



**CQMF
QCAM**

COLLOQUE ÉTUDIANT
STUDENT SYMPOSIUM

Le VENDREDI, 8 DÉCEMBRE 2023
FRIDAY, DECEMBER 8TH 2023

**CARNET DE RÉSUMÉS
ABSTRACT BOOKLET**

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1. Commanditaires/Sponsors



**Fonds de recherche
Nature et
technologies**

Québec 



UQTR









Université du Québec
à Trois-Rivières

Nous remercions chaleureusement nos commanditaires du Colloque annuel du CQMF 2023 pour leur soutien.

We sincerely thank our sponsors of the 2023 QCAM Annual Symposium for their support.

Programme

9:30-10:00	 Inscriptions 		Atrium
10:00-10:30	CQMF concours vidéo et vote		1200 Albert-Tessier
	Session 1 - Énergie 1026 Ringuet	Session 2 - Énergie et Développement Durable 1200 Albert-Tessier	Session 3 - Auto-assemblage Moléculaire et Biomédical 1092 Ringuet
10:30-10:50	Fola S. Akogun <i>Molecular Carbazole-based complexes as catalysts for CO₂ reduction reaction</i>	Brunilda Rica <i>Introducing the concept of low-concentration organic acid leaching to recycle graphite from failed anodes</i>	Johann Sosoe <i>Towards molecular materials derived from benzenetetramine and related compounds</i>
10:50-11:10	Maryam Alihosseini <i>In-situ study of surface modification on Ti₃C₂ as a catalyst for hydrogen evolution reaction</i>	Amir Khojastehnezhad <i>Rapid, Mild and Catalytic Synthesis of 2D and 3D Covalent Organic Frameworks</i>	Aaron Gabriel Nunez Avila <i>Exploring Polymorphism: Hydrochloride Salts of Pitolisant and Analogues</i>
11:10-11:30	Mohammad Masaellii <i>Enhanced hydrogen storage properties of TiZrVHfNb_{1-x}Fe_x high-entropy alloys by modifying the Fe content</i>	Faranak Hosseini <i>Effect of Zr on hydrogen storage characteristics of TiFe alloy</i>	Babak Omranpour Shahreza <i>Sustainable development in biocompatible metals: Nanostructured tantalum with enhanced tribological and mechanical properties</i>
11:30-11:50	Ludmila dos S. Madalena <i>Oxygen Reduction Reaction on Graphene Oxide Functionalized with Aminobenzoic Acid</i>	Issa Malam Mahamadou <i>One-spot NiTe₂@GO Transition-Metal Dichalcogenides electrocatalyst for hydrogen evolution reaction (HER)</i>	
12:00-12:20	 Pause café 		Atrium
12:20-13:00	Atelier: Équité, diversité et inclusion en recherche.		1200 Albert-Tessier
13:00-14:00	 Pause Dîner 		Atrium

14:00-14:20

Session 4 - Énergie

1026 Ringuet

Imane En-Najien
The Impact of Oxygen Vacancies in WO₃ Photoanodes Engineered through a One-Step Electrochemical Treatment for Efficient Photoelectrochemical Water Splitting

Session 5 - Nanosciences

1200 Albert-Tessier

Pedro Mena-Giraldo
Near-infrared remote-driven Janus micromotors for photon upconversion applications

Session 6 - Polymères

1092 Ringuet

Ahmad Al Shboul
Advancing Temperature Sensing Technology: Gt/PS Nanocomposite based Wearable Sensor for Dynamic Environments

14:20-14:40

Ngara Diouf

Matériaux Magnétiques Micro-Poreux N-Hétérocycliques Fonctionnalisés par Nanoparticules de Au, Pt, Ag pour des Performances améliorées dans le Stockage d'Énergie des Supercondensateurs

Jaspal Singh

Boosted photocatalytic and SERS Capability of Ag nanoparticles functionalized MoS₂ nanoflakes

Olivier Roy

Nanofiber Materials with High Reflectance and Polarization Contrast in the Mid-Infrared Spectral Range

14:40-15:00

Zujhar Singh

Effect of Increasing Ligand Conjugation in Cu(I) Photosensitizers on NiO Semiconductor Surfaces

Lebar Ghizelane

Étude des effets de différents COF 2D liés à l'imine pour une élimination efficace de la rhodamine b

15:00-15:20

Samuel Lemay

Simulations numériques de catalyseurs moléculaires pour la production d'hydrogène

Hichem Gamraoui

Enhanced Catalytic Efficiency of Nitrophenol Reduction through Size-Controlled Synthesis of Gold Nanoparticles within Covalent Organic Frameworks

15:20-16:40

Visite du plan pilote, Innofibre

Visite simultanée en sous-groupes de 10 à 12 personnes

Départ du devant des cubes



Session d'affiches



Atrium

16:40-18:00

Auto-assemblage Moléculaire

- 1) PohYing Fong
- 2) Louise Gourdelier
- 3) Mostafa Eesae
- 4) Maryam Lormahdiabadi
- 5) Heriniaina Randriamiharisoa

Polymères

- 12) Imen Hamouda
- 13) Nkana Nkanagilbert Romeo
- 14) Cephas Amoah
- 15) Masoud Tayefi
- 16) Saba Goharshenasmoghadam

Énergie

- 18) Giuliana Lazzaro
- 19) Brittany Pelletier-Villeneuve
- 20) Alborz Bavandsavadkouhi
- 21) Manon Saget
- 22) Rupinder Kaur
- 23) Arindam Saha
- 24) Houssam-Eddine Nemamcha
- 25) Adela Abidi
- 26) Natalia Vargas Perdomo

Développement Durable

- 6) Safa Ladhari
- 7) Payman Ghassemi
- 8) Lucia Švandová
- 9) Bendhiba Badredineberfai
- 10) David Nadeau
- 11) Luis Alfonso Paramo Serrano

Matériaux pour applications biomédicales

- 17) Dridi Donia

2. Mot de bienvenue/Welcoming remarks

C'est avec grand plaisir que le comité étudiant du QCAM vous accueille à l'Université du Québec à Trois-Rivières pour le Symposium étudiant du QCAM 2023. Ce sera l'occasion de mettre en valeur les travaux de recherche des étudiants de notre communauté et de stimuler le dialogue entre professeurs et étudiants.

Ce carnet de résumés contient l'horaire de la journée, le concours de vidéos scientifiques CQMF/QCAM, l'atelier équité, diversité et inclusion (EDI), la visite de l'usine pilote (Innofibre), les résumés des exposés des étudiants (triés par séance de présentation), les titres des présentations par affiches.

Nous encourageons les conversations et les discussions en réseautage entre étudiants diplômés, postdoctorants et professeurs pour renforcer la recherche au Québec. Nous vous invitons également à rester jusqu'à la fin de la journée pour célébrer les lauréats du concours de vidéos scientifiques, des présentations orales et par affiches,

Le comité étudiant du QCAM

It is with great pleasure that the QCAM student committee welcomes you to the Université du Québec à Trois-Rivières for the 2023 QCAM Student Symposium. This will be an opportunity to highlight the research work of students from our community and to stimulate dialogue between professors and students.

This *abstract booklet* contains the schedule for the day, CQMF/QCAM science video competition, equity diversity and inclusion (EDI) workshop, pilot plant visit (Innofibre), abstracts of the student talks (sorted by presentation session), titles of the poster presentations.

We encourage networking conversations and discussion among graduate students, post docs and professors to strengthen the research in Quebec. We also invite you to stay until the end of the day to celebrate the awardees from the science video contest, oral and poster presentations,

The QCAM student committee

3. Activities

CQMF/QCAM science video contest

Inside the laboratory

Check out the submissions for this year video contest, where students, postdocs and researchers had the opportunity to share the exciting research happening in their laboratories.

French

Marco Assis, ETS: <https://youtu.be/ojgs11SrvsM>

Caroline St-Antoine, UdeM: <https://www.youtube.com/watch?v=yxdhAVTrsRw>

English

Ameer Nizami, Concordia: <https://www.youtube.com/watch?v=m5Zq85RMsfq>

Yiwei Jiang, McGill: <https://youtu.be/TPZIZfvZ-0Q>

To vote for the video you liked the most, please follow the link below or scan the QR code which will direct you to the voting form.

https://form.jotform.com/qcam_cqmf/voting-contest-based-on-video



Flash poster presentation (1 min each)

Manon Saget: NEW BIO-BASED COATINGS FOR OPV ENCAPSULATION

Safa Ladhari: Évaluation de l'activité biologique de nouveaux matériaux textiles antimicrobiens et biodégradables pour les équipements de protection

EDI workshop

Équité, diversité et inclusion en recherche.

Geneviève Côté, M.A. (elle, she, her) |Conseillère en équité, diversité et inclusion
Service du développement humain et organisationnel |Université du Québec à Trois-
Rivières

Pilot plant visit

Innofibre "biomass-based eco-products and eco-fuels"

Innofibre's pilot plant concerns pulp and paper process and cellulosic products development. In addition, I2E3 and innofibre have research labs on biomass valorization, éco-products and energy that will be visited.

4. Résumés des présentations/Talks abstracts

Séance/Session 1 – Energie

Oxygen Reduction Reaction on Graphene Oxide Functionalized with Aminobenzoic Acid

Ludmila dos S. Madalena, Fausto Eduardo Bimbi Junior^b, Yuting Leia, Benjamin Diby Ossoyona, Jiyun Chena, Marcos R. V. Lanzab, Ana C. Tavaresa

Institut National de la Recherche Scientifique - Énergie Matériaux Télécommunications

Nowadays, most of the hydrogen peroxide (H_2O_2) production is intended for the paper/cellulose and textile industries, as well as environmental remediation [1]. The H_2O_2 can be produced electrochemically in adjustable concentration through the oxygen reduction reaction (ORR). This electrochemical reaction allows for the decentralized production of H_2O_2 , overcoming the main environmental and safety challenges of the traditional anthraquinone process [2,3]. The use of selective catalytic materials capable of reducing oxygen exclusively to H_2O_2 via a two-electron process is required. Considerable attention has been given to graphene-based materials, because of their high specific surface area, good electrical conductivity, tunable chemistry, and high activity for ORR [4].

Here we will present our studies on the electrocatalytic activity for ORR of graphene-based catalysts produced by one-step electrochemical exfoliation of graphite foil in the presence of 4-aminobenzoic acid in different concentrations (from 0 to 40 mM) [5]. The graphene oxide materials (EGO) modified with 4-ABA (EGO-ABA) had their electrochemical performances evaluated by cyclic voltammetry (CV) and linear sweep voltammetry (LSV) techniques, using the Rotating Ring Disk Electrode (RRDE) in alkaline and acid media [5].

The cyclic voltammograms recorded in alkaline medium for the EGO-ABA's catalysts showed a higher electrochemical surface area for EGO-ABA-5mM catalyst compared to unmodified EGO. Among the catalysts, EGO-ABA-10 showed the highest ORR activity in alkaline medium with a more positive onset potential for ORR (-0.245 V vs SCE vs -0.265V V vs SCE for unmodified EGO). However, EGO exhibited ca. 82% of selectivity for H_2O_2 electrogeneration, thus larger than that of the EGO-ABA's materials with values varying between 64% and 71%. Instead in acid medium, all catalysts were found to reduce oxygen mostly to H_2O (four-electron process) which is of relevance for fuel cells. The highest selectivity for H_2O was also found for EGO-ABA-10 (93% vs 80% for EGO). The effect of the composition of the EGO and EGO-ABA catalysts on their activity and selectivity for ORR in the different media will be discussed.

In-situ study of surface modification on Ti_3C_2 as a catalyst for hydrogen evolution reaction

Maryam Alihosseini, Guillaume Goubert, Samaneh Salek Esfahani, Joshua Byers

Université du Québec à Montréal

Since the discovery of graphene, two-dimensional (2D) materials have become an active area of research in material science and chemistry. As a result, new 2D materials like transition metal dichalcogenides (e.g. MoS_2 , WS_2), layered double hydroxides (LDHs) or black phosphorous have been introduced. MXenes are a family of two-dimensional materials of transition metal carbides or nitrides, they have the general formula $M_{n+1}X_nT_x$ where M is a transition metal, X is carbon or nitrogen and T_x is surface terminations, such as -O, -OH, -F or -Cl. MXenes are synthesized by selective etching of A layers from a MAX phase precursor ($M_{n+1}AX_n$), where A is an element from the group IIIA or IVA, usually Al.¹

A diverse combination of transition metals and C/N leads to the expansion of the MXene family with interesting functional properties. Surface-active sites, high conductivity, hydrophilic nature, optical properties, and easy production are the major reasons that make MXenes a promising material for energy storage systems and electrocatalytic applications². However, poor stability in oxidating environments and restacking limit their performance. It has been shown that modification of surface termination T_x and defect engineering are promising avenues to enhance the electrocatalytic activity of MXenes.³

In this work, the titanium carbide ($Ti_3C_2T_x$) was synthesized as single flakes through a soft delamination method in which a solution of HF and HCl is used as an etchant solution and KOH was used for post-synthetic modification. KOH helps reducing the presence of -F terminations to improve activity towards the Hydrogen Evolution Reaction (HER). The electrocatalytic activity of modified and unmodified $Ti_3C_2T_x$ was studied in bulk electrochemical cells as well as using Scanning Electrochemical Cell microscopy (SECCM) to study the behavior of single flakes. *In situ Raman* spectroscopy allowed us to follow the change in the chemical nature of the $Ti_3C_2T_x$ surface with the presence of KOH and with the applied potential.

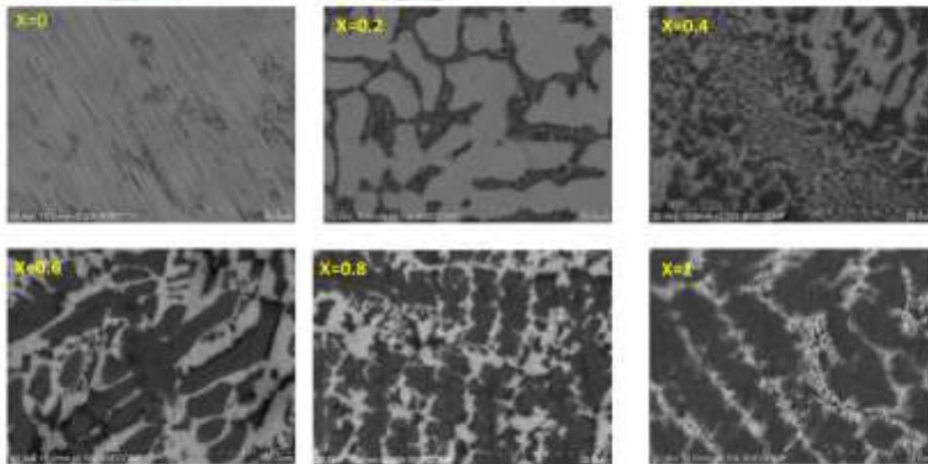
Our *in-situ* studies combining spectroscopy and electrochemical microscopy offer unique opportunities to guide the synthesis of higher-performance electrocatalytic materials, in agreement with the *advanced materials for energy applications* research theme of CQMF.

Enhanced hydrogen storage properties of $\text{TiZrVHfNb}_{1-x}\text{Fe}_x$ high-entropy alloys by modifying the Fe content

Mohammad Masaeli, Jacques Huot

Universite du Québec à Trois-Rivières

Hydrogen has emerged as a promising energy carrier for a sustainable and clean energy future. One of the key challenges in harnessing hydrogen's potential lies in efficient and safe storage methods. High-entropy alloys (HEAs) have gained significant attention due to their exceptional structural stability and tunable properties. ZrTiVHfNb high-entropy alloys have shown great potential as a hydrogen storage material due to their appreciable capacity. In this study, transition metal Fe was used to improve the hydrogen storage properties of the equimolar ZrTiVHfNb alloy by substituting Nb by Fe to form alloys of compositions $\text{ZrTiVHfNb}_{1-x}\text{Fe}_x$ ($x = 0, 0.2, 0.4, 0.6, 0.8, 1$). The microstructure evolution and hydrogen storage properties. The results show that the $\text{ZrTiVHfNb}_{1-x}\text{Fe}_x$ alloys are composed of a hexagonal C14 Laves phase and a Body-centered Cubic (BCC) phase. The fraction of the C14 Laves phase increases with increasing iron content. The $\text{ZrTiVHfNb}_{1-x}\text{Fe}_x$ alloys show enhanced hydrogenation kinetics and activation in room temperature. Notably, the ZrTiVHfNb alloy can reversely absorb 2.1 wt. % hydrogen at 350°C under 2 MPa H_2 . The increased fraction of the C14 Laves phase lead to the increase of hydrogenation rates. Moreover, the increased Fe content leads to easy activation even at room temperature and under 1.2 Mpa of hydrogen pressure.

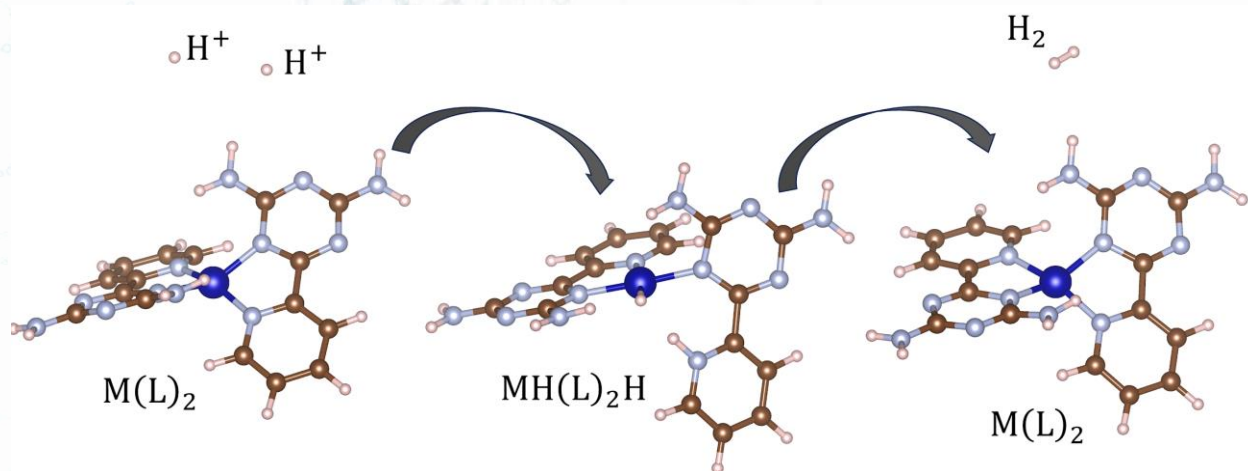


Simulations numériques de catalyseurs moléculaires pour la production d'hydrogène

Samuel Lemay, Gabriel Antonius

Université du Québec à Trois-Rivières

Les catalyseurs moléculaires peuvent être utilisés afin d'améliorer de façon significative l'efficacité de la réaction d'évolution d'hydrogène (HER) dans les systèmes d'électrocatalyse et de photocatalyse [1,2]. Nous étudions une classe de catalyseurs sans métaux nobles composés d'un métal de transition et de deux ligands organiques de formule chimique $M(L)_2$ où $M=Co, Cu, Ni$. Cette classe de molécules possède de bonnes propriétés catalytiques à la fois pour l'électrocatalyse et la photocatalyse [3,4]. Nous utilisons la théorie de la fonctionnelle de la densité, afin de simuler pour plusieurs de ces catalyseurs les différents cycles catalytiques possibles. Ces calculs nous permettent ainsi de déterminer quels sont les cycles énergétiquement favorables et quelles sont les étapes limitantes. Nous utilisons le logiciel Orca afin de déterminer l'énergie électronique, les contributions des différents modes de vibrations à l'énergie libre et l'effet du solvant.

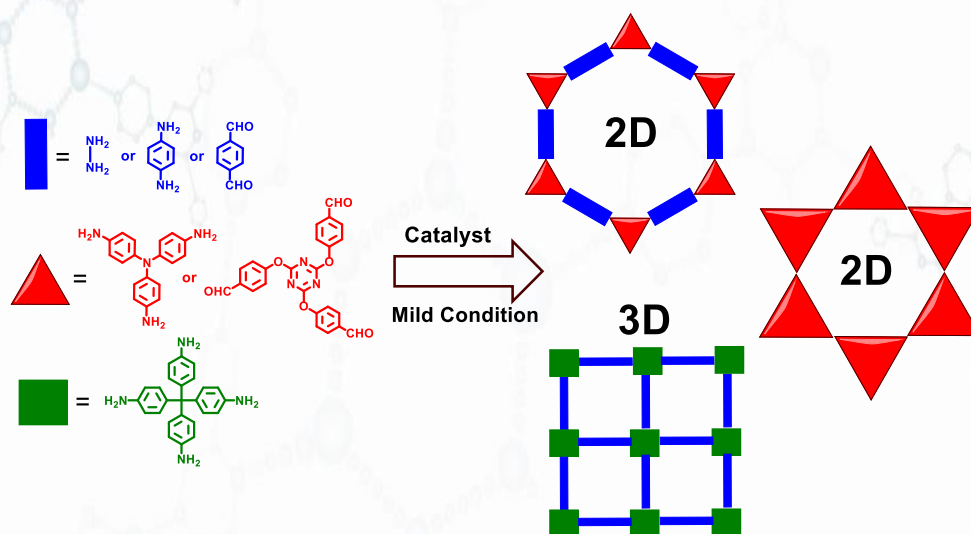


Rapid mild and catalytic synthesis of 2D and 3D covalent organic frameworks

Amir Khojastehnezhad, and Mohamed Siaj

Université de Québec a Montréal

In this research, a new approach based on Keggin heteropoly acids (HPAs) has been presented for the mild and fast synthesis of five different structures of imine and azine-linked two-dimensional (2D) and three-dimensional (3D) covalent organic frameworks (COFs). Traditionally, these crystalline materials have been synthesized via the Schiff base polycondensation reaction between different aldehydes and amines at harsh condition and in the presence of acetic acid [1-3]. Herein, the Keggin-type heteropolyacid has been used as catalyst to speed up the synthesis of 2D and 3D COFs and improve their materials quality. The catalyst led to prepare the imine and azine-linked COFs with high crystallinity and porosity under mild condition and short reaction time. According to the results, the amine building blocks with two amine functional groups, formed the COFs with higher crystallinity, porosity, and yield compared to amine with three functional groups and non-planar structure.



Introducing the concept of low-concentration organic acid leaching to recycle graphite from failed anodes

Brunilda Rica, Elsa Briqueleur, Denis Mankovsky, Ilona Royer, Mickael Dollé and Karen C.

Université de Québec à Montréal

Recycling graphite from Li-ion battery (LIB) waste plays an important role in increasing accessibility of graphite resources and sustainable recovery. This study aims to purify graphite from failed anodes in LIB manufacturing by focusing on the most common contaminant: copper, used as the current collector in LIB anodes.

A new, three-step scalable and environmentally friendly treatment approach was used: mechanical sieving to eliminate Cu chunks ($> 45 \mu\text{m}$), then dilute organic acid leaching of Cu residues and finally low-temperature thermal treatment. This approach provides a cost-effective and sustainable method in industrial settings to recycle failed (i.e., out-of-specification) anodes during the early stages of battery manufacturing.

The following experimental parameters were studied to evaluate Cu leaching efficiency: solid-to-liquid ratio, temperature, concentration, time and stirring speed. Leaching efficiency was quantified by measuring the Cu concentration in leachates by Microwave Plasma – Atomic Emission Spectroscopy (MP-AES). The surface morphology and elemental composition of leached and thermally treated purified graphite were analysed by Scanning Electron Microscopy-EDS (SEM) and Laser Induced Breakdown Spectroscopy (LIBS). The specific surface area and crystallographic parameters of the purified graphite were measured by Braunauer–Emmett–Teller Analysis (BET) and X-Ray Diffraction (XRD), respectively. The electrochemical performance of our purified graphite was evaluated by galvanostatic cycling with potential limitation *versus* Li^+/Li .

This study on sustainable recycling of graphite from failed anodes addresses two important issues. The first is the [upcoming](#) LIB recycling regulations, which will impose the recycling of graphite and other LIB components within the region of waste generation. The second is the increasing demand for metallic Cu and graphite in the global supply chain and demand for LIB increases.

Hydrogen storage characteristics of TiFe alloy

Faranak Hosseini, Jacques Huot

Université du Québec à Trois-Rivières

Hydrogen as an energy carrier is increasingly coming into focus in industry, as part of the promotion of renewable energies for environmental protection. Various hydrogen storage technologies are being explored. Metal hydrides are known as good candidates for solid-state hydrogen storage due to their sufficiently high gravimetric hydrogen capacity, extraordinarily high volumetric capacity, and desirable working temperature and pressure Conditions. FeTi-based alloys have shown great potential for hydrogen storage applications due to their high hydrogen storage capacity of 1.86 wt.% at low pressure at room temperature. First hydrogenation or activation of FeTi is usually slow at room temperature due to FeTi being highly sensitive to air and a passivation layer formed on the surface which acts as a barrier for hydrogen diffusion. The first stage of activation somehow disrupts the oxygen film and initiates hydrogenation. In this research, the hydrogen absorption properties of FeTi and FeTi+4wt.%Zr will be compared. Both of the alloys were prepared by arc-melting in argon atmosphere. FeTi alloy was not activated at 90 °C, and a hydrogen pressure of 4000 kPa. But FeTi+4wt.%Zr was activated without any previous heat treatment and reached the capacity of 1.6 wt.%.

One spot NiTe₂@GO transition metal dichalcogenides electrocatalyst for hydrogen evolution reaction (HER)

Issa Malam Mahamadou, Sujitra Poorahong, Mohamed Siaj

Université du Québec à Montréal

The hydrogen evolution reaction (HER) is an effective method for hydrogen production, addressing energy challenges. In this context, NiTe₂@rGO electrocatalyst has been prepared. Given tellurium's classification as a chalcogen, when combined with a transition metal, it can create an electrocatalyst suitable for HER. The synthesis of NiTe₂@rGO was achieved through the hydrothermal method. Experiments in acidic conditions with both NiTe₂ and NiTe₂@rGO revealed that NiTe₂@rGO exhibits satisfactory performance in HER. It has an overpotential of 325 mV against RHE, with a Tafel slope of 44.7 mV.dec⁻¹ compared to platinum (Pt), which has a Tafel slope of 33.6 mV.dec⁻¹. Moreover, NiTe₂@rGO demonstrates notable stability, maintaining effectiveness over 16 hours of testing. This efficiency is attributed to its interconnection with rGO, resulting in commendable conductivity. Thus, NiTe₂@rGO emerges as a potential alternative to platinum in the hydrogen evolution reaction.

Séance/Session 3 – Auto-assemblage Moléculaire et biomédical

Exploring polymorphism: Hydrochloride salts of Pitolisant and Analogues

Jessica Patel, Zachary Leduc, **Aaron Gabriel Nunez Avila**, Joseph A. Glover, Kelin Wu, Yuxing Zhang, Jing Zhang, Xiaoting Zhai, Alex M. Chen, Daniel Chartrand, Thierry Maris, Graeme M. Day, and James D. Wuest

Molecular organization is the key aspect dictating physicochemical properties of a given material. In the pharmaceutical industry, different forms of an active pharmaceutical ingredient (API) are routinely screened in goal to discover the most adequate form for commercialization according to their solubility, stability, and other properties.

Pitolisant hydrochloride is used to treat excessive daytime sleepiness in adults with narcolepsy. The drug is formulated as a crystalline solid, and a monoclinic P21 form has been claimed in patents, but little additional information about the structure and polymorphism of the compound has been published. No new forms were obtained when we grew crystals from solution under various conditions. Reexamination of the crystals revealed a disordered and partially hydrated structure that resembles the one reported earlier but is not identical. Further insight was obtained by synthesizing analogues of pitolisant with its Cl substituent replaced by Me, F, and Br, followed by structural analysis of the hydrochloride salts by X-ray diffraction.

Pitolisant hydrochloride and its three analogues showed very similar solid-state behavior, and each compound yielded new metastable forms when crystallized from melts. The lifetime of metastable Form III of pitolisant hydrochloride could be extended significantly by adding small amounts of the fluoro analogue, but none of the metastable forms could be obtained as single crystals suitable for structural analysis. Computational predictions of the polymorphic landscapes of pitolisant hydrochloride and its analogues identified possible structures of the metastable forms. Dual experimental and computational approaches are already widely used in polymorphic screening, but our work shows the value of broadening these searches to include sets of structural analogues.

Sustainable development in biocompatible metals : Nanostructured tantalum with enhanced tribological and mechanical properties

BABAK O' SHAHREZA, EDGAR O' GARCIA SANCHEZ , MARCO HERNANDEZ RODRIGUEZ ,LEMBIT KOMMEL ,FJODOR SERGEJEV ,JACQUES HUOT

Université de Québec à Trois-Rivières

Tantalum is a non-allergenic, biocompatible metal with a high melting point and high corrosion resistance which has been used in the jewelry industry, implants, and the coating of other biocompatible materials. As-received tantalum, however, exhibits a textured and inhomogeneous microstructure due to the casting method. Consequently, various post-processing techniques are required to address this heterogeneity and enhance mechanical properties. Severe Plastic Deformation (SPD) has proved effective in modifying the microstructure and improving material properties. In this work, we implemented a new Severe Plastic Deformation technique called Indirect Extrusion Angular Pressing (IEAP) to refine the microstructure of tantalum and improve the mechanical and tribological properties. Results showed that a considerable refinement in microstructure was achieved. The grains were reduced from large-elongated grains of 11 microns to refined-equiaxed grains of 500 nm after processing, and the hardness increased more than two times. Results of wear testing showed that the wear and tribological properties of the material improved and a reduction of more than 50% was achieved in the volume loss and wear rate of the material after IEAP. This enhancement in the wear resistance in a biocompatible material is important especially when it comes to the application of such a material as an implant, as it ensures prolonged durability and reduced degradation over time.

TOWARDS MOLECULAR MATERIALS DERIVED FROM BENZENETETRAMINE AND RELATED COMPOUNDS

Johann E. O. Sosoe, Cédric Malveau, Thierry Maris, Radu Iftimie, James D. Wuest.

Université du Québec à Montréal

People have never been able to travel and communicate as swiftly and extensively as they do now. Modern transportation and telecommunication democratize these capabilities, but they also cause depletion of natural resources, giving rise to global environmental and socio-economic concerns. Some of these challenges can be addressed by designing new sustainable electronic materials. To make these materials by design, strategies for controlled bottom-up construction are desirable. Molecular moieties such as benzenetetramine (BTA) and its derivatives represent an attractive class of starting materials for predictable construction. Indeed, such motifs can take part in defined supramolecular interactions, as well as in reversible redox processes. Despite the structural simplicity of BTA derivatives, their reactivity and organization in the solid state are little studied. We show how a deeper understanding of these aspects was achieved by using a combination of improved methods of synthesis, computation, spectroscopic studies, and structural analyses. Such new knowledge is expected to accelerate exploitation of the compounds in areas of materials science where desirable properties can only be attained by properly controlling the organization of molecular components.

Séance/Session 4 – Énergie/Energy

Molecular Carbazole-based complexes as catalysts for CO₂ reduction reaction

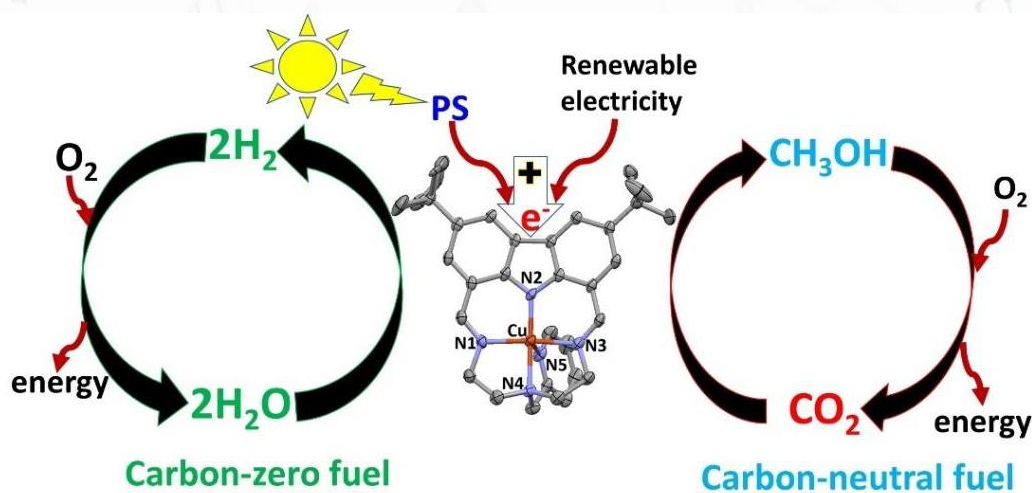
Fola S. Akogun, Garry S. Hanan, Sally Brooker

Université de Montréal

Scientists are providing a new perspective on carbon dioxide (CO₂), opening our eyes to the idea of embracing it as an asset – as a feedstock that can be converted into value-added chemicals, materials, and fuels for a future carbon neutral energy cycle – rather than viewing it as a liability with regard to global climate change.

Most molecular catalysts can reduce CO₂ to the two-electron products, CO and/or formate (HCO₂H), usually along with H₂ from the reduction of the protons present in the reaction mixture.¹ Transition metal complexes based on noble metals have been proven to be efficient homogeneous catalysts for the reduction of CO₂ to CO under photocatalytic conditions.² However, their first-row analogues are desirable because first-row transition metals are abundant in nature, exhibit low toxicity, and are economically cost-effective compared to second- and third-row ones.

In this talk, I will discuss the effects of water, a proton source, on the photocatalytic CO₂ reduction reaction (CO₂RR) and suppression of competitive HER using carbazole-based molecular complexes. Also, optimization of CO over H₂ as well as stability, efficiency, and selectivity aspects will be highlighted.



The Impact of Oxygen Vacancies in WO₃ Photoanodes Engineered through a One-Step Electrochemical Treatment for Efficient Photoelectrochemical Water Splitting

Imane En-Naji, Peng, Zhiyuan, Su, Yilu, Mohamed Siaj

University of Quebec at Montreal

This research focuses on optimizing the fabrication of tungsten oxide (WO₃) nanoplates on FTO substrates for superior photoanode performance. By varying the synthesis conditions—specifically temperature and duration—we sought to refine the hydrothermally prepared tungsten oxide, which was further processed through calcination in air. To elevate the electrochemical attributes of the WO₃ photoanode, an electrochemical treatment was applied, resulting in a notable enhancement, with photocurrents reaching as high as 0.8 mA/cm².

The electrochemical reduction technique was instrumental in promoting effective charge transport and collection in WO₃ layers during photonic absorption and charge separation, leading to a significant increase in photocurrent density. The methodology presented in this study lays out a straightforward, fast, scalable, and safe protocol for the production of high-efficiency metal oxide photoanodes.

Matériaux magnétiques Micro-poreux N-hétérocycliques fonctionnalisés par des nanoparticules de Au, Pt, Ag pour des performances améliorées dans le stockage d'énergie des supercondensateurs

Ngara Diouf, Amir Khojastehnezhad, and Mohamed Sijaj

University of Quebec at Montreal

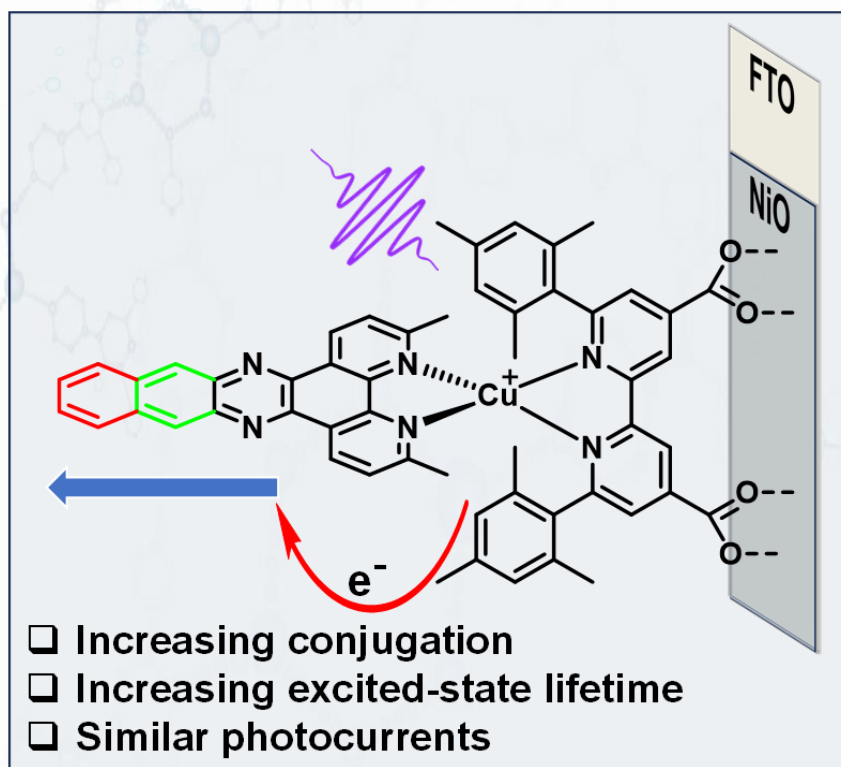
En raison de leurs hautes densités de puissance et leurs cycles de charge et décharge rapides, une variété de supercondensateurs ont été développées en utilisant des matériaux à base de carbone pour le stockage d'énergie. Par ailleurs, l'enrichissement de ces matériaux carbonés avec des hétéroatomes est une stratégie prometteuse pour améliorer les capacités de stockage. Des hétéroatomes comme l'azote ne se contentent pas de modifier les propriétés électroniques des matériaux carbonés, mais servent également de sites actifs pour des réactions redox, conduisant à des performances pseudo-capacitives accrues. Néanmoins, une exploration synthétique plus approfondie est nécessaire pour ces matériaux en structure à base de carbone poreux dopés à l'azote, non seulement pour élargir la diversité des méthodes, mais aussi pour un contrôle plus précis des caractéristiques des matériaux, comme la création de coquille magnétique fonctionnalisée. Au cours de cette présentation, nous explorerons les avancées réalisées dans la synthèse de matériaux magnétiques micro-poreux N-hétérocycliques (MON) qui intègrent un anneau hétérocyclique de triazine (schema 1). La particularité de ces matériaux MON réside dans leur anneau de triazine en surface, qui a permis la création de complexes N-hétérocycliques. Ces complexes ont été fonctionnalisés avec divers métaux, notamment l'or (Au), le platine (Pt) et l'argent (Ag), grâce à une technique de modification post-synthèse. Ces nouveaux matériaux se caractérisent par une surface spécifique étendue, les rendant particulièrement adaptés pour diverses applications dans les domaines du stockage d'énergie.

Effect of increasing ligand conjugation in Cu (I) photosensitizers on NiO semiconductor surfaces

Zujhar Singh, Marek B. Majewski

Concordia University

Dye-sensitized photoelectrochemical cells may be used as heterogeneous catalysts for fuel-forming and redox reactions. We describe the synthesis, characterization, and study of ground and excited state properties of three Cu(I) complexes involving three different ligands with varying electron accepting capacities. Femtosecond and nanosecond transient absorption studies confirm the formation of a singly reduced acceptor ligand after photoexcitation of the Cu(I) centre. These complexes are surface anchored onto nanostructured NiO on conductive fluorine-doped tin oxide on glass to fabricate photocathodes. It was found that even though the ligands with increasing conjugation have effects in the formation of final excited state in solution, but they exhibit almost similar photocurrents upon white light illumination suggesting hole transfer to NiO happening in advance of the formation of the final excited state.



Boosted photocatalytic and SERS Capability of Ag nanoparticles functionalized MoS₂ nanoflakes

Jaspal Singh, and Phuong Nguyen-Tri

Université du Québec a Trois-Rivières

We report the preparation of Ag nanoparticles functionalized MoS₂ nanoflakes by using the chemical reduction method followed by the hydrothermal method. Field emission scanning electron microscopy and elemental mapping reveal the uniform functionalization of Ag nanoparticles with MoS₂ nanoflakes. The high density of Ag plasmonic nanoparticles onto MoS₂ nanoflakes demonstrates tremendously improved charge separation behavior in Ag–MoS₂ nanohybrids. The photodecomposition capability of plasmonic Ag–MoS₂ nanohybrids was explored by the decomposition of industrial pollutant molecules, showing a direct correlation between the Ag content over the MoS₂ surface with their photodecomposition ability. The SERS-based detection profiles of the plasmonic were investigated by the ultra-low detection of MB molecules. The Ag–MoS₂ nanohybrids SERS substrate manifests the detection of MB molecules solution up to a concentration of 10⁻⁹M with an enhancement factor of 10⁷. In the current study, we proposed and elucidated the probable efficient charge transfer mechanism for improved photocatalytic behavior and SERS-based sensing performance.

Near-infrared remote-driven Janus micromotors for photon up-conversion applications

Pedro Mena-Giraldo, Mannu Kaur, Steven L. Maurizio, Gabrielle A. Mandl and John A. Capobianco

Université de Concordia

Micromotors (also referred to as microrobots) are devices that produce motion through *in situ* mass transfer or external stimuli, increasing their interaction with the medium for spatiotemporal control and enhanced kinetic efficiency of the involved processes. Near-infrared (NIR)-activated micromotors are attractive fuel-free systems that offer high spatiotemporal control using the properties of NIR irradiation.¹ Photophoretic motion of micromotors occurs by generating temperature gradients in the medium under NIR excitation, enabling micromotor movement from cold to hot regions.² NIR irradiation is also a driving force behind photon up-conversion commonly achieved by lanthanide-doped upconverting nanoparticles (UCNPs), which convert NIR to ultraviolet and visible light, demonstrating uses in a variety of applications. The micromotors developed herein are assembled with Fe₃O₄ nanoparticles, NaGdF₄:Yb³⁺, Er³⁺/NaGdF₄:Yb³⁺, and LiYF₄:Yb³⁺, Tm³⁺ UCNPs. The Fe₃O₄ nanoparticles were localized to one hemisphere of a chitosan microsphere to produce a Janus architecture that facilitates improved up-conversion luminescence, with the UCNPs distributed throughout the micromotor volume. Under 976 nm excitation, Fe₃O₄ nanoparticles generate a temperature gradient to activate the photophoretic motion, while the UCNPs produce visible light that was used for micromotor tracking and triggering reactive oxygen species generation. The motion and the photon up-conversion applications of these micromotors were performed using a single excitation wavelength. Curcumin was adsorbed to the micromotor surface to demonstrate the practicality of this system and degradation of Rhodamine B was achieved with kinetic rates that were more than doubled relative to static microcarriers. Together, this system provides a versatile approach to achieving NIR-driven motion while taking advantage of the many potential applications of up-conversion luminescence.

Advancing Temperature Sensing Technology: Gt/PS Nanocomposite-based Wearable Sensor for Dynamic Environments

Ahmad Al Shboul, Ricardo Izquierdo

École de Technologie Supérieure

Wearable temperature sensors have emerged as crucial tools in modern sensing technology, providing real-time data for applications ranging from healthcare to environmental monitoring. This study introduces an innovative temperature sensor utilizing a thermistor nanocomposite comprising graphite (Gt) and polystyrene (PS) [1-3]. Systematic optimization yielded a sensing nanocomposite with 50 mg mL⁻¹ Gt and 250 mg mL⁻¹ PS, a 10-minute sonication time, and a curing temperature of 180°C for 10-15 minutes. The resulting sensor exhibited exceptional thermal stability and film integrity, demonstrating a sensitivity of 0.3% °C⁻¹ and reversibility across the temperature range of -10°C to 60°C, as shown in **Figure 1**. Impressively, it showcased a rapid response/recovery time of 0.97/1.3 minutes at a heating/cooling rate of 60°C/minute, maintaining minimal baseline drift even under varying humidity levels.

The sensor's capacity to adapt to dynamic environmental conditions underwent thorough examination through extensive bending cycles at a 30° angle. This evaluation underscored its mechanical flexibility and unwavering stability across a temperature spectrum from -10°C to 60°C. This adaptability was further substantiated by a comprehensive analysis of loss/storage moduli and tan(delta). Moreover, the sensor's exceptional chemical and physical stabilities were evident, affirming its robust resilience in demanding environments, including exposure to corrosive gases and prolonged immersion in tap water.

Real-world tests confirmed its practical utility, demonstrating precise temperature measurements in liquid media and accurate breath temperature monitoring. These results suggest promising applications in healthcare, environmental monitoring, and diverse IoT applications. The Gt/PS nanocomposite-based temperature sensor signifies a significant advancement in temperature sensing technology, addressing key performance aspects such as thermal stability, sensitivity, response time, mechanical flexibility, and chemical and physical stabilities.

Enhanced Catalytic Efficiency of Nitrophenol Reduction through Size-Controlled Synthesis of Gold Nanoparticles within Covalent Organic Frameworks

Hichem Gamraoui, Amir Khojastehnezhad, Marilynne Bélanger-Bouliga, Ali Nazemi, and Mohamed Siaj

Université de Québec à Montréal

In this study, a covalent organic framework (COF) functionalized with gold nanoparticles (Au NPs) was developed. We initially synthesized a novel N-heterocyclic carbene (NHC) compound, followed by the creation of a mesoionic NHC-Au(I) complex. The resulting complex was used as Au NPs precursor. The findings indicated that synthesizing Au NPs concurrently with the COF precursors resulted in smaller nanoparticles than forming the Au NPs subsequent to the COF assembly. Electron microscopy confirmed the successful incorporation of Au NPs into the COF, revealing nanoparticle sizes under 5 nm and over 50 nm for the two methods, respectively. Furthermore, N₂ adsorption-desorption analysis (BET) showed a substantial decrease in surface area, dropping to 1106 m²/g and 910 m²/g for the respective methods post-gold integration, down from an initial 1885 m²/g. The resultant heterogeneous Au NP catalysts demonstrated the capability to facilitate the reduction of nitrophenol rapidly with high efficiency at ambient temperature. Moreover, the analysis demonstrated that smaller-sized Au NPs embedded within the COF exhibited superior catalytic efficacy compared to their larger counterparts.

Étude des effets de différents COF 2D liés à l'imine pour une élimination efficace de la rhodamine B

Lebar Ghizelane, Khojastehnezhad Golmakani, Amir, Mohamed Siaj

Université du Québec à Montréal

La pollution par les colorants organiques est un problème environnemental important qui a largement suscité l'intérêt de la communauté des chercheurs. Récemment, la méthode d'adsorption a été largement utilisée comme une approche efficace et simple pour éliminer les colorants des eaux usées. Dans cette étude, trois cadres organiques covalents (COF) différents appelés TPT-PDA, TPT-HZ et TAPA-TPT COF avec une structure triazine ont été préparés en utilisant différents blocs de construction via une réaction de polycondensation d'imine pour éliminer les colorants cationiques tels que la rhodamine B, le Crystal Violet et le bleu de méthylène de l'eau. L'analyse BET a révélé une surface et une taille de pore différentes pour ces trois COF, de l'ordre de 1438, 825 et 120 m²/g, respectivement. Les observations PXRD, également en accord avec l'analyse BET, ont montré des structures cristallines différentes pour ces COF préparés. D'après les résultats obtenus, il a été démontré que les matériaux COF ayant une surface plus grande ainsi qu'une structure cristalline plus développée ont une capacité d'absorption supérieure pour éliminer les colorants présents dans l'eau. L'étude souligne également l'importance de tenir compte de la taille des molécules de colorants organiques et de la taille intrinsèque des pores du matériau COF lors de la conception d'adsorbants efficaces à base de COF. La diversité structurale des matériaux COF et la compréhension de l'encapsulation des colorants organiques sur les COF offrent une voie prometteuse pour le développement de nouveaux adsorbants COF en vue d'une élimination efficace des polluants organiques des eaux usées.

Nanofiber Materials with High Reflectance and Polarization Contrast in the Mid-Infrared Spectral Range

Olivier Roy, Arnaud W. Laramée, Christian Pellerin.

Université du Québec à Montréal

Highly reflective materials in the mid-infrared (MIR) atmospheric transparency window (8 to 14 μm) possessing adequate mechanical properties, such as strength-to-weight ratio, flexibility, and robustness, are crucial for camouflage and sensing technologies development.¹ For sensing technologies such as hyperspectral polarimetric detection, materials require a high polarization contrast in addition to a strong reflectance in the MIR. While metamaterials offer ideal optical responses for these purposes, their fabrication cost limit widespread application.¹ This stresses the need for alternatives, such as polymers, which we believe can provide an all-encompassing solution.

Polyoxymethylene (POM) was chosen for its high reflectance in the MIR atmospheric window, which originates from polaritonic modes,² its strong chemical resistance, and its robustness. To achieve flexible materials exhibiting a polarization contrast, we collected aligned mats of oriented electrospun POM nanofibers.³ To improve the optical response of the mats, they were subjected to four treatments, namely compression (C), drawing (D), submersion with a non-solvent (S), and incorporation of an index-matching medium (I). Through adjustment of treatment parameters and strategic combinations (D-C, D-C-I, S-D-C-I), we created a mat with a reflectance of $60 \pm 8\%$ and a corresponding polarization contrast (DOLP) of 0.52 ± 0.01 . To assess the material's robustness, the performances of compressed mats were monitored under simulated on-field conditions. Optical responses of selected mats were measured over time to evaluate durability. The promising performance of these mats make them potential candidates for military applications and beyond.

5. Présentations par affiche/Poster presentations

Auto-assemblage Moléculaire

- 1) PohYing Fong - TOWARDS SPATIO-TEMPORAL RESOLUTION OF COPPER ASPARTATE IN GEL
- 2) Louise Gourdelier - Odd-Even Effect in the Molecular Orientation in 2D and 3D Phospholipid Assemblies
- 3) Mostafa Eesaee - Crystallization Dynamics and Lamellar Structuring of Poly(ϵ -caprolactone) on Natural Fiber : A Micro and Nanoscale Analysis
- 4) Maryam Lormahdiabadi - Impact of Antibacterial Carbon Dots on the Biophysical Properties of Pulmonary Surfactant
- 5) Heriniaina Randriamiharisoa - Synthesis, characterization, and potential applications of coordination compounds based on aromatic polypyridine carboxylic acid ligands

Développement Durable

- 6) Safa Ladhari - Évaluation de l'activité biologique de nouveaux matériaux textiles antimicrobiens et biodégradables pour les équipements de protection
- 7) Payman Ghassemi - Advancing Green Chemistry: Crystallization Strategies in Biodegradable PHB/PLA Polymer Blends
- 8) Lucia Švandová - Atmospheric pressure plasma treatment of cellulose nanofibril films : analysis of chemical functionalization and etching Biomédical
- 9) Bendhiba Badredineberfai - Adsorption des ions de cérium par des nanofibres électrofilées de chitosane/PEO
- 10) David Nadeau - Numerical investigation of the electrostripping of lithium geometry defects in an all-solid-state cell
- 11) Luis Alfonso Paramo Serrano - CuS and CuInS Quantum Dots as Green Alternatives for Solar Cells

Polymères

- 12) Imen Hamouda - Analyse des données d'essais thermiques et mécaniques pour estimer la durée de vie des élastomères
- 13) Cephas Amoah - Nanofibrillar Conducting Polymers for Stretchable Electrodes

- 14) Masoud Tayefi - Mechanical Properties Evaluation of Elastomeric Industrial Parts Upon High Temperature Exposure
- 15) Saba Goharshenasmoghadam - Revolutionizing Ionic Liquids : Enhancing Anti-icing properties Achieved by Designing Hydrophilic or Hydrophobic Surface
- 16) Gilberto Romeo Nkana Nkana - Développement de cryogels poreux de carboxyméthylchitosane sous forme d'un réseau interpénétré d'acide polyacrylique et de polythiophène pour l'élimination de la fluoxétine en milieux aqueux.
- 17) Vahideh Akbari - Biobased chemical densification of three hardwoods by Michael addition reaction

Matériaux pour applications biomédicales

- 18) Drirdi Donia – Recent progress on the synthesis and characterization of efficient and harmless antibacterial-agents based on silver nanoparticles
- 19) Fazia Mechaj - Room Temperature Synthesis of Zinc Oxide Nanomaterials for Improved Detection of Gases in Human Breath Profiles

Énergie

- 20) Giuliana Lazzaro - Ru-based Photosensitizers and Co-based Catalyst : A Promising Systems for Light-driven Hydrogen Evolution
- 21) Brittany Pelletier- Villeneuve - The microwave cavity perturbation technique to study battery materials
- 22) Alborz Bavandsavadkouhi - Synthesis and Characterization of Cyanopyridines Followed by Subsequent Hydrolysis to Form Amide-Pyridines and Nicotinic Acids
- 23) Manon Saget - NEW BIO-BASED COATINGS FOR OPV ENCAPSULATION
- 24) Rupinder Kaur - Electroactive coatings for energy storage devices from perylene derivatives
- 25) Arindam Saha - Photocatalytic hydrogen production from water using Pt (II) complexes with ligands forming 6-membered chelate rings : effects in N^NN and N^CN coordinated complexes
- 26) Houssam-Eddine Nemamcha - Development of highly efficient biomass-based catalysts for the removal of industrial pollutants from water (rhodamine dye)
- 27) Adela Abidi - Visible-light-driven photocatalytic CO₂ Reduction Performed by Coordination Polymers Based on the 1,2-di(4-pyridyl) ethylene Ligand and First-row Transition Metals
- 28) Natalia Vargas Perdomo - A Simple Triboelectric Nanogenerator - Using a Salad Spinner as a Power Source

6. Résumés des présentations par affiche/Poster presentations abstracts

(2) Odd-Even Effect in the Molecular Orientation in 2D and 3D Phospholipid Assemblies

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Abstract: The preparation and characterization of organized organic ultrathin films, such as self-assembled monolayers (SAMs) chemisorbed to metal or semiconductor surfaces, is fundamental to the booming field of molecular electronics. The study of SAMs can further our understanding of surface hydrophobicity, charge transport and charge storage, which are crucial for the design of novel electronic devices. The challenge is to correlate the molecular organization of the monolayer with its macroscopic properties. The parity or odd-even effect is any structural or orientational change that correlates with the chain length or chain parity of the molecules forming the SAM. Odd-even effects have been observed in the surface/interface properties of SAMs, such as wettability, friction, and electron transfer rate, which are key to designing new materials.

This investigation aims to demonstrate the parity effect in the molecular organization of 2D and 3D assemblies of phosphatidylcholines (PCs), namely Langmuir-Blodgett (LB) monolayers and multi-lamellar vesicles (MLVs). We studied (n:0 PC) with $n = 12-18$, where n is the number of repetitive carbon units forming the PC tails. The floating LB monolayers were formed by spreading and laterally compressing the PC molecules at the air/water interface on a water subphase contained in a Langmuir-Blodgett trough. Surface pressure-molecular area (π -A) isotherms (Langmuir isotherms) were recorded during monolayer compression for each chain length. The PC monolayers were transferred at constant surface pressure from the air/water interface onto a germanium crystal substrate by the LB technique. The chain conformational order and orientation in the solid-supported PC monolayers were characterized by Attenuated Total Reflection-Fourier Transform Infrared (ATR-FTIR) spectroscopy. Finally, a series of aqueous MLV suspensions were also prepared using the same series of PCs and their thermotropic properties were characterized by Differential Scanning Calorimetry (DSC). The ATR-FTIR and VP-DSC results show that PCs with an even number of carbons adopt a different molecular orientation in both two- and three-dimensions compared with PCs with an odd number of carbons. We conclude that the parity effect exists in PC assemblies.

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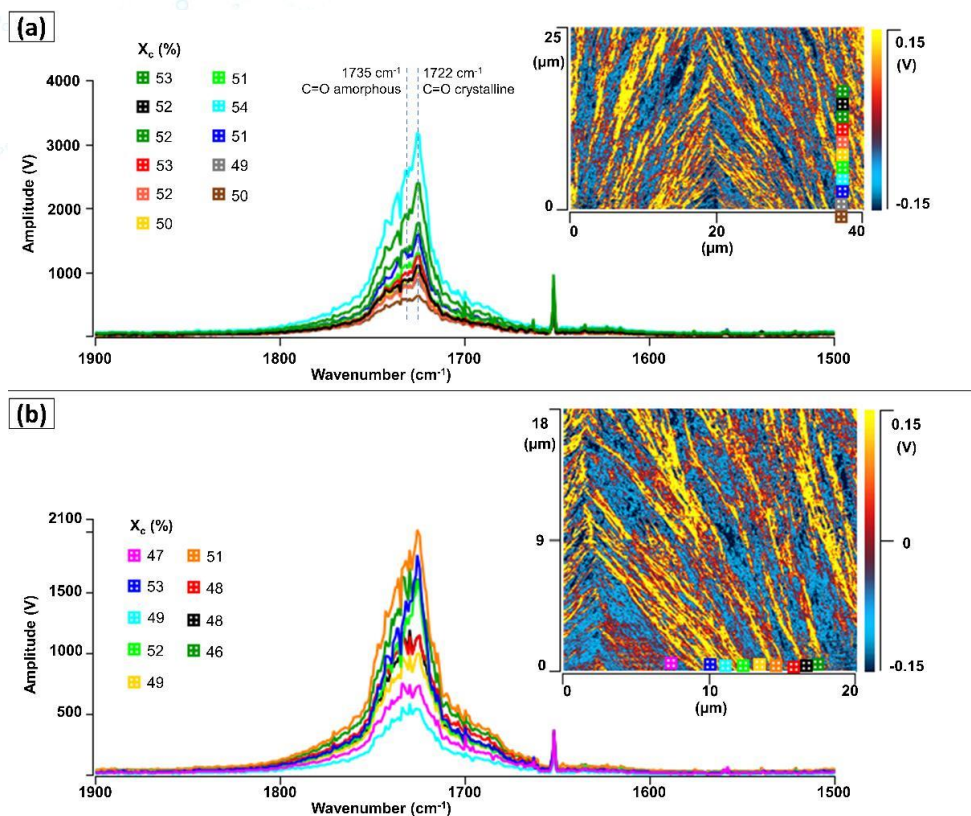
(3) Crystallization Dynamics and Lamellar Structuring of Poly(ϵ -caprolactone) on Natural Fiber: A Micro and Nanoscale Analysis

Mostafa Eesaee, Phuong Nguyen-Tri

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Abstract:

This conference abstract presents a study on the micro and nanoscale morphological development and lamellar structure of biodegradable poly(ϵ -caprolactone) (PCL) in conjunction with a natural fiber. The research focuses on how graphene oxide (GO) treatment of MW fiber influences the crystallization and formation of a transcrystalline (TC) layer of PCL. Microscopic techniques have provided insights into the lamellar growth of PCL around the MW fiber and to examine the morphology and kinetics of PCL crystallization. The real-time observation of lamellar growth using *in-situ* AFM provided insights into the dynamic processes and time evolution of these structures. This TC layer development, from initial nucleation to lamellar orientation perpendicular to the fiber, underscores the intricate interplay between the fiber's physical presence and PCL crystallization dynamics. The study reveals how the natural fiber's presence impacts the lamellar assembly, causing newly formed PCL lamellae to reorient and branch into a sheaf-like structure. Additionally, AFM-IR was used to explore variations in PCL crystallinity, offering insights into the interlamellar structure and amorphous region distribution.



AFM-IR spectra of PCL semi-spherulites grown from MW fiber surface, shown by color-filled squares, in different directions: (a) perpendicular to the fiber surface, (b) parallel and very close to the fiber surface.

(4) Impact of Antibacterial Carbon Dots on the Biophysical Properties of Pulmonary Surfactant

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Abstract:

One of the most common types of pulmonary infection diseases is bacterial pneumonia which can cause mild to life-threatening illness in people of all ages. Presently, antibiotics are used as first-line drugs to treat pneumonia. Due to the limitations of systemic administration methods, inhalation, as a targeted administration route, can deliver the drug directly to infected cells. [1]

Inhaled nebulized nanomedicines (NMs) are gaining attention among researchers due to being transported into the deep lung deposition at the alveoli region. However, the pulmonary fate of inhaled NMs is affected by the bio-nano interactions with pulmonary surfactant (PS) at the air/alveoli fluid interface, which alters the fate of inhaled therapeutic NMs and the lung's physiological function. Since the role of PS is reducing the surface tension at the air/alveoli interface to ease the breathing process, whatever affects the standard functionality of PS could cause respiratory problems. Therefore, the interaction of NMs with PS can cause changing surface tension, PS phase structure, and reservoir formation. The consequences of each alteration have a diverse impact on the breathing system. [2]

Recently, the antibacterial cysteine-carbon dots (cys-CDs) have been successfully developed [3]. Antibacterial properties of these cys-CDs against different strains of bacteria show promising results toward generating new ideas in the field of antibiotics.

In this research project, the effects of different concentrations of antibacterial cys-CDs on the phase behavior and lateral structure of lung surfactant binary mixture model (DPPC:POPG) were investigated at the air/water interface using surface pressure-area isotherms and Brewster angle microscopy, respectively. Additionally, atomic force microscopy was used to image the morphology of films transferred onto a mica substrate with nanometer resolution. The results revealed that the presence of cys-CDs resulted in hindering lipid packing and loss of material resulting in shifts to higher molecular area during early compression for monolayer isotherms. However, further studies are aimed at looking over the more complex lung lining membranes.

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(5) Synthesis, characterization, and potential applications of coordination compounds based on aromatic polypyridine carboxylic acid ligands

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There are still numerous unexplored aspects regarding the utilization of flexible aromatic pyridine-carboxylic acid ligands in crystal engineering for the construction of coordination polymers and metal-organic frameworks (MOFs), as well as their applications in various areas, including photocatalytic reactions, hydrogen evolution reactions (HER), carbon dioxide reduction, oxygen evolution reactions (OER), sensing and luminescence devices.[1]

Four novel coordination compounds comprising transition and rare earth metal ions were successfully synthesized using a solvothermal process, spanning from discrete coordination complexes to coordination polymers.[1] In this study, the choice of aromatic polypyridine carboxylic acid ligands was motivated by the wide range of coordination modes exhibited by the carboxylic and pyridyl functionalities.[2] The metal ions Co(II), Zn(II), Cd(II), and Nd(III) were selected based on their oxidation states and their affinity towards the ligand.[3], [4] The compounds were subjected to characterization utilizing a range of analytical techniques, including Fourier transform infrared spectroscopy (FT-IR), ultraviolet-visible spectroscopy (UV-Vis), single crystal X-ray diffraction (SCXRD), powder X-ray diffraction (PXRD), and thermogravimetric analysis (TGA). The characterization of the compounds showcases their variety, flexibility, thermal stability, and fascinating topologies.

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(6) Évaluation de l'activité biologique de nouveaux matériaux textiles antimicrobiens et biodégradables pour les équipements de protection

Safa Ladhari, Alireza Saidi, Phuong Nguyen-Tri

Au cours des crises sanitaires, telles que la pandémie COVID-19, l'utilisation des équipements de protection (EP) jetables (masques, blouses, etc.) engendre des problèmes à long terme, accroissant le volume de déchets dangereux qui doivent être gérés en toute sécurité. Par conséquent, la production de matériaux antimicrobiens et biodégradables est vivement souhaitable pour réduire l'utilisation d'EP qui devraient être considérés comme des déchets dangereux. Les déchets contaminés menacent la santé humaine et environnementale, exposant un besoin crucial d'améliorer les pratiques de gestion des déchets. De plus, les matériaux fréquemment utilisés pour les EP sont en plastique non biodégradable. Par conséquent, l'objectif ultime de cette étude est de remplacer les plastiques à base de pétrole par des bioplastiques offrant une meilleure biodégradabilité.

Dans cette étude, nous avons développé un nouveau matériau antibactérien et biodégradable pour les EPs. Des films PHB-AgTiO₂ électrofilés antibactériens ont été testés pour la première fois pour désactiver les bactéries Gram-négatives *Escherichia coli* et les bactéries Gram-positives *Staphylococcus epidermidis*. Tout d'abord, des fibres PHB de taille 1-2 micromètre ont été produites en utilisant la technique émergente de l'électrofilage. Ensuite, les films électrofilés ont été modifiés en surface par traitement au plasma et ensuite chargés avec des nanoparticules hybrides AgTiO₂ par trempage. Les résultats de caractérisation indiquent la réussite du dépôt de nanoparticules AgTiO₂ sur la surface des fibres électrofilées PHB. Les tests biologiques révèlent une excellente propriété antibactérienne des films PHB traités, avec une efficacité bactérienne supérieure à 99,8 %. Ces propriétés sont améliorées lorsque les films revêtus sont exposés à une lumière blanche (xénon). De plus, les films traités peuvent être utilisés jusqu'à trois fois sans perte significative d'efficacité antibactérienne. Enfin, le taux de dégradation du sol des films nanocomposites a atteint près de 99 % après seulement six semaines.

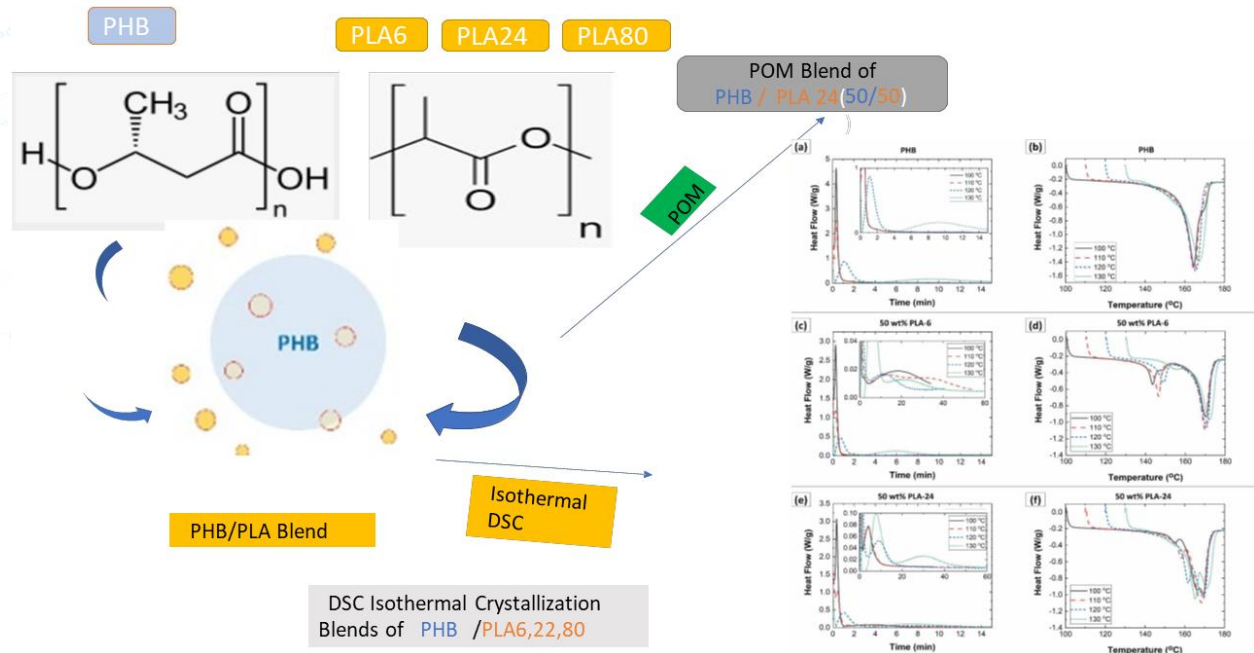
(7) Advancing Green Chemistry: Crystallization Strategies in Biodegradable PHB/PLA Polymer Blends

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Abstract:

This study delves into the crystallization kinetics and thermal behavior of Polyhydroxy butyrate (PHB) and Polylactic Acid (PLA) blends, shedding light on their phase interactions and potential for enhanced biopolymer applications. Using Differential Scanning Calorimetry (DSC), we have charted the isothermal crystallization paths and melting transitions, revealing that crystallization behavior is intricately linked to thermal conditions. Our findings underscore the significant impact of temperature on the crystallization kinetics of PHB, with the crystallization peak broadening and shifting to higher temperatures as the crystallization temperature increases. Polarized Optical Microscopy (POM) has been instrumental in visualizing spherulite formation within thin film blends, allowing us to explore the competitive nucleation phenomena, where PHB and PLA exhibit tendencies to crystallize independently. Atomic Force Microscopy (AFM) further complements our study by illustrating the surface morphology, providing a microstructural perspective on the spherulitic growth and phase behavior under varying thermal conditions. Collectively, our research advances the understanding of PHB/PLA blend behavior, paving the way for developing sustainable and high-performance biopolymers tailored for diverse industrial applications.



(8) Atmospheric pressure plasma treatment of cellulose nanofibril films: analysis of chemical functionalization and etching

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Abstract:

Cellulose is the most abundant biopolymer and, therefore, one of the most promising sources for future eco-friendly and biocompatible products. However, parameters like water absorption and low adhesion have been limiting the possible uses. Large-scale surface modifications are also necessary to scale up the use of this material for industrial applications [1]. In this context, surface modifications, atmospheric pressure plasma treatments are among the most versatile and sustainable strategies available today. In this study, the authors studied the cellulose-plasma interactions and highlighted significant modifications under different treatment times.

Chemical changes were observed for the short treatment times (5s) by using a novel coplanar barrier discharge [2]. The functionalization resulted in increased wettability and the creation of new COO functional groups just after the plasma interaction. A new peak at 1728 cm⁻¹ in the FTIR spectra of treated samples was observed, suggesting the protonation of carboxylate groups. Slight decrease in roughness was also noted. With increasing treatment times, a sudden modification of morphology was observed, suggesting the start of deeper chemical etching of the material. This is also supported by AFM maps showing structures with 300nm depths occurring at 60s of plasma treatment. For very long treatments (over 10 minutes), a complete etching of the surface layer and powder-like residue was observed. The morphological changes followed a significant shift in the FTIR spectrum, suggesting more crystalline structures. These observations support a hypothesis of anisotropic etching of CNFs leading to almost complete etching of amorphous parts while leaving cellulose nanocrystals behind. This is preliminary observations will be confirmed by further analysis such as XRD and X-ray computed tomography.

In conclusion, the authors present for a first time a study on the anisotropic modification induced on CNF film by atmospheric pressure CDBD plasma in air. These results provide insights into plasma-material interaction and possible explanations of observed differences for short and long treatments.

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(9) Adsorption des ions de cérium par des nanofibres électrofilées de chitosane/PEO

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Ces dernières années, la quantité des déchets électroniques a augmenté à un rythme élevé et la pollution qui leur est associée est devenue un problème majeur. Les minéraux critiques et stratégiques (MCS) dont les éléments du groupe du platine et les éléments des terres rares qui se trouvent dans ces déchets sont toxiques et nocifs pour la santé humaine et peuvent provoquer des maladies et même un danger sur l'environnement lorsqu'ils ne sont pas recyclés. Par contre, ils présentent une richesse lorsqu'on les récupère grâce à leurs valeurs économiques car ils sont essentiels à l'économie et à la sécurité nationale du Canada. De plus, la transition énergétique vers une économie faible en carbone causera une hausse de la demande de ces MCS [1]. Le recyclage est proposé pour valoriser ces éléments dans une approche d'économie circulaire visant à mieux utiliser la matière première et réduire l'impact environnemental des chaînes de production et de réduire nos besoins d'exploitation des ressources naturelles. L'adsorption s'avère une approche ayant fait ses preuves pour capter des métaux critiques et stratégiques en milieu aqueux [2]. Plusieurs études ont été menées pour le développement d'un matériau adsorbant pour récupérer certains MCS en solutions aqueuses, mais elles ont été confrontées au coût élevé de production, la consommation d'énergie et la génération de sous-produits. Par conséquent, il est primordial d'orienter les efforts de recherche vers la mise au point de matériaux adsorbants qui surpasseront ces contraintes techniques. Les polymères renouvelables dérivés de la biomasse attirent une attention particulière pour la récupération des MCS car ils possèdent des groupes chélateurs de surface contenant de l'oxygène et de l'azote et sont biodégradables. Ils peuvent éliminer efficacement divers composés organiques et inorganiques. Pour ces raisons on a choisi le chitosane qui est l'un des polymères biodégradables naturels les plus abondants dans la nature et aussi un déchet de l'industrie de la pêche. En raison de l'abondance et de la disponibilité de ce déchet, il présente une solution moins coûteuse que les adsorbants disponibles sur le marché [3]. L'objectif de cette étude consiste à développer une matrice d'adsorption perméable à partir de biopolymère issu de biomasse marine. Une technique d'électrofilage est utilisée pour fabriquer une membrane de nanofibres non-tissé. Plusieurs paramètres, tels que les paramètres de solution, les paramètres de processus et les conditions ambiantes, ont été étudiés pour contrôler la morphologie et les propriétés des nanofibres produites. Ces paramètres ont été optimisés pour obtenir des nanofibres avec les propriétés souhaitées. La morphologie et le diamètre des nanofibres ont été déterminés par microscopie électronique à balayage (MEB). La capacité de captation d'un MCS modèle, le Ce(III), a été mesurée par des essais en cuvée (Batch). Une méthode de mesure du Ce(III) en solution aqueuse a été mise au point pour estimer l'efficacité d'adsorption des nanofibres. Les résultats ont montré que les nanofibres ont une capacité d'adsorption élevée pour le Ce(III). L'effet du pH, du temps de contact et de la température sur la capacité d'adsorption des nanofibres envers le cérium a également été évalué dans l'étude.

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(10) Numerical investigation of the electrostripping of lithium geometry defects in an all-solid-state cell

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Abstract:

All-solid-state batteries with a lithium negative electrode and a ceramic electrolyte are key to high capacity and energy density. The experimental methodology must be combined with the numerical modeling approach to ensure safe, fast, accurate, and cost-effective technological development. This work proposes and describes an electrochemical model of a $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$ (LLZO) and Ni-rich NMC-based lithium cell with a deformable lithium negative electrode. The volumetric deformation strategy is supported by a theoretical validation of the mass balance, the deposit velocity, the ohmic polarization, and the mesh deformation. The cell's discharge potential is decomposed by considering the equilibrium potential and the polarizations of the main components of the cell. To demonstrate the scope of the modeling work, simulations are computed using the finite element method at different operating conditions. Discharge rate tests, deformation tracking, geometry defects investigation, and polarization decomposition are described.

(11) CuS and CuInS Quantum Dots as Green Alternatives for Solar Cells

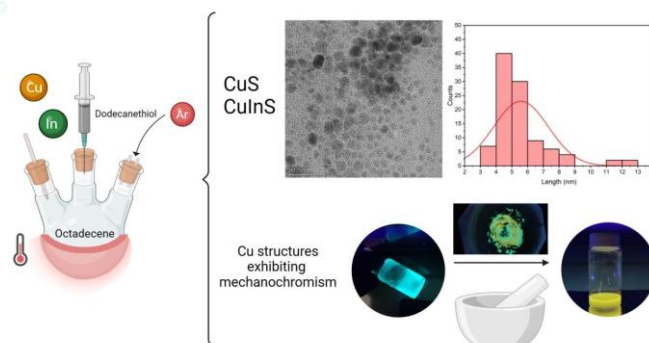
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Due to their size, quantum dots possess physical and chemical properties that make them attractive for applications in the conversion of solar energy to electrical energy [1]. However, the biggest problem concerning these is that the highest efficiencies are obtained using quantum dots made of heavy metals such as lead or cadmium, which are highly toxic elements [2]. As an alternative to these materials, chalcogenide compounds such as CuS and CuInS allow the use of infrared wavelengths with a lower environmental impact due to their low toxicity compared to quantum dots based on heavy metals [3]. The synthesis of the QDs was carried out using a hot injection method where Cu and In salt were dissolved in dodecanethiol and injected into a flask containing octadecene preheated at temperatures ranging from 120-210°C. The obtained QDs were isolated and purified using organic washes. Modifying the synthesis conditions such as temperature, the absorption and emission properties of wavelengths can be tuned and are related to the size of the quantum dot [4]. At the same time, the synthesis proposed in this work allows for the production of other copper-based structures using only DDT at low temperatures (50°C), creating novel materials that possess unique properties such as mechanochromism, which can be exploited in applications other than solar energy conversion [5].



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(12) Analyse des données d'essais thermiques et mécaniques pour estimer la durée de vie des élastomères

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L'objectif principal de cette étude est d'obtenir un aperçu complet du comportement en compression des élastomères dans diverses conditions de température et durées afin de tirer des conclusions sur la compréhension des mécanismes dominants de vieillissement des matériaux et de prédire avec précision leur durée de vie. Nous examinerons méticuleusement comment des facteurs tels que la température et la durée de vieillissement affectent la compression et les comportements chimiques, mécaniques et d'amortissement des élastomères qui sont facteurs cruciaux influençant leur durée de vie.

La méthodologie de recherche proposée impliquera une approche systématique de la sélection, de la préparation et des tests expérimentaux rigoureux pour étudier le comportement des élastomères sous compression. Les paramètres critiques tels que la courbe contrainte-déformation, le jeu de compression et les propriétés thermodynamiques seront méticuleusement enregistrés et analysés. Nous appliquerons également des techniques innovantes pour déterminer la durée de vie des élastomères sur la base des données de compression recueillies à différentes températures et durées de traitement. Grâce à ces méthodologies, nous prévoyons de parvenir à une compréhension plus approfondie du comportement de compression des élastomères permettant de prédire leur durée de vie de manière plus fiable. Nous nous attendons à ce que les résultats aient des implications substantielles pour les industries où les élastomères sont largement utilisés, conduisant à une conception améliorée des produits, à une fiabilité accrue et à une durée de vie prolongée.

(13) Nanofibrillar Conducting Polymers for Stretchable Electrodes

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Abstract:

In recent years, research efforts have focused on developing sustainable electronics by diverging from conventionally used metals such as ITO for conductive layers. Efforts have also been dedicated to replacing glass substrates because of their limited mechanical properties. As such, new materials with improved mechanical properties such as stretchability and bendability are of interest. ITO must also be replaced as the conductive layer in electrodes because of its brittleness. The electrospinning of conductive layers as nanofibers is an appropriate technique for producing mechanically compliant conductive layers that can potentially be used in stretchable electronics. In this study, the potential of nanofibers that are prepared from a conductive polymer without a dispersing polymer for use in stretchable devices is explored. A self-doped conductive polymer (poly ProDOT-sulfate) was prepared, and it was electrospun into nanofibers on a stretchable and bendable substrate. Both the conductivity after spinning and mechanical properties will be evaluated towards using the stretchable electrode in flexible electrochromic device.

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(14) Mechanical Properties Evaluation of Elastomeric Industrial Parts Upon High Temperature Exposure

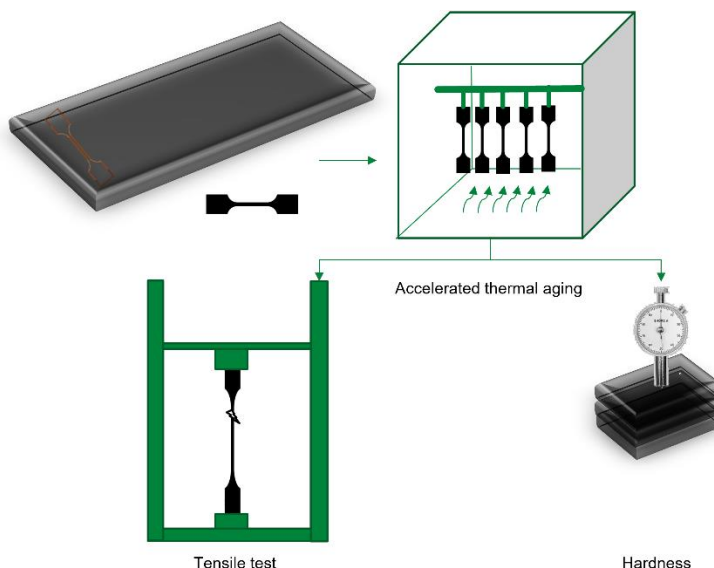
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Elastomers play a central role in modern industrial applications due to their unique properties including elasticity, flexibility and wear resistance. However, over time, these elastomer parts undergo aging which can lead to a drop in their mechanical performance, ultimately compromising the efficiency and reliability of the systems. The aging of elastomers is a complex phenomenon that can be influenced by several factors [1].

This article presents an investigation of the aging process of industrial elastomeric parts, with particular emphasis on the importance of accelerated aging techniques and the resistance of elastomers to temperature-induced aging. The study aims to improve the understanding of the impact of aging on the mechanical properties of elastomeric materials, in particular their tensile and hardness properties. Tensile properties, such as tensile strength and elongation at break, provide valuable information about the material's ability to withstand mechanical stress. Hardness, on the other hand, is a measure of the resistance of the material to indentation or penetration. The analysis of the evolution of these properties during aging will make it possible to understand the degradation mechanisms and to predict the service life of industrial elastomer parts.



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(15) Revolutionizing Ionic Liquids: Enhancing Anti-icing properties Achieved by Designing Hydrophilic or Hydrophobic Surface

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There is a substantial demand for durable anti-icing coatings capable of withstanding extremely low temperatures. Exploring the dynamic interplay between ice and the substrate opens exciting possibilities for altering interactions to minimize ice adhesion [1,2]. The innovative concept of dynamic interface melting has garnered significant interest for its extraordinary approach, incorporating a continuous antifreezing-releasing capacity into the interface to facilitate ice removal even after formation [3,4]. Ionic liquids (ILs), emerging as novel antifreeze materials, have been chosen for their unique properties in contributing to melting interfaces [5,6]. The increased mobility of ionic liquids (ILs) within coatings, combined with their solubility and compatibility in water, creates a pathway for ions to migrate to the surface. Beyond the physicochemical attributes of ionic liquids (IL), the inherent characteristics of the matrix play a crucial role in influencing ion transportation [7]. Our study explores the potential of ionic liquids (ILs) in anti-icing coatings for subfreezing applications. We investigate how matrix hydrophobicity influences IL mobility at low temperatures. Wettability results highlight the crucial role of IL anion hydrophobicity. The study demonstrates higher IL mobility in coatings with increased water absorbency, resulting in enhanced ionic conductivity. Additionally, the coatings exhibit a significant reduction in ice formation to -23.5 °C and low ice adhesion strength (~15 kPa). The durability of coatings is assessed under various conditions, emphasizing the importance of matrix selection in designing effective subfreezing coatings.

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(16) Développement de cryogels poreux de carboxyméthylchitosane sous forme d'un réseau interpénétré d'acide polyacrylique et de polythiophène pour l'élimination de la fluoxétine en milieux aqueux.

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La santé mentale est une réelle préoccupation pour l'organisation mondiale de la santé (OMS). Elle rapporte qu'en 2019, un milliard de personnes étaient atteint de troubles mentaux dans le monde et a noté une augmentation de la dépression et de l'anxiété de 25% [1]. Au Canada, l'organisation de coopération et développement économique (OCDE) a observé une hausse de 17% de la consommation d'antidépresseur entre 2019 et 2022. Cette augmentation a notamment été aggravée par la pandémie de Covid-19 entraînant une croissance des ventes d'antidépresseur dans le monde évalué à 15.87 milliards de dollars en 2021 [2]. Par conséquent, des concentrations plus importantes d'antidépresseurs et de métabolites secondaires sont observées dans les affluents des stations d'épuration des eaux usées (STEP). Malheureusement, les procédés de traitements actuellement utilisés sont peu efficaces pour retirer convenablement ces résidus toxiques avant leur rejet dans le milieu récepteur. Leur présence constitue alors un danger pour la biodiversité et la faune aquatique [3]. De nombreuses méthodes d'élimination ont été mises au point pour suppléer les traitements conventionnels, dont l'adsorption s'avère être l'une des plus prometteuses. Toutefois, les adsorbants conventionnels disponibles proviennent essentiellement de sources pétrolières et sont discutables du point de vue environnemental. Le développement d'adsorbants à base de biopolymères représente une alternative attrayante pour remplacer ces adsorbants traditionnels. Nos travaux portent sur la mise au point de matrices d'adsorption novatrices telles que des hydrogels et des cryogels à partir de dérivés de chitosane. Ces polysaccharides possèdent des caractéristiques chimiques particulières qui pourraient favoriser l'adsorption d'une large gamme d'antidépresseurs [4]. Cette étude a pour but de fabriquer des cryogels poreux de carboxyméthylchitosane sous forme d'un réseau interpénétré d'acide polyacrylique et de polythiophène pour l'élimination de la fluoxétine en milieux aqueux.

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(17) Biobased chemical densification of three hardwoods by Michael addition reaction

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The construction sector is a major contributor to global greenhouse gas emissions, accounting for 40% of the total, with building materials and construction alone responsible for 10% of these emissions [1]. This trend is expected to grow significantly by 2030. To address these environmental concerns, the adoption of green materials, particularly wood products, offers a promising solution to reduce energy consumption and carbon emissions in construction.

Wood, commonly used in residential buildings (71% market share), faces limitations in non-residential structures due to hardness and flammability concerns [2]. Wood densification, a technique aimed at enhancing wood density and hardness, presents a promising solution for expanding wood's use across various applications [3,4]. Current densification methods, however, have limitations in terms of cost and environmental impact [5]. This project introduces an environmentally friendly approach involving in-situ polymerization using Michael-addition reaction between biobased acrylate and malonate monomers. This reaction, conducted in mild conditions with reducing energy and solvent consumptions, aims to enhance wood densification while minimizing environmental impact.

Various malonate-acrylate systems are formulated, optimized, and tested on three different North American hardwoods. The study aims to advance sustainable wood-polymer composites to enhance wood properties, particularly hardness and potentially reducing greenhouse gas emissions associated with the sector.

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(18) Update review on the synthesis and characterization of efficient and harmless antibacterial-agents based on silver nanoparticles

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Abstract:

Pathogens along with multidrug resistance have recently been responsible for widespread diseases, fatalities, and economic distress [1,2]. Nanotechnology driven advancements via the engineering of well-sized and shaped Nanoparticles provided a hope to patients as well as physicians in solving complicated bacterial infections. Silver nanoparticles AgNPs have been widely emerged as a cost-effective and efficient antibacterial agent to combat both of bacterial contamination and multidrug-resistance issues through its ability to easily penetrate bacterial cell walls, damage their membranes, yield reactive oxygen species, and interfere with DNA replication as well as protein synthesis. This review tackle for the first time the key role of the synthesis strategies on the size and shape of targeted Ag NPs as well as exhibiting their cons and pros. At another hand, aiming to address the toxicity and the aggregation problems encountered with the solely use of silver NPs in medicinal applications, this review summarizes all the well-engineered silver-based nanocomposites through the combination of silver NPs with other antibacterial agents including the inorganic and inorganic nanomaterials. These reported silver-based nanocomposites could be used as antibiotic-free strategies in the fight against bacterial infections which could act with multiple simultaneous mechanisms to efficiently treat or prevent contaminations.

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(19) Room Temperature Synthesis of Zinc Oxide Nanomaterials for Improved Detection of Gases in Human Breath Profiles

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Gas sensors have found diverse applications, with recent emphasis on their significance in advancing breath analysis—an increasingly attractive research avenue for non-invasive health monitoring. Sensors designed for breath analysis have to meet strict requirements, requiring exceptional sensitivity to trace gas levels in parts per billion (ppb), high selectivity, quick response times, and robust anti-humidity properties. These sensors need to perform consistently well across various operating conditions to ensure reliable sensing capability. In our recent research at Prof. Izquierdo's lab, we've been at the forefront of developing state-of-the-art sensing technology [1-3]. This includes a simple nanocomposite blend comprising sensing materials (metal oxide nanoparticles, polymers, organic compounds), graphite flakes (Gt), and polystyrene (PS). Importantly, the sensors undergo a brief one-hour mixing process and a low-temperature curing process at 60°C for an additional hour, simplifying the fabrication process to just two hours.

Our research centers on utilizing zinc oxide (ZnO) nanomaterials as the core sensing component. These materials, derived from zinc acetate salt employing diverse room temperature techniques, are intended to enhance sensing capabilities. Initially, we contrasted ZnO nanomaterials produced through a straightforward co-precipitation method involving zinc acetate and deionized water in an ultrasonic bath at room temperature, varying pH levels (pH = 7, 9, 11, and 13). This approach eliminates resource-intensive steps such as calcination or hydrothermal reactions. Following this, adjustments to the preparation method involved probe sonication for different durations (0.5, 1, 5, and 10 minutes) at pH = 13, which previously showed the most promising results among the mentioned pH levels. This modification significantly reduced the preparation time from 2 hours to minutes. The resultant ZnO nanomaterials displayed varied physical structures (nanoflakes and nanoparticles), ranging in size from 30 nm to 460 nm, with surface areas spanning from 30 m² g⁻¹ to 53 m² g⁻¹, contingent upon the specific preparation conditions.

While our research is ongoing, ZnO-based gas sensors' preliminary findings underscore a notable responsiveness to styrene gas. However, it's crucial to note that secondary sensitivities to acetone and benzene display nuanced variations based on specific preparation conditions (such as pH levels, bath and probe sonication methods, durations, and initial materials). These early insights reveal the intricate relationship between the sensing material and target gases, stressing the necessity for further exploration and optimization to fully comprehend the sensor's response profile. As our investigations progress, a comprehensive understanding of these nuanced interactions will contribute to refining and enhancing the overall efficacy of the gas sensors in diverse applications, especially in applications like breath analysis.

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(20) Ru-based Photosensitizers and Co-based Catalyst: A Promising Systems for Light-driven Hydrogen Evolution

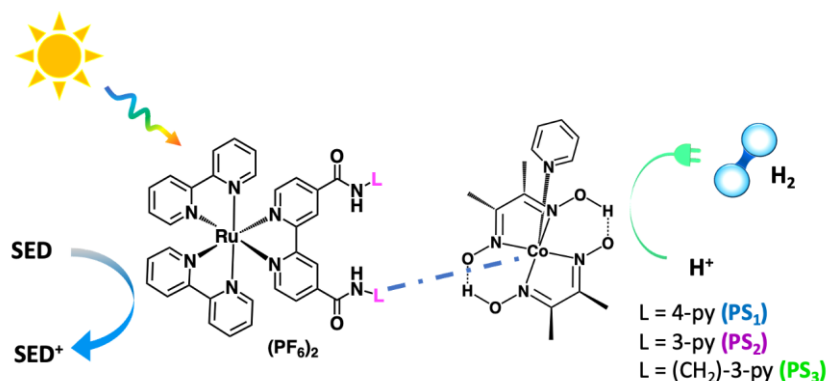
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Molecular hydrogen is considered the most powerful and sustainable energy source, characterized by its eco-friendly energy carrier properties, high energy density, lack of CO₂ emission and with water production as its combustion by-product. Consequently, in the field of artificial photosynthesis, particularly in the reductive half-reaction of the overall water-splitting, it has been emerging as a one of the most interesting energy storage system.[1] Therefore, the development of a Hydrogen Evolution Reaction (HER) system represents a significant challenge for the scientific community. To evaluate the photocatalytic performance of the H₂-evolution system,[2][3] three essential components are typically used: a photosensitizer (PS), a proton-reduction catalyst and a sacrificial electron-donor. This work is focused on the photosensitizer aspect with the aim to improve its photophysical properties with respect the archetypal [Ru(bpy)₃]²⁺. [4] Specifically it involves the design, synthesis and the optimization of the photophysical properties of a series of Ru-based amide polypyridine hetero-complexes of the type [Ru(L)(bpy)₂]²⁺ (L = [2,2'-bipyridine]-4,4'-dicarboxamide), by properly tuning the ligand L. To evaluate the rate of mechanism and the stability of the photocatalytic system when compared to [Ru(bpy)₃]²⁺, the light-driven H₂-production was investigated using each photosensitizer combined with a cobaloxime catalyst, under different Light-Emitting-Diodes (LEDs).



Scheme 1. Illustrative scheme of H₂-evolution system.

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(21) The microwave cavity perturbation technique to study battery materials

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Abstract:

As the shift to green energy occurs, the need for efficient batteries becomes progressively more urgent. To improve lithium-ion batteries, specifically their power and energy density which entails improving their ionic and electronic conductivity. In this study, we used the microwave cavity perturbation technique to study the electronic conductivity of battery materials. Without this technique, the conductivity of nanomaterials is hard to measure mainly because it is difficult to electrically connect to the sample. This technique removes the need to make contact by remote sensing with an electromagnetic field. This technique is non-invasive, requires a few milligrams and allows us to control the temperature, the pressure and the gas environment. Our research focuses on widely used materials such as lithium iron phosphate (LFP), a cathode material, and lithium lanthanum zirconium oxide (LLZO), a solid electrolyte, at different temperatures. Our measurements have shown that for LFP, there is a significant change in conductivity when the material goes from triphylite and heterosite phases? to a disordered solid solution.¹ The conductivity change is also affected by the degree of lithiation of the materials with the biggest gap being for the half lithiated LFP. For LLZO, our measurements indicate that the electronic conductivity does not change as the temperature increases up to 900°C.

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(22) Synthesis and Characterization of Cyanopyridines Followed by Subsequent Hydrolysis to Form Amide-Pyridines and Nicotinic Acids

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Cyanopyridines, amide pyridines, and nicotinic acid have attracted significant attention among researchers in the fields of material science, coordination chemistry, and pharmaceuticals due to their versatile applications.^{1–3}

In this project, we synthesized cyanopyridines through a nucleophilic reaction with good yields. Subsequently, we hydrolyzed them to form both their amide and carboxylic acid counterparts under basic conditions. The ratio of amide to carboxylic acid was dependent on reaction conditions such as temperature and reaction time. Purification was achieved without the use of column chromatography, and water served as the only solvent during hydrolysis. All these compounds were thoroughly characterized using NMR and FTIR spectroscopy. Additionally, their thermal stability was assessed through TGA analysis. To delve deeper into the structural aspects and intermolecular interactions of these molecules, single-crystal X-ray diffraction (ScXRD) was used to determine their precise structures in the solid state. Furthermore, a Hirshfeld study was conducted to investigate and better understand the intermolecular interactions.

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(23) NEW BIO-BASED COATINGS FOR OPV ENCAPSULATION

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Organic photovoltaics (OPV) are the third generation of solar cells and are more and more attractive for industrial applications. OPV present numerous advantages, such as flexibility, low cost, light weight, large-area production.[1,2] Nonetheless, OPV are not as efficient as the conventional crystalline silicon photovoltaic (PV) cells. Recently, power conversion efficiency (PCE) has reached 18% for OPV, while conventional PV remains around 30% [3]. In this sense, additional works are necessary to improve their processability. Moreover, components of OPV are highly sensitive to water or oxygen, which strongly affect OPV stability in time when used in harsh conditions. Therefore, development of new barrier coatings are today essential to reduce OPV degradation and increase their shelf life. According to the literature, encapsulation can be performed following three strategies: (i) glass-glass encapsulation, (ii) flexible polymer lamination and (iii) thin film direct deposition. Glass-glass encapsulation provides great protection, with good optical properties but it remains fragile and is not compatible with roll-to-roll processes. On the other hand, although, flexible polymer lamination is suitable for roll-to-roll processes, adhesion between the front and back barriers is still complex to deal with, leading sometimes to partial encapsulation, thus increasing OPV degradation. Finally, direct deposition allows to obtain thin films with excellent optical and oxygen and humidity barrier properties. To date, most of thin layers are synthesized under vacuum [1,2]. This work focus on the development new barrier coatings at atmospheric pressure, compatible with roll-to-roll processes using bio-based material (*i.e.*, cellulose nanofibrils) with excellent oxygen barrier properties [4]. Being hydrophilic, the surface of cellulose nanofibrils have been modified to improve the water barrier properties. Wettability modification (WCA ~ 140°) was successfully achieved with an atmospheric pressure dielectric barrier discharge to control the fragmentation/reticulation of 2,4,6,8-Tetramethylcyclotetrasiloxane (TMCTS).

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(24) Electroactive coatings for energy storage devices from perylene derivatives

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Abstract:

Solar energy is clean and renewable energy source which can meet global energy needs. Nonpolluting sources of electricity such as solar cells have gain interest because of their low cost and increasing efficiency. However, the major drawback associated with derived electricity from solar power is that it is reliant on the availability of the sun. Therefore, electricity must be stored for dark periods because of their intermittency. A traditional photovoltaic battery system is bulky as it involves operating a photovoltaic (PV) and battery as two independent units that are electrically connected by wires which leads to energy loss and requiring more space.

A photo-rechargeable electric energy storage system can be an efficient solution for storing the electricity captured from the sun. Such a system harvests the sunlight energy, converts it to electricity, and stores it in a battery. Energy storable dye-sensitized solar cells (ES-DSSC) are suitable systems as they are sustainable and nonpolluting sources of energy with low fabrication costs. This energy system is versatile by operating even under at low light intensity. The energy storage devices used for ES-DSSC can be either redox flow batteries or Li-ion batteries.

In this work, we detail the synthesis of a molecular dye i.e., perylene derivatives that can both harvest sunlight and convert the energy for storage in a battery. For this, the dye will be combined with a monomer for developing light harvesting coatings on conventional redox active rechargeable battery components. The potential application of these materials will also be presented.

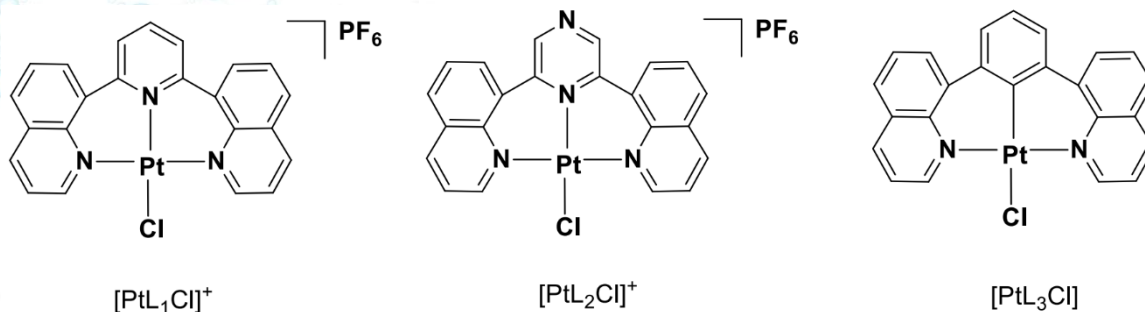
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(25) Photocatalytic hydrogen production from water using Pt (II) complexes with ligands forming 6-membered chelate rings: effects in N[^]N[^]N and N[^]C[^]N coordinated complexes

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Hydrogen has emerged as a clean and renewable source of energy and is a promising candidate as a substitute for fossil fuels. Huge efforts are being made to develop photosystems for HER (Hydrogen Evolution Reaction). Herein, we have utilized Pt(II) based complexes consisting of N[^]N[^]N and N[^]C[^]N chelate systems for the photocatalytic hydrogen production from HBF₄:H₂O. The complexes absorb between 315 to 380 nm in the UV-Vis spectra and have excited energy state lifetimes in the microsecond range. Using TEOA as the sacrificial electron donor for our reactions, we have excited each Pt(II) complex alone using 395 nm LEDs. Interestingly, [PtL₁Cl]⁺ (L₁= 2,6-di(quinolin-8-yl)pyridine) showed a turnover number of 190 in 40 hrs. Inspired by the results, we then coupled the complexes with [Ru(bpy)₃]²⁺ and [Co(dmgH₂)(py)Cl]. The [PtL₁Cl]⁺ complex showed a massive TON of 1200 when coupled with [Co(dmgH₂)(py)Cl] and a TON of 775 with [Ru(bpy)₃]²⁺ representing the best results to date under similar conditions. This proves that the [PtL₁Cl]⁺ complex is efficient both as a photosensitizer and a reduction catalyst for HER. The [PtL₂Cl]⁺ (L₂= 2,6-di(quinolin-8-yl)pyrazine) complex also acts as a fairly good catalyst. However, the cyclometalated [PtL₃Cl] (L₃= 1,3-di(quinolin-8-yl)benzene) shows surprisingly, very poor photosensitization and catalytic performance.



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(26) Development of highly efficient biomass-based catalysts for the removal of industrial pollutants from water (rhodamine dye)

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The spectacular increase in the world population has increased the demand for pure water, according to the UN, water needs will increase by 50% by 2030. At the same time, there is increasing industrialization which pollutes enormous quantities of water from the release of toxic and hazardous chemical substances. The presence of these contaminants in ground and surface water becomes a very serious problem and poses a threat to organisms and human health [1, 2].

Rhodamine B, (RhB, C₂₈H₃₁ClN₂O₃), mostly widely used in the textile industry, is a stable organic compound soluble in water, toxic, and non-biodegradable [2]. Therefore, several recent works have been carried out to remove or reduce the level of RhB in wastewater. Recently, nanomaterials derived from biomass have attracted particular interest due to their special properties (Nanometric size, porosity, catalytic activity, etc.) [1-4].

Against this backdrop, the present work involves the preparation of biomass-based catalysts with exceptional characteristics for the elimination of RhB molecules in wastewater. Graphitic carbon nitride/Carbon dots photocatalysts were successfully prepared using an eco-friendly synthesis method. The photodegradation process of Rhodamine B molecules under visible light was conducted at different irradiation times. The results obtained from UV-Visible spectroscopy demonstrated that the as prepared photocatalyst exhibited an exceptional efficiency of 99.8% for 30 min of photodégradation reaction. This remarkable outcome can be attributed to the homogeneous distribution of carbon dots on g-C₃N₄ sheets, which facilitates the adsorption of RhB molecules onto the catalyst's surface. The presence of carbon dots can enhance the transfer of photogenerated electrons to the active sites and effectively prevents the recombination of charge carriers (electron-hole).

In conclusion, biomass can serve as a renewable source for the development of efficient green photocatalysts that can be used for the removal of organic pollutants from wastewater.

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(27) Visible-light-driven photocatalytic CO₂ Reduction Performed by Coordination Polymers Based on the 1,2-di(4-pyridyl)ethylene Ligand and First-row Transition Metals

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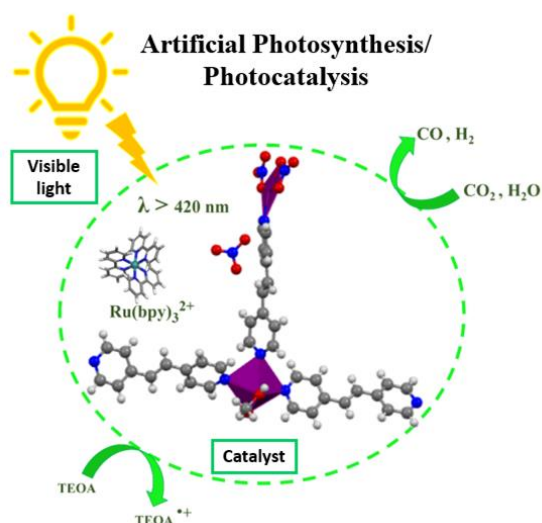
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Coordination polymers (CPs) are a rapidly emerging class of solid-state materials and offer unlimited possibilities for the design of chemical and physical properties depending on the topology of the overall structure.¹ These hybrid crystalline materials are formed by the coordination of a metal cation and organic ligands resulting in infinite hybrid networks such as zeolites² and MOFs (Metal-Organic Frameworks).³ CPs have attracted the interest of the scientific community since the advent of reticular chemistry and offer tremendous potential applications such as gas storage and separation,⁴ photoluminescence,⁵ catalysis,⁶ photocatalysis,⁷ magnetism,⁸ and drug delivery.

A series of coordination polymers were synthesized by the assembly of organic ligand 1,2-di(4-pyridyl) ethylene with divalent metal cations Cu²⁺, Co²⁺, Ni²⁺, and Zn²⁺ through solvothermal reactions. They were characterized using various techniques, including infrared spectroscopy (IR), single crystal X-ray diffraction (SCXRD), powder X-ray diffraction (PXRD), thermal analysis (TGA) and UV-vis spectroscopy. These coordination polymers exhibit interesting optical properties resulting from the interaction between the organic ligand and the metal cation. The application of these materials as catalysts in photocatalytic systems for carbon dioxide reduction was tested and yielded promising results.



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(28) A Simple Triboelectric Nanogenerator - Using a Salad Spinner as a Power Source

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As new and innovative electronic technologies continue to evolve, there is a growing need for microelectronics and efficient devices that are sustainable and environmentally friendly.¹ In 2012 this necessity was addressed by Wang. *et al.* by designing a triboelectric nanogenerator (TENG), which is a device that transforms and harvests wasted mechanical energy into electrical energy.² The working principle of these devices is based on contact electrification, where the friction or contact between two materials produces charges that are induced through a pair of electrodes, converting mechanical energy into power.^{2,3} This new technology allows for the development of light-weight, low cost, and high-power density devices.⁴ Herein a new type of rotatory TENG based on a salad spinner (SS-TENG) is reported as a power source. Specifically, wool or fur (material 1) is attached to the inner basket of a salad spinner to allow contact between the wool or fur and the styrene-acrylonitrile (outer plastic; material 2), as the triboelectric pair. Opencircuit and short-circuit measurements were performed to evaluate the generated output by using four interdigitated electrode configurations. Additionally, a series of LEDs were illuminated and the output difference between the wool and the rabbit fur SS-TENG was compared with other related rotary TENGs.

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