogen conversion. Few studies, however, have mentioned encapsulation resulting from "strong metal-support interaction" (SMSI) in the context of photocatalysis. Therefore, further investigations should be performed to understand the effect of photocatalyst designs, the intrinsic activities of metallic nanoparticles, to name but a few, in photocatalytic redox reactions. From a perspective of reaching optimal photon-to-hydrogen conversion yield when anatase TiO_2 is coupled with plasmonic gold nanoparticles (NPs), two key factors are of pivotal importance: i) the efficiency of electron transfer among active sites and ii) the available reactive surface. In this study, we accomplish the construction of artificial SMSI-like nanostructures through a soft-chemistry process whereby a thin TiO_2 overlayer covers Au NPs highly dispersed on the surface of SiO_2 nanospheres. Comprehensive characterizations involving spectroscopy, microscopy, and electrochemistry evidenced that the synergetic metal–support interactions offer significant effect on the electronic properties, guarantee efficient photogenerated electron transfer and plasmonic charge carrier injection through SMSI region. In addition, we proposed a schematic mechanism to pinpoint the selectivity towards photo-redox pathways regarding photocatalyst configuration that produce hydrogen and value- added compounds – formaldehyde and acetaldehyde – on account of C-H activation and C-C coupling.



POSTER #32

Bioremoval of dyes in a microbial fuel cell by the fungus Trichoderma harzianum: a sustainable approach in energy production

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Large volumes of water are used in processing operations of textile industries. The presence of dyes, degrades the drinkability of the water. Among this group we found Violet crystal (VC) and methylene blue (BM). VC has been classified as potential carcinogenic compound as MB is a dye used in several applications like in medicine, biology, and textile industries. It is suspected to interfere with photosynthetic activity and the growth of biota. Dye removal with physical chemical methods are not sufficient for a complete removal and generate a large amount of sludge containing secondary pollutants. Biological methods are now well appreciated because they are very useful and often low-cost. Among them, microbial fuel cells (MCF) could be also considered for dye degradation and particularly using fungi (Mbokou[1]). MFC are bioelectrochemical systems. They can produce electricity by degradation of chemical compounds using microorganisms. After microorganism colonization, the bioanode can produce power by oxidation of the substrate. Microorganisms are often bacteria but sometimes fungi. The aim of this work was to develop an MFC using the fungi *Trichoderma harzianum* fungus for efficient VC and BM removal associated with high electrical performances*.* *T. harzianum* possess enzymes (i.e., laccase) that allow the degradation of molecules containing aromatic rings like MB and VC (Shabani[2]). The present MFC developed consisted in dual chambers separated by a cationic exchange membrane. The anode was made by *T. harzianum* cultivated on a carbon cloth, the cathode a carbon cloth. Two carbon clothes were tested (KIP and CSV). Results in Fig. 1

(as example for KIP) showed that MB was almost completely removed from the 100 mg.L^{-1} solution after 22h whatever the carbon cloth. VC was not completely removed, respectively 52% and 57% with KIP and CSV. The difference was explained by the difference in the number of aromatic structures in the two dyes. Maxima power densities observed were higher with KIP (65 W.m^{-3} with MB and 230 W.m^{-3} with VC). (Fig. 1 (b)) compared to CSV. External resistance with MB and VC were respectively 300 and 200 Ohms. KIP has a lower resistance and is thicker permitting a faster electrons collection and is more hydrophobic allowing better interaction with *T. harzianum* which is hydrophobic. So, KIP carbon cloth gave more intensity and power density than CSV.

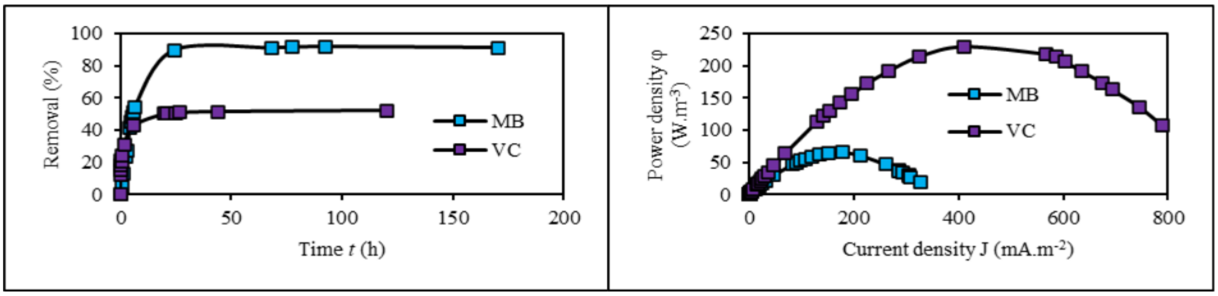

Figure 1 (a) Evolution of percentage of MB and VC removal through time. (b) Maxima power densities produced with MB and VC

POSTER #33

GaN nanowire-based piezoelectric devices for energy harvesting: Impact of the NW/polymer matrix composite

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Piezoelectric devices based on nanomaterials are a promising solution for energy harvesting applications. Due to their high-crystalline quality and their large surface-to-volume ratio, 1D-nanostructures present stronger piezoelectric response in comparison with their bulk and 2D-film counterparts. Piezoelectric active layer embedding NWs are consequently characterized by enhanced electromechanical conversion per surface unit. Combined with the specific properties of GaN, namely its high chemical and thermal stability as well as its radiation resistance, GaN NWs-based nanogenerators are perfectly suitable for powering micro-sensors and micro-actuators in medical or hostile environments.

Nanowire-based piezo-nanogenerators have shown their potential, with power densities in the µW/cm^2 under conditions close to what is found in the environment. Nevertheless, micro-devices often need electrical power in the hundreds of µW up to mW, either in continuous or in intermittent powering. Consequently, these nanogenerators need to be further improved to make the sensors and actuators autonomous. That amelioration requires an optimization of the active layer and of the design of the harvester, which are intrinsically linked. It must be conducted in regards of the environmental conditions in which the micro-device operates -frequencies and forces present-, and of their power need.

Our nanogenerators consist of a vertically oriented GaN NWs array embedded into a polymer matrix. The choice of the matrix is crucial to fully take advantage of the conversion efficiency of the NWs considering the given solicitation input. Moreover, besides influencing the mechanical response of the composite (NWs+matrix), the matrix also impacts its piezoelectrical response. For that reason, nanogenerators must be developed considering the composite NWs+matrix in the optimization with respect to the solicitation conditions and energy requirements.

We have investigated the influence of different polymer matrixes embedding the GaN NWs on the device conversion capacities. Their Young modulus and their influence on the surface charge density of the NWs, known to strongly affect the output voltage, have been considered. In addition, active layers without NWs -without the piezoelectric effect- were also considered to identify the other possible electromechanical effects. In the objective of applicative use, the transducers composed of the different NW/matrix composites were mechanically compressed in permanent contact mode, with forces and frequencies corresponding to environmental conditions: a few N in the 10-200 Hz range. The output voltage and output power were investigated, and the effect of the load resistance was also studied.

Heterometallic (M^{IV}/M^{II}) MOFs as a versatile platform for the photocatalytic overall water-splitting reaction

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Hydrogen is considered a serious alternative to fossil energy as it burns without producing any pollutants. Today, more than 90% of the hydrogen produced is from the steam reforming of fossil fuels (known as black hydrogen or grey hydrogen). Hydrogen production by electrolysis of water using electricity generated from renewable energy sources such as solar energy and wind energy is currently the primary source of green hydrogen. Photocatalytic overall water splitting produces hydrogen, converting solar energy into green hydrogen in one step. This simple, low-energy-intensive, and sustainable hydrogen production process can enrich the existing green hydrogen production system and provide more possibilities for green hydrogen production.

Metal-organic frameworks (MOFs), also known as porous coordination polymers (CPs), are crystalline solid materials formed by the orderly coordination of metal ions/clusters and organic ligands. Heterometallic metal-organic frameworks (HMOFs) are usually self-assembled by no less than two metals and organic ligands in an ordered synergistic array. Their high crystallinity, high porosity, and multifunctional catalytic sites promote HMOFs as potential candidates as heterogeneous catalysts, especially in the field of photocatalysis. In our quest for the development of MOFs suitable for photocatalytic hydrogen evolution reaction, we synthesized a series of high-valence (Zr, Ce, Hf) heterometallic metal-organic frameworks, in which unique Cu metallo-ligand and Ni metallo-ligand help these MOFs significantly improve the utilization of visible light. In this communication, the highly versatile structure of these heterometallic MOFs will be presented together with the photocatalytic studies that have shown very promising properties (up to 4.26 mmol H_2 $gcat^{-1}$ in 23 h) in overall water splitting under simulated sunlight irradiation.

POSTER #35

Ionic analysis of phosphorus doped-diamond homoepilayers grown with different carbon isotopic abundances

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Diamond has exceptional properties that make it a promising material for many applications in several fields. For several decades, many studies have been carried out to study the nature and the impact of impurities in diamond films synthesized by chemical vapor deposition (CVD). Doping impurities can be added in a controlled manner into the gas mixture during the growth process and incorporated into CVD diamond films. Among them, phosphorus is a donor when it replaces carbon of the crystal lattice. To date, it gives the highest n-type electronic conductivities. Nitrogen is also a well-known impurity in synthetic diamond. Coupled with vacancies (missing carbon atoms in the lattice, denoted V), it forms interesting N-V complexes for optically active centers, such as colored centers or single photon sources.

Recently, phosphorus donors in homoepitaxial diamond have been shown to increase the coherence time of N-V centers [1], paving the way for new applications in quantum technology. This breakthrough was achieved thanks to the progress made on the quality of CVD diamonds and in particular techniques allowing the elimination or reduction of undesirable defects such as the nuclear spins of the isotope 13 of carbon (^{13}C), obtained in a low range of doping in phosphorus ($< 1\mathrm{x}10^{17}$ at/cm^3) [2].

For several years, GEMaC studies n-type diamond through the synthesis of phosphorus-doped diamond films thanks to microwave plasma assisted CVD. Recently, a gas line dedicated to methane isotopically depleted in ^{13}C (^{13}C/^{12}C = 0.01% instead of 1.10% for natural methane) has been installed. Using standard growth conditions, homoepilayers were synthetized on commercial HPHT Ib (100) diamond substrates with a gaseous mixture of methane either isotopically depleted in ^{13}C, or of natural isotopy.

Samples were analyzed by secondary ion mass spectrometry (SIMS). Compared to the layer grown with natural isotopic carbon, nitrogen is detected in the ^{13}C-depleted layers which have higher thicknesses and higher phosphorus contents. These results suggest nitrogen contamination of the layer from the new gas line. The ionic analysis also gives the isotopic ratio of carbon in the layers grown with natural methane or ^{13}C isotopically depleted methane. The carbon-12 isotopic purity reaches 99.99966% (i.e. 0.00034% in ^{13}C) in ^{13}C-depleted homoepilayer against 99.989% for natural isotopic homoepilayer (i.e. 0.011% in ^{13}C). To our knowledge, this value is currently a record.

[1] E.D. Herbschleb et al. Nature Communications, 10, 3766 (2019).
[2] A. Watanabe et al., Carbon, 178 (2021), 294-300.

POSTER #36

Locally Ion Implantation and Annealing Effects in Diamond

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Diamond has demonstrated interesting properties for high power applications. However numerous technological obstacles make difficult the fabrication of power devices on diamond. Diamond doping in-situ gas phase is today the most efficient technique. In fact, the possibility to dope locally by ion implantation is indispensable for establishing a diamond manufacturing chain in particular to achieve the highest possible doping.

In 2014 successful incorporation of implanted phosphorus in (100) diamond donor sites show promising perspectives to process convinced implanted n-type doping [1]. However, the absence of dopant electrical activation after implantation and thermal annealing is a technological obstacle to be removed to achieve localized n-type and p-type doping.

In this work, we focus our attention on boron over-doped implanted diamond layer. We performed implantation on (100)-oriented diamond single crystals by high temperature beam line ion implantation and by beam line followed by a co-implantation plasma immersion ion implantation (PIII). The boron depth profiles in the implanted diamonds are measured by secondary ion mass spectrometry (SIMS). They confirm an almost constant concentration of implanted species at a 200 nm depth (box-profiles): 1.6×10^{20} B/cm3 for high temperature implantation. Plasma immersion ion implantation (PIII) add a boron concentration peak of $2\text{-}3\times10^{20}$ B/cm3 at diamond extreme surface. Transmission Electron Microscopy (TEM) images performed on as implanted samples indicate damages on diamond crystal induced by implantation, but no amorphization. After high thermal annealing at 1700°C during 30 min, SIMS analysis evidences the loss of the boron surface peak obtained by PIII while diamond recrystallization is observed by TEM together with an increase of the diamond surface roughness.

The comparison between the four-probes measurements on as implanted samples and after annealing shows a decrease of the measured sheet-resistance. This demonstrates a benefit of thermal annealing on the electrical activation of implanted boron. Hall measurements will complete these first results to evaluate the efficiency of both boron implantation and annealing conditions.

[1] Barjon et al. Physical Review B 89 (2014) 045201

Molecular engineering of hole transporting molecules for high efficient and enhanced thermal stability perovskite solar cell

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We report here the design and synthesis of different series of conjugated molecules for use as charge transporting materials in halide perovskite solar cells. The thermal, morphological, optical and electrochemical properties of all prepared compounds have been investigated in detail and a comparative discussion has been presented. Their characteristics have suggested that these molecules could be suitable for use as hole transporting materials in perovskite photovoltaic devices. The preliminary photovoltaic application have given devices with power conversion efficiency (PCE) around 17 %. Selected molecules have been subjected for further device optimization and in deep interface engineering (between the perovskite and hole transport layers) improving PCE to higher than 23 % and this champion PCE is even higher than that of the Spiro-OMeTAD-based device. Thermal stability test at 85°C for over 1000 h showed that the PSC employed novel HTM retains 86% of initial PCE, while the Spiro-MeOTAD-based PSC degrades unrecoverably. Time-of-flight secondary ion mass spectrometry studies combined with Fourier transformed infrared spectroscopy reveal that novel HTM shows much lower lithium ion diffusivity than spiro-MeOTAD due to a strong complexation of the lithium ion with HTM, which is responsible for the higher degree of thermal stability. Under optimized condition, the perovskite solar cells employed additive-free HTM gave a PCE of ca. 16%. This work delivers an important message that capturing mobile Li^+ in hole transporting layer is critical in designing novel HTM for improving thermal stability of PSCs. In addition, it also highlights the importance of interfacial engineering on the non-conventional HTM.

Capturing Mobile Lithium Ion in Molecular Hole Transporter Enhances Thermal Stability of Perovskite Solar Cells. S.-G. Kim, T. H. Le, T. de Monfreid, F. Goubard, **T.-T. Bui,** N.-G. Park *Advanced Materials* **2021**, *33,* 2007431.
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Selective Aqueous Electrocatalytic CO_2-to-CO Reduction with a Cobalt-based Molecular Cathode

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Electrochemical conversion of CO_2 into hydrocarbons and/or useful chemicals using clean electricity from renewable energy sources is a promising strategy to close the carbon cycle.[1] The preparation of molecular heterogeneous catalysts stands as an attractive alternative. These hybrid catalysts combine the robustness of material-based heterogeneous catalysts with the ease of tuning molecular structures which usually showcase better selectivity at lower overpotentials.[2] Various hybrid molecular catalysts relying on earth-abundant metals have been developed. In particular, Co-based ones showed great promises for CO_2 conversion once incorporated to electrolysers devices.[3] Over the past decade, the cobalt complex based on a tetraaza macrocyclic ligand (Figure 1) have shown promising activity for electrochemical CO_2 reduction under homogeneous organic conditions.[4,5] We modified the ligand scaffold of this complex in order to introduce a pyrene anchoring unit to allow its smooth immobilisation onto multi-walled carbon nanotube (MWCNT) based electrodes. The modified electrodes were fully characterised using standard electrochemical techniques. This new molecular cathode was then investigated for electrocatalytic CO_2 reduction in neutral aqueous media and showed currents up to 7 mA cm^{-2} and reasonable stability over time at a relatively low overpotential of 450 mV. From these electrolysis measurements a high CO selectivity and faradaic efficiency above 95% could be obtained, corresponding to TOF_{CO} values up to 3.00 s^{-1}. This hybrid catalyst matches the benchmark activities of other state-of-the-art cobalt catalysts.[3]

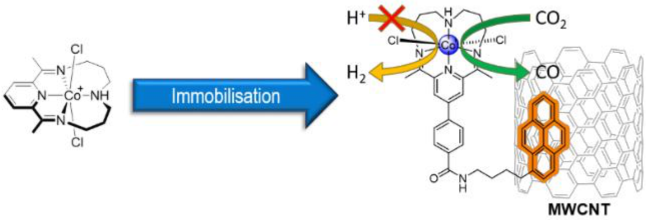

Figure 1: The tetraaza macrocyclic Co-complex (left) and the modified tetraaza macrocyclic complex for immobilisation onto MWCNT (right).

References

[1] O. S. Bushuyev, P. De Luna, C. T. Dinh, L. Tao, G. Saur, J. van de Lagemaat, S. O. Kelley, E. H. Sargent, *Joule* **2018**, *2*, 825–832.
[2] L. Sun, V. Reddu, A. C. Fisher, X. Wang, *Energy Environ. Sci.* **2020**, *13*, 374–403.
[3] K. Torbensen, B. Boudy, D. Joulié, N. von Wolff, M. Robert, *Current Opinion in Electrochemistry* **2020**, *24*, 49–55.
[4] D. C. Lacy, C. C. L. McCrory, J. C. Peters, *Inorg. Chem.* **2014**, *53*, 4980–4988.
[5] W. Nie, D. E. Tarnopol, C. C. L. McCrory, *J. Am. Chem. Soc.* **2021**, *143*, 3764–3778.

Structure-Engineered TiO_2: Harvesting Light for Photocatalytic H_2 Production

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Solar energy, as renewable energy with abundant resources, is the most attractive alternative to fossil fuels. Photocatalysis is a promising strategy to convert solar energy into green hydrogen energy.[1] Titanium dioxide (TiO_2) is the most popular photocatalyst due to its low cost, low toxicity and high chemical stability. However, the low solar energy utilization and the rapid photogenerated charge carriers recombination greatly restrict its industrialization progress. Designing highly efficient and inexpensive photocatalysts is an important topic in solar energy conversion technology.[2]

Structuring photocatalysts into photonic crystals or mesoporous structures are promising approaches to improve their photocatalytic activity. Inspired by Nature, we aim to artificially imitate the hierarchical structures, like in green leaves, to improve light scattering for efficient solar-to-hydrogen energy conversion. To this end, we proposed a one-pot method to design photonic mesostructured TiO_2 materials by taking advantage of the ability of cellulose nanocrystals (CNCs) to self-assemble into chiral nematic (CN) structures during solvent evaporation. This straightforward method can be easily spread to the coupling of TiO_2 with different metal oxides, such as Cu_xO, NiO, Bi_2O_3, etc.[3] Moreover, we designed novel black TiO_{2-x} film and TiO_x/C microsphere systems with CN structures to extend the light absorption region and light harvesting capability.[4]

1. G. D. Gesesse et al. *Nanoscale* **2018**, 20140-20146.
2. G. D. Gesesse et al. *Chem Mater* **2019** , 4851-4863.
3. C. Wang et al. *J Mater Chem A* **2020**, 1077 -10786.
4. C. Wang et al. *Chem Mater* 2021, 33, 17, 625–633.

POSTER #40

ZnO nanostructures based photocatalytic civil engineering materials development for urban pollution remediation

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Sustainable city development is facing many problems such as the pollution management. Hence, efforts have been made to reduce emission and to develop purification process, which are efficient and not energy consumer. Therefore, photocatalytic processes are being studied extensively as air and water treatments due to their ability to remove pollutants at different scales and places without requiring complex and expensive infrastructures. Photocatalytic infrastructures are indeed particularly attractive and suitable because they could use only solar energy (renewable and green energy) and a photocatalyst, which is mostly a wide bandgap metal oxide semiconductor, to degrade and mineralize pollutants. Therefore, the development of photocatalytic urban infrastructures (PUI) has emerged as a promising solution to address environmental pollution directly near emission sources, thereby avoiding pollutant accumulation and dispersion in urban areas. Due to the high surface-to-volume ratio and their excellent properties, since past years, research was focused on PUI development with TiO nanoparticles. Other semi-conductors were only explored recently. Due to its properties closed to TiO, ZnO nanostructures (NSs) appeared as a new promising candidate.

Therefore, we invested on development of ZnO NSs appropriate growth strategies by hydrothermal route depending on the substrate for developing PUI. Results demonstrated that tiling and aggregates could be functionalized by three simple operating steps: ( ) a seed layer deposition by horizontal impregnation in zinc acetate ethanolic solution followed by an annealing at C for min to create ZnO nucleation sites; ( ) a hydrothermal growth in presence of zinc salt and hexamethylenetetramine at C for h to obtain ZnO NSs; ( ) a post-annealing in min at C to improve the ZnO crystallinity. Whereas for the concretes and zinc roofs, a short seedless hydrothermal growth in h without post-annealing step is enough to produce ZnO NSs based photocatalytic surface. Characterization works demonstrated ZnO Wurtzite phase obtention with a band gap from . eV to . eV depending on the synthesis conditions and the substrate nature. The efficiency of theses smart materials was evaluated under solar light at laboratory scale for dye degradation and proved its good efficiency. Then, by scaling-up the process, a few square meters paved with tiling and bitumen road were easily produced to evaluate their photocatalytic activity at large scale under solar lamp in a climatic chamber (Sense-City, m) to reflect real atmospheric situations. Observations provided insights into their ability to remove simultaneously various pollutants from a real car exhaust. Thus, we propose to present work on appropriate and up-scaled ZnO NSs synthesis development depending on the substrate nature and the proved of efficiency for water depollution and for air pollution remediation under solar light at large scale.

POSTER #41

Why are photovoltaic/thermal solar collectors (PVT) yet on the way to be a key technology of buildings energy transition, especially for DHW preparation?

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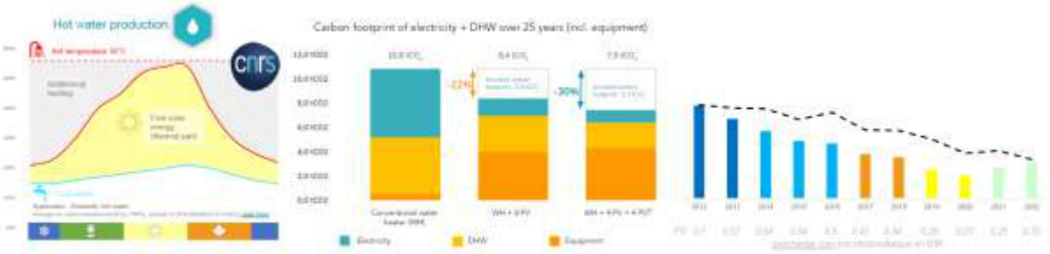
Photovoltaic-thermal solar technology (PVT) is the combination of a classic PV panel with a heat exchanger. Thus, such a hybrid panel both produces electricity and collects the excess heat from the solar irradiation. There is a wide range of concepts regarding the heat transfer fluid, the glazing, the presence of a light concentration add-on, the material of the heat exchanger, etc. [1] The focus of this work is the integration of unglazed water-based PVT collectors (like the one made by DualSun) in assisted domestic hot water (DHW) preparation systems. We want to show that the stars are aligned so that such a system for new buildings or in energy renovation becomes a major game player of energy transition.

First, in such a configuration, it is now recognized that this technology, in most scenarios, corresponds to a significant gain of energy production compared to a reference scenario with the same area of PV panel only. From [2], [3] and additional DualSun monitoring data, it could go up to 100% of reference scenario if it is well sized and controlled. Possible total autonomy over 4 months of the year is possible when it is south of Lyon (see Fig. 1) It was demonstrated that there is no risk of stagnation and even a possible slight increase of electricity production due to cooling. **Second**, a study conducted by ZHAW University in [4] demonstrates that these PVT panels for DHW preparation have a lower environmental impact compared to equivalent production by combining photovoltaic and solar thermal side by side. This study has been deepened from additional monitoring and modelling data so that we are able to quantify carbon footprint of any installation and configuration as Fig. 2 shows. **Third**, two mechanisms makes solar-assisted DHW preparation systems economically relevant for the end customer: the context of rising gas – and energy – prices (x2.3 in Dec. 2022 compared to 2016-2019 mean price for natural gas futures in [5]) and the PVT industry learning curve which have been driving prices down over the past ten years (see Fig. 3)



Figures- 1,2, 3: Solar thermal energy production over 1 year, carbon footprint of 3 configurations for DHW preparation in Lyon, DualSun PVT learning curve (€/Wp) and ratio on PV prices

PVT technology provides buildings renewable electricity and hot water in a significant amount at low cost and low carbon footprint. Such systems are robust, durable (at least 25 years like PV) and require low maintenance. However, it should be kept in mind that sizing, installation, connection, commissioning, and control strategy are at stake to ensure expected performance and durability. Ultimately, this study would benefit from the study of many other systems in which they are suitable to be integrated (e.g., PVT-HP for production of hot water for collective housing or even individual space heating).

POSTER #42

Nickel based anodes for the electro-oxidation of urea and synthetic urine in alkaline media

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The nitrogen removal biological process used in wastewater treatment plants (WWTPs) is energy intensive and not fully efficient. However, 85% of the nitrogen reaching WWTPs comes from urea in urine. Hence, a selective urine collection coupled with an electrochemical (EC) treatment could be an interesting alternative. Urea electrolysis can be performed efficiently on Ni catalysts in alkaline media, according to the overall reaction [1]:

$$CO(NH_2)_2\ (aq) + H_2O \rightarrow N_2\ (g) + 3H_2\ (g) + CO_2\ (g) \qquad (1)$$

Overall, nitrogen is removed from the solution as N_2 gaz. The degradation of urea (pollutant) at the anode is coupled to the production of H_2 (green fuel) at the cathode. At the anode, $Ni(OH)_2$ is first oxidized to NiOOH, then NiOOH chemically oxidizes urea, thus forming a catalytic cycle :

$$(E) \qquad 6Ni(OH)_2\ (s) + 6OH^- \rightarrow 6NiOOH\ (s) + 6H_2O + 6e^- \qquad (2)$$

$$(C) \qquad CO(NH_2)_2\ (aq) + 6NiOOH\ (s) + H_2O \rightarrow 6Ni(OH)2\ (s) + N_2\ (g) + CO_2\ (g) \qquad (3)$$

During EC cycling at anodic potentials, a layer of $Ni(OH)_2$/NiOOH is established on the Ni electrode surface. However, this native layer is very thin and made of the most compact allotropic forms (β-$Ni(OH)_2$/ β-NiOOH), which limit the number of available Ni catalytic sites. To increase this number, we studied the anodic deposition of NiOOH at the surface of Ni electrodes. Different charges have been tested and under optimal conditions, it allows to increase the number of active Ni sites by a factor of 50, thanks to the preferential formation of the less compact α-$Ni(OH)_2$/γ-NiOOH phases. These phases also have the advantage of being further away from the electro-oxidation wall of water, which limits the current fraction involved in this competing reaction.

Electrolysis of urea and synthetic urine solutions were performed at different potentials using these Ni/NiOOH electrodes. Compared to bare Ni, the average current was three times higher after NiOOH electrodeposition. Gaseous product analysis (GPC) confirmed the formation of N_2 and O_2 at the anode. However, ionic liquid chromatography of the electrolyte solutions revealed the formation of nitrites and cyanates indicating other routes than reaction (3) [2]. These results demonstrate the advantage of the electrochemical deposition of NiOOH to improve the performance of Ni electrodes for urea oxidation. In the future, it will also be necessary to improve their selectivity towards N_2 gas formation in order to avoid nitrogen processing in WWTPs.

[1] E. Urbańczyk et al., *J. Appl. Electrochem.* 46 (2016) 1011.
[2] L. Rebiai et al., *Electrochimica Acta,* 10 (2023) 141516.

The way to 100% MW scale renewable power systems: future challenges and promising solutions

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Under the Paris Agreement goal of achieving net-zero emissions by 2050, an increased share of solar, wind generations and other renewable technologies is on course to accelerate over the coming years. The technical control design of power electronics-based resources (PEs) that interface these technologies will be crucial for the stable operation of the electrical power system, considering frequency and voltage control loops at much faster timescales compared to synchronous machines. The existing power converters control schemes for such systems focus mostly on the stable operation of small-scale power system, which have different requirements from the Mega-Watt (MW) scale power system perspective. The main contribution of this work is to identify the future challenges of large power scale power systems and propose promising solutions for future low-inertia power systems that will be dominated by high penetration of different PEs control strategies; grid support, grid-following and grid-forming inverters.

Smart Building Simulation and Control

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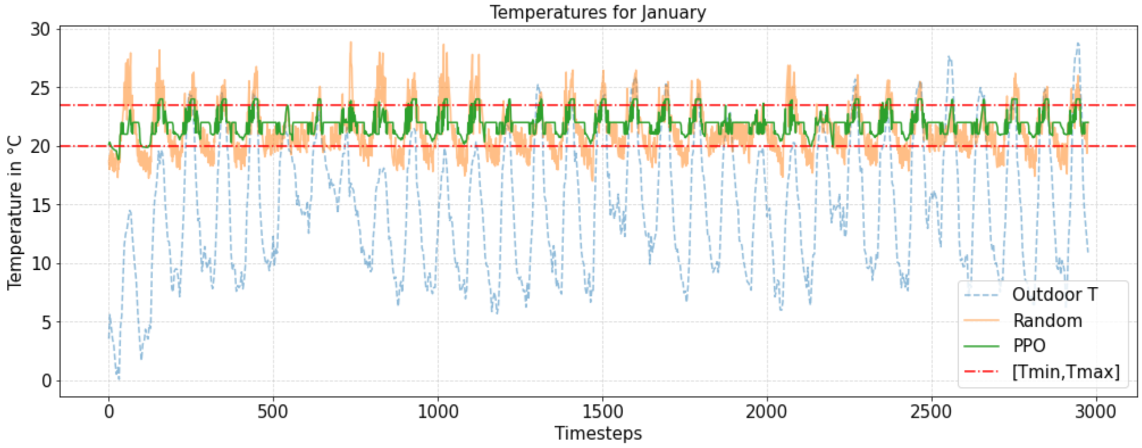
The electrification of energy needs of households (including heating, transportation and cooking) comes at a cost for our electrical system. As the storage of electricity remains costly, and new renewable electricity production (including photovoltaic cells and wind turbines) cannot be piloted, we must make our power consumption more flexible than before. However, this increased flexibility should have a minimal impact on comfort in order to be widely adopted.

The problematic is boiled down to an optimization problem, where comfort and energy consumption is in the target, and controllable devices such as heating, battery state of charge (Soc) etc. are in the actions. Data shortage is an expected difficulty, as raw data needs pre-processing to be meaningful. It would be too human intensive to treat all potential buildings. To solve this issue, our approach is to use thermal simulation and machine learning technics to create automatically the digital twin of any building, with limited data overhead.
Another potential issue is computation resource shortage for optimization purpose. The actions of shedding, charging or inner temperature regulation etc. are determined for each controllable device, and optimally in real-time. The increased demand of computational resource is non-negligible. In plus, some sensitive data cannot leave its locality and thus optimization should run locally with even less resources. Our solution is to run deep-learning based algorithm as deep reinforcement learning, which is computationally intensive during preparation phase but lightweight in deployment.

In short, we enter an era of increased power optimization needs, in which machine learning algorithms coupled with physics models can help us find the right strategies balancing user comfort, energy consumption, budget and carbon footprint in an automatic manner.



How R&D Can Help us Transform into a Clean H_2 Economy

Nicolas Dubouis

Programme Hydrogène, OneTech R&D, TotalEnergies

Reaching net-zero by 2050 is key to keep global warming under the ambitious target of 2°C by 2100. To develop this carbon free economy, one of the key challenges is to massively deploy renewable energy and cope with their intermittency. This technical challenge is an exciting challenge for scientists and especially for electrochemists who are leveraging their skills to develop cheap and efficient electricity storage solutions.

Electrolyzers and batteries will play a key role in this transition, and will be highlighted during the introduction of this seminar. Despite decades of research on batteries and electrolyzers, plenty of mystery remains regarding their behavior. Electrochemistry and material science will surely bring incremental improvements to these devices. But, to deploy them at the multi-GW scale by 2030, many industrial challenges will also need to be tackled. We will thus explain during this talk how the R&D department of a multi-energy company TotalEnergies can accompany this transition towards a GW-scale H_2 economy.

POSTER #46

Vertically aligned carbon nanotubes on aluminum foils: one-step synthesis from bio-sourced precursors and electrochemical characterization

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In order to meet the growing demand for devices able to store efficiently electrical energy, supercapacitors are emerging as good candidates due to their attractive balance between their energy density and their power density. However, their performance remains to be improved, which is highly dependent on the material of the electrodes.

Vertically aligned carbon nanotubes (VACNT) have been used instead of activated carbon as electrode for supercapacitors applications. Indeed, owing to their anisotropy, VACNT offer easy ionic diffusion pathway and great specific power [1]. The Aerosol Assisted Catalytic Chemical Vapor Deposition method allows the controlled one-step growth of Vertically Aligned Carbon Nanotubes (VACNT) carpets on conductive substrates [2,3]. This process has been optimized for the growth of dense VACNT on aluminium foils at low temperature (580 to 615°C) with acetylene as carbon precursor, leading to a single-step process that meets industrial requirements for the development of low cost, highly conducting and light supercapacitors electrodes[4]. In order to meet the challenges of energy transition, the industrial sector urgently needs to develop more acceptable processes from the point of view of environmental preservation and decarbonisation. The aim of this work is to replace the current carbon precursor (acetylene) by bio-based carbon sources compatible with an industrial process. Our approach is to first identify the most relevant carbon sources and to develop the synthesis conditions adjusted to these carbon sources in order to achieve VACNT growth at a temperature as low as the one required on thin Al collectors. The challenge is a better control of the growth process under these conditions where the physico-chemical phenomena at work can be modified or slowed down. Different bio-based precursors and their association (liquids and gas) were selected for a parametric study in order to assess the interest in term of VACNT growth. We will present first results on controlled growth of VACNT i e m f CNT le g h de i diame e a d a al e f he c e di g electrochemical storage performances (capacitance).

[1] H. Zhang, G. Cao, Y. Yang, Z. Gu, Comparison Between Electrochemical Properties of Aligned Carbon Nanotube Array and Entangled Carbon Nanotube Electrodes, J. Electrochem. Soc. 155 (2008) K19. https://doi.org/10.1149/1.2811864.

[2] M. Pinault, V. Pichot, H. Khodja, P. Launois, C. Reynaud, M. Mayne-L He mi e, E idence of Sequential Lift in Growth of Aligned Multiwalled Carbon Nanotube Multilayers, Nano Lett. 5 (2005) 2394 2398. https://doi.org/10.1021/nl051472k.

[3] C. Castro, M. Pinault, D. Porterat, C. Reynaud, M. Mayne-L He mi e, The role of hydrogen in the aerosol-assisted chemical vapor deposition process in producing thin and densely packed vertically aligned carbon nanotubes, Carbon. 61 (2013) 585 594. https://doi.org/10.1016/j.carbon.2013.05.040.

[4] F. Nassoy, M. Pinault, J. Descarpentries, T. Vignal, P. Banet, P.-E. Coulon, T. Goislard de Monsabert, H. Hauf, P.-H. Aubert, C. Reynaud, M. Mayne-L He mi e, Single-Step Synthesis of Vertically Aligned Carbon Nanotube Forest on Aluminium Foils, Nanomaterials. 9 (2019) 1590. https://doi.org/10.3390/nano911159

POSTER #47

Operation of Power Diodes at Cryogenic Temperature

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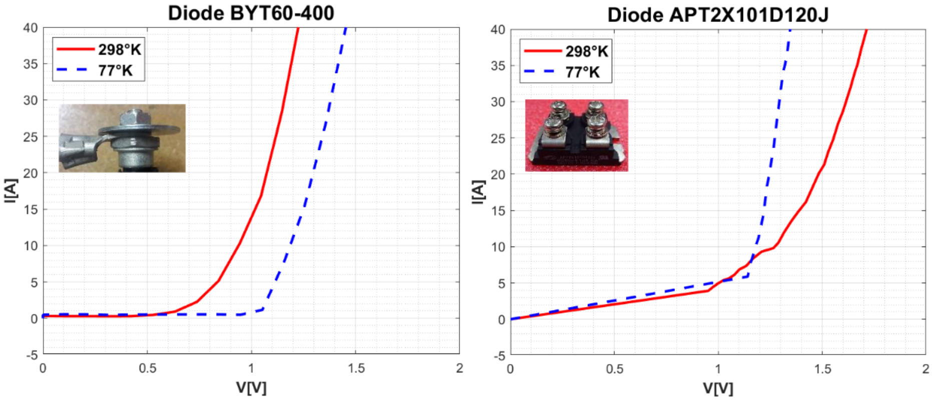
Power converters working at cryogenic temperature (Cryo-converters) can present several advantages, so studies related to this area has been of great interest to the aviation sector [1], notably if the refrigeration system is considered as free of charge as currently envisaged in the future aircraft.

This paper deals with the diode bridge operation maintained at a cryogenic temperature (77°K). Measurements carried out on different power diodes show that the electrical characteristic differs from one diode to another in the bridge at room and cryogenic temperature. These tests show that different types of diode technology are more conducive to operation at cryogenic temperatures than others.

For example, the BYT60-400 diode tested in the laboratory has a higher dynamic resistance and threshold voltage at cryogenic temperature than in room temperature (Figure 1a) when in comparison with the APT2X101D120J (Figure 1b). This result is coherent with the literature [2]. It is therefore essential to choose the best diode for the desired application.

Continuing, using only the APT2X101D120J diode, a 97 kW three-phase diode bridge was simulated in MATLAB/Simulink to compare the operation at the two temperatures using the diode characteristics obtained in the previous measurements. The simulation showed that a power gain of 80 W can be obtained by considering only the electrical characteristic of the diode and that the cooling is provided free of charge.

Considering these advantages, the next step will be to carry out a technical-economic analysis to compare both solutions in terms of their life cycle.



(a) (b)

Figure 1. Diode electrical characteristics in environmental and cryogenics temperature.

[1] Airbus Newsroom, “Cryogenics and superconductivity for aircraft, explained”. Disponible in: https://www.airbus.com/en/newsroom/stories/2021-03-cryogenics-and-superconductivity-for-aircraft-explained

[2] A. Elwakeel, Z. Feng, N. McNeill, M. Zhang, B. Williams and W. Yuan, "Study of Power Devices for Use in Phase-Leg at Cryogenic Temperature," in IEEE Transactions on Applied Superconductivity, vol. 31, no. 5, pp. 1-5, Aug. 2021, Art no. 5000205, doi: 10.1109/TASC.2021.3064544.

Semiconducting conjugated oligomers for photo-driven water oxidation

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Conjugated polymer (CP) nanostructures appear as **a new class of photocatalytic nanomaterials** that are very active under visible light for water treatment and photocatalytic solar water splitting (PSW). Previously we had developed the synthesis of conjugated ***polydiphenylbutadiyne*** (PDPB) nanowires using soft templates and studied their photocatalytic properties [1][2] The e PDPB a i e he i ed b UV -irradiation in mesophases, are very active photocatalysts under visible light for water depollution and water oxidation, without the presence of any sacrificial electron donors/acceptors or any co-catalysts. We showed that nanostructuration is the key factor for their photocatalytic activity [3][4]. In this study, a new monomer ***bis(pyridyl)butadiyne*** (BPB) containing pyridyl moieties that can form hydrogen bonds with water molecules, was synthesized using Sonogashira and Glaser coupling reactions. Introduction of hydrophilic functions like pyridyl can enhance dispersity in aqueous solutions while maintaining or even improving the photocatalytic activity, compared with the previously investigated PDPB. The new monomer BPB was synthesized and characterized by UV-Vis spectroscopy, nuclear magnetic resonance (NMR) and Fourier-transform infrared spectroscopy (FTIR). Using soft template method he ag al me ha e a d UV -irradiation, the monomer molecules were polymerized in the confined oil domain of mesophases to give new nanostructures ***poly(bis(pyridyl)butadiyne)*** (PBPB). Herein, we developed different PBPB nanostructures that were characterized by UV-Vis spectroscopy and FTIR. The photocatalytic activity of these nanostructures for water oxidation and H_2O_2 generation was studied using the triiodide method.

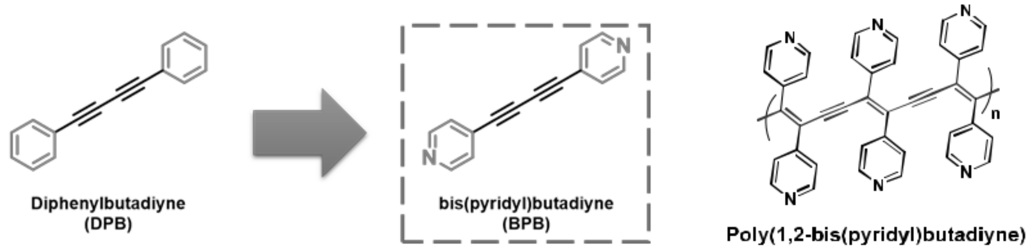

Figure 1. Structure of the new monomer BPB and the proposed structure of PBPB.

[1] Ghosh, S.; et al., New J. Chem. 2015, 39, 8311.
[2] Geetarani, S., et al., Chem. Mater. 2005, 17, 1505-1514
[3] Ghosh, S.; et al., Nat. Mater. 2015, 14 (5), 505-11.
[4] Patel, J.; et al., Chem. Sci. 2020, 11 (28), 7324-7328.

POSTER #49

Thermoelectric Properties of high-entropy rare-earth cobaltates

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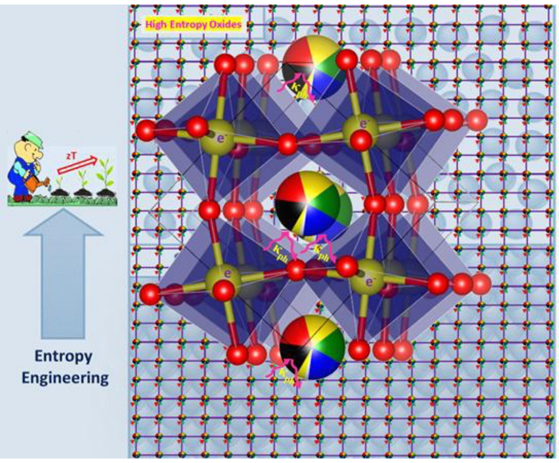
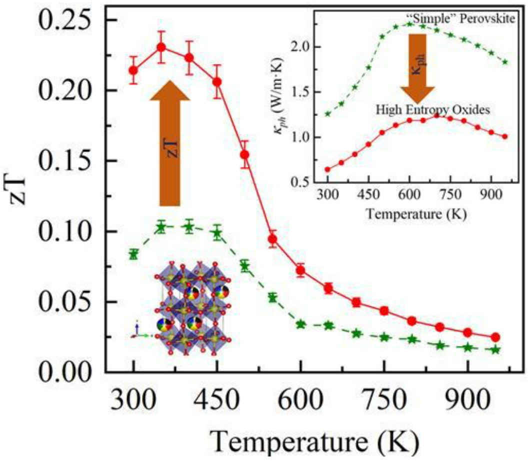
High-entropy concept introduced with a promising paradigm to obtain exotic physical properties has motivated us to explore the thermoelectric properties of Sr-substituted high-entropy rare-earth cobaltates i.e., $(LaNdPrSmEu)_{1-x}Sr_xCoO_3$ (0 x 0. 0). The structural analysis of the samples, synthesized using the standard solid-state route, confirms the orthorhombic structure with the *Pbnm* space group. The Seebeck coefficient and electrical resistivity decrease with rising Sr concentration as well as with an increase in temperature. The multiple A-site ions in high-entropy rare-earth cobaltates result in an improved Seebeck coefficient (α) compared to $La_{0.95}Sr_{0.05}CoO_3$, associated with a decrease in the Co-O-Co bond angle, which further enhances the power factor. The random distribution of cations at the rare-earth site results in a significant lowering of phonon thermal conductivity. As a result, a maximum figure of merit (zT) of 0.23 is obtained at 350 K for $(LaNdPrSmEu)_{0.95}Sr_{0.05}CoO_3$, which is one of the highest values of zT reported at this temperature for oxide materials. This study shows promise to decouple thermoelectric parameters using the high-entropy concept in several materials.





POSTER #50

3rd gas revolution: challenges and prospects for the development of renewable gases

Clothilde MARIUSSE, head of renewable gases – West Parisian Area, GRDF

As France's main natural gas distribution system operator, GRDF distributes natural gas to more than 11 million customers every day for heating, cooking, mobility and industrial processes, regardless of their supplier. Performing a public service mission, we build, operate, and maintain the largest gas distribution network in Europe (200,715 km) safely, with the highest standards of quality. We are committed to promoting the use of renewable gas as a crucial part of the energy transition.

Methanization (of agricultural residues, biowaste, sewage sludge), regulated in France since 2010, is experiencing significant growth: at the end of November 2022, nearly 500 anaerobic digestion sites are in operation; representing 8.5 TWh of renewable gas injected into the grid. This dynamic translates into 2 to 3 commissioning of biogas plants in France per week. The deposit of methanizable organic residues would even reach 140 TWh of biomethane produced by 2050 according to a study conducted in recent years by ADEME and network operators[1].

The development of local green gas production is made possible by significant sectoral crossovers between the energy sector and the sectors of:

- Agriculture (agricultural methanization)
- Waste (sewage sludge, …)
- Industry, in view of the forthcoming advent of second-generation green gases (pyrogasification and methanation), whose deposits will, among other things, be industrial and to be defined locally.

This sectoral convergence is also underpinned by local authorities promoting the emergence of projects, both from the point of view of energy planning, financing or local acceptability.

As a public service player, GRDF proposes to provide its testimony on the challenges and prospects in the development of green gases and to support the observation of sectoral convergences and the decentralization of green gas production.

POSTER #51

Photo-induced Fe(III)-hydroperoxo generation for oxygen atom transfer reaction

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Performing oxidation of organic substrates with atmospheric O_2 instead of hazardous chemical oxidants is highly desirable.[1] A viable approach is to use metal complexes as a platform to bind dioxygen and generate high valent metal-oxo species for oxygen atom transfer (OAT). Bioinspired non-heme complex $[(L_5)Fe^{II}]^{2+}$ has widely been studied for both O_2 and H_2O_2 activation, and reactive intermediates have been chemically generated and characterized.[2-4] In this work, the non-heme $[(L_5)Fe^{II}]^{2+}$ catalyst has been coupled with a photoredox module to perform photocatalytic OAT to 4-styrenesulfonate as a model substrate (Figure 1).[5] For the first time, we were able to characterize the photo-produced Fe(III)-hydroperoxo (Fe^{III}-OOH) intermediate in aqueous medium with EPR and UV-visible spectroscopies at different pH. The photocatalytic activity under these experimental conditions was confirmed by ^{1}H-NMR and HRMS.

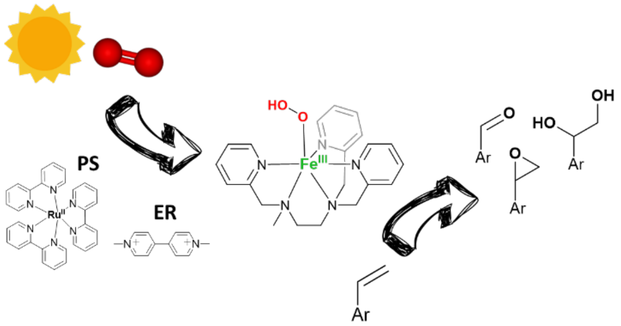

Figure 1: Schematic representation of the photo-generation of Fe(III)-hydroperoxo intermediate (**Fe^{III}-OOH**) from $[(L_5)Fe^{II}]^{2+}$ complex and oxygen atom transfer to the substrate. Photosensitizer (**PS**), electron relay (**ER**).

[1] Teles, J. H. Ch. 7 *Oxidation. In Applied Homogeneous Catalysis with Organometallic Compounds: A Comprehensive Handbook in four volumes*; **2018**; pp 465–568.
[2] A. J. Simaan, S. Döpner, F. Banse, S. Bourcier, G. Bouchoux, A. Boussac, P. Hildebrandt and J.-J. Girerd, *Eur. J. Inorg*, **2000**, *2000*, 1627–1633.
[3] A. Bohn, C. Chinaux-Chaix, K. Cheaib, R. Guillot, C. Herrero, K. Sénéchal-David, J.-N. Rebilly and F. Banse, *Dalton Trans*., **2019**, *48*, 17045–17051.
[4] A. Bohn, Theses, Université Paris Saclay (COmUE), **2018**.
[5] E. Pugliese, N. T. Vo, A. Boussac, F. Banse, Y. Mekmouche, J. Simaan, T. Tron, P. Gotico, M. Sircoglou, Z. Halime, W. Leibl, A. Aukauloo, *Chem. Sci*., **2022**, *13*, 12332-12339.

POSTER #52

Molecular imprinted butterfly-shaped micromotors for selective target recognition

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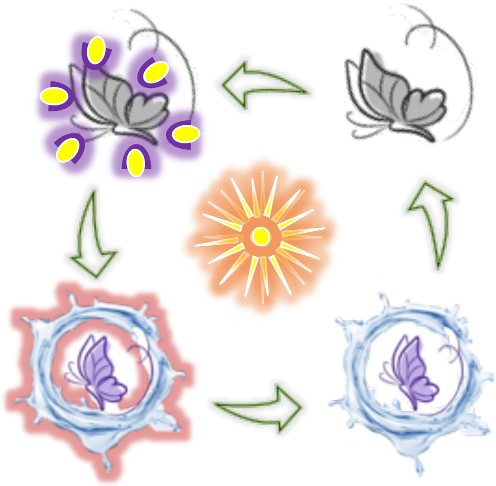
Analogue to photosynthetic systems, photoactive semiconductor-based micro/nanomotors display biomimetic features that enable unique light harvesting, energy conversion and interactions with the surroundings.[1] However, these artificial swimmers usually exhibit a non-selective character and ineffective target recognition, yielding poor surface analyte binding that affect the overall reactivity and motion efficiencies. Here, we present surface engineering of light-driven butterfly shaped micromotors by molecular imprinting polymer (MIP) for selective target recognition. Owing to the embedding of surface recognition sites, the micromotors showed a specific ability to degrade the target molecule in a mixture but also enabled their self-propulsion in the solution without requiring toxic fuels. This approach shows that a tailor-made design of semiconductor-based micromotors with specific target recognition cavities in their surface is a promising strategy to achieve selective catching of desired molecules that leads not only to higher reaction efficiencies but also to enable the motion in such compound. [2] The outcome of this investigation can be extended to other approaches involving sensing and detection of enzymes, proteins, viruses for biotechnological purposes. On the other hand, it also represents a unique strategy to enhance motion capabilities of single-component micromotors in a specific chemical environment containing more than one molecule in the matrix.



[1] K. Villa, H. Sopha, J. Zelenka, M. Motola, L. Dekanovsky, D. C. Beketova, J. M. Macak, T. Ruml, M. Pumera, *Small* **2022**, 2106612.

[2] X. Yuan, R.F. Campos, F. Garcés, K. Villa, *Small*, **2022**, 2207303.

POSTER #53

High-rate CO_2 Reduction to Formic Acid using Bismuth-based electrocatalysts

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Electrochemical reduction of CO_2 (CO_2R) into fuels and valuable chemical feedstocks using low-carbon electricity sources is a promising route to recycle CO_2 emissions. Formic acid has some of the highest market values among CO_2R products[1], due its wide range of applications in industrial processes, and particularly its excellent properties as a safe and convenient H_2 carrier[2,3]. In our study, we synthesized a bismuth catalyst for the selective electroreduction of CO_2 to formic acid. The catalyst activity was investigated using different type of electrochemical cells, from a standard H-type cell to more advanced systems enabling the production of formic acid at high rates with industrially-relevant current densities superior to -100 mA cm^{-2}. We also studied the influence of pH which is a key parameter for the catalytic performance of the system. While most studies only use neutral or alkaline electrolytes to inhibit the competitive hydrogen evolution reaction (HER), our catalytic system could maintain high selectivity of CO_2R in acidic conditions (pH 1). Acidic CO_2R has recently gathered a lot of interest as a way to improve the carbon efficiency of CO_2R processes by suppressing the formation of (bi)carbonate salts in the electrolyte and thus eliminating excessive costs related to electrolyte regenaration[4].

1. Nitopi, S. *et al.* Progress and Perspectives of Electrochemical CO2 Reduction on Copper in Aqueous Electrolyte. *Chem. Rev.* **119**, 7610–7672 (2019).
2. Aligoli, B., Nazmi, A. & Consultants, T. Chemical profile: Formic acid. *ICIS Chem. Bus.* **1**, 39 (2006).
3. He, T., Pachfule, P., Wu, H., Xu, Q. & Chen, P. Hydrogen carriers. *Nat. Rev. Mater.* **1**, (2016).
4. Huang, J. E. *et al.* CO2 electrolysis to multicarbon products in strong acid. *Science (80-.).* **372**, 1074– 1078

POSTER #54

New insights on the charge storage mechanism of thin films electrode materials by Raman spectroscopy

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Thin film solid-state Li-ion micro-batteries (TFMB) are promising candidates to power miniaturized sensors for Internet of Things (IoT) applications. Such applications have created a high demand for the battery systems to provide larger power and energy densities. To fulfil the performance requirements, both positive and negative electrodes with high storage capacities should be developed. A promising candidate for the positive electrode is the spinel $LiMn_{1.5}Ni_{0.5}O_4$ (LMNO) which exhibits a mean operating potential of 4.75 V vs. Li/Li^+, a theoretical specific capacity of 147 $mAh\cdot g^{-1}$, and is inexpensive due to use of high amount of low cost and environmentally benign manganese. On the other side, TiO_2 (anatase) is of great interest as negative electrode for TFMB because of its interesting capacity of 168 $mAh\ g^{-1}$ and operating potential of 1.5 V vs. Li^+/Li . Other advantages of TiO_2 are its rapid discharge and charge properties as well as its low cost and non-toxicity.

In this work, Raman spectroscopy is carried out to explore the short range environment in sputtered disordered LMNO and ALD- deposited TiO_2 thin films during the electrochemical process. Significant and reversible evolution of the Raman spectra is displayed in both cases during the electrochemical cycle, signifying reversible change in the metal-oxygen bond strength on Li^+ extraction/insertion. In the case of Li_xMNO ($0 \leq x \leq 1$), pertinent descriptors of the $Ni^{2+}/Ni^{3+}/Ni^{4+}$ species are identified in the Raman spectra, and a proper analysis of the Raman features gives access to their relative ratio in the LNMO thin film. The obtained results demonstrate that Raman spectroscopy is able to probe the electrode state of charge (SOC), which makes it an efficient and simple diagnostic tool to measure the self-discharge phenomenon occurring in the LMNO cathode. On the other hand, a Raman spectroscopy study performed on the anatase Li_xTiO_2 system ($0 \leq x \leq 0.5$) shows the homogeneous nature of the lithium insertion process in TiO_2 thin film electrodes. The structural transition from tetragonal TiO_2 to orthorhombic titanate Li_xTiO_2 is clearly evidenced by Raman spectroscopy. For the first time in the thin film configuration, the rich Raman fingerprint of the pure orthorhombic $Li_{0.5}TiO_2$ phase, made of 20 components, is fully observed for $x = 0.5$. The high quality of the Raman spectra obtained on the thin film electrodes allows quantifying the amount of orthorhombic phase at different oxidation-reduction states, showing again the efficiency of Raman spectroscopy to evaluate the SOC of the TiO_2 thin film electrode material.

NOTES

NOTES

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