CQMF
QCAM

COLLOQUE ÉTUDIANT
STUDENT SYMPOSIUM

Vendredi, 1 novembre 2024

Friday, November 1st 2024

CARNET DE RÉSUMÉS
ABSTRACT BOOKLET

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2. Mot de bienvenue/Welcoming remarks

C'est avec grand plaisir que le comité étudiant du CQMF vous accueille à l'Université Concordia pour le Symposium étudiant du CQMF 2024. 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, la conférence plénière de la Dre Valentina Guccini, les résumés des conférences des étudiants (classés par session de présentation) et les titres des présentations par affiches.

Nous encourageons les conversations et les discussions entre les étudiants diplômés, les postdoctorants et les professeurs afin de renforcer la recherche au Québec. Nous vous invitons également à rester jusqu'à la fin de la journée pour célébrer les lauréats des présentations orales et affichées.

Avez-vous déjà envisagé de rejoindre le comité des étudiants du CQMF?

C'est l'occasion d'apporter de nouvelles perspectives, d'enrichir votre CV et de faire partie d'un environnement dynamique et collaboratif. Si vous êtes passionné par la promotion du développement académique et que vous voulez faire la différence, pensez à nous rejoindre pour façonner des événements futurs inspirants.

Le comité étudiant du CQMF

It is with great pleasure that the QCAM student committee welcomes you to Concordia University for the 2024 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, the plenary talk by Dr. Valentina Guccini, abstracts of the student talks (sorted by presentation session) and 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 oral and poster presentations.

Have you ever considered joining the QCAM Student Committee?

It's an opportunity to bring new perspectives, enhance your CV and be part of a dynamic, collaborative environment. If you're passionate about fostering academic development and making a difference, consider joining us to shape inspiring future events.

The QCAM student committee

Programme

9:00-9:45 (Toute la journée)	**Inscriptions**	Pavillon RF 100
9:35-9:45	**Notes de bienvenue**	Pavillon RF 110
	Présentations des étudiants Session 1 - Énergie	Pavillon RF 110
9:45-10:00	**Influence of Graphene Oxide on mechanical and Morphological properties of Nafion® Membranes** Carlos Ceballos Alvarez, et al. École de Technologie Supérieure (ETS)	
10:00-10:15	**π-Donor ligands to the rescue: influence of the metal-ligand covalency on photophysical properties** Arindam Saha, et al. Université de Montréal (UdeM)	
10:15-10:30	**Investigating Pulsed Laser Annealing of Hafnia-Zirconia Using a Dynamic Transmission Electron Microscope** Aida Amini, et al. Institut National de Recherche Scientifique (INRS)	
10:30-10:45	**Lithium-ion batteries electrolyte salts concentration profiles using a laboratory source** Brittany Pelletier-Villeneuve, et al. Université du Québec à Montréal (UQAM)	
10:45-11:00	**Titania Nanotube Semiconductor Arrays for Copper(I)-Bis(diimine) Sensitized** Joseph Daniel Chiong, et al. Concordia University	
11:00-11:15	**Pause café**	Pavillon RF 100
	Présentations des étudiants Session 2 - Énergie et Nanosciences	Pavillon RF 110
11:15-11:30	**Metal–Organic Frameworks for the Adsorptive Removal of Oxyanions in Nuclear Power Plants** Christopher Copeman, et al. Concordia University	
11:30-11:45	**Effects of Doping on the Self-Assembly of CsPbX3 Perovskite Supercrystals** Victoria Lapointe, et al. Concordia University	
11:45-12:00	**Single particle electrocatalysis using Scanning Electrochemical Cell microscopy (SECCM)** Samaneh Salek, et al. Université du Québec à Montréal (UQAM)	
12:00-12:15	**The versatility of micromotors: a perspective for new research in Quebec** Pedro Mena-Giraldo, et al. Concordia University	
12:15-13:00	**Pause Dîner**	Pavillon RF 100

13:00-13:45	**Plenary speaker** **Dr. Valentina Guccini** **Exploring the Structure-Property Relationship of Soft Matter to Enhance their Performance** **Uppsala University**	Pavillon RF 110
	Présentations des étudiants **Session 3 - Nanosciences et Développement Durable**	Pavillon RF 110
13:45-14:00	**Insight exploration of efficient charge transfer in boosting photocatalytic of Ag-WS2 plasmonic nanohybrids toward textile and pharmaceutical waste** Jaspal Singh, et al. Université du Québec à Trois-Rivières (UQTR)	
14:00-14:15	**In situ Electron Energy Loss Spectroscopy (EELS) Studies of Laserinduced Graphene Oxide Reduction in a Dynamic Transmission Electron Microscope (DTEM)** Israt Ali, et al. Institut National de Recherche Scientifique (INRS)	
14:15-14:30	**Routes to improve persistent luminescence in NaLuF4 nanoparticles.** Camilo Garcia Henao, et al. Concordia University	
14:30-14:45	**Computational Investigation of Potential-Dependent Competition of NRR and HER via Grand Canonical Ensemble DFT** Mehdi Shamekhi, et al. Concordia University	
14:45-15:00	**Pause café**	Pavillon RF 100
	Présentations des étudiants **Session 4 - Auto-assemblage Moléculaire et Biomédical**	Pavillon RF 110
15:00-15:15	**Tuning the Photosensitization Activity of Fluorenone-Based Materials** Léo Boivin, et al. Université de Sherbrooke (UdeS)	
15:15-15:30	**On the Development of Praseodymium-Doped Radioluminescent Nanoparticles and Their Use In X-Ray Mediated Photodynamic Therapy Of Glioblastoma Cells** Gabrielle Mandl, et al. Concordia University	
15:30-15:45	**MRI-assisted Monitoring and Explantation of Alginate Microbeads Encapsulating Insulin-producing Cells along with Magnetic Nanoparticles** Samila León Chaviano, et al. Université Laval (ULaval)	
15:45-16:00	**The Development of Aptasensors for Costimulatory Protein Receptors Detection** Sirirat Khemasiri, et al. Université du Québec à Montréal (UQAM)	
16:00-16:15	**First-Ever Integration of Ionic Liquid Crystal Elastomers (iLCEs) For biomedical Microelectromechanical (MEMS) Sensors** Elaheh Asgari, et al. École de Technologie Supérieure (ETS)	
16:15-16:30	**Pause café**	Pavillon RF 100

Présentations des étudiants

Session 5 - Polyméres

Pavillon RF 110

16:30-16:45

Préparation et caractérisation de mélanges polymère:photosensibilisateur

Ramzi Zidani, et al. Université de Montréal (UdeM)

16:45-17:00

Development of a polymersome blood ammonia assay coupled with a portable near-infrared fluorometer

Marie-Lynn Al-Hawat, et al. Université de Montréal (UdeM)

17:00-17:15

Caractérisation locale des phases dans les polymères semicristallins imprimés

Maxime Goulet, et al. Université de Montréal (UdeM)

17:15-17:30

Towards a better understanding of the polymer – salt coordination phenomenon in solid polymer electrolyte

Tristan Perodeau, et al. Université de Montréal (UdeM)

17:30-17:45

Azatriangulene-based Conductive C=C Linked Covalent Organic Frameworks with Near-Infrared Emission

Ehsan Hamzehpoor, et al. University of British Columbia

17:45-18:00

Invited speaker

Dr. Olivier Rynne

Volt-Age

Concordia University

Pavillon RF 110

18:00-19:45

Session d'affiches

Pavillon RF 120

Énergie

1) Elizabeth Lamothe
2) Aaron Gabriel Nunez Avila
3) Oubaha Ilyes
4) Qihang Yu
5) oseph F. Ricardo-Noordberg
6) Orlando Ortiz
7) Orlando Ortiz
8) Ameer Nizami
9) Zhao Yang
10) Vivian Alexandra
11) Rupinder Kaur
12) Ilies Seddiki
13) Donia Dridi
14) Mohammad Masaeli
15) Maryam Alihosseini
16) Anna Thinphang-nga

Développement Durable

17) Ahmed Azrrar
18) Cristina Pomillio

Auto-assemblage Moléculaire et Biomédical

19) Mahdokht Akbari Taemeh
20) Raquel Espino-López
21) Anne-Frédéric Laurin
22) Nishadi Lokuge
23) Souheib Zekraoui
24) Myriam Lessard

Polymères

25) Sacha Porlier
26) Ghazal Minoofar
27) Sofia Nieves Casillas-Popova
28) Rachid Amrhar
29) Gabriel Mercier
30) Fateme Eslampanah

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Remise des prix & Mots de remerciements

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Liste des intervenants pour les présentations orales

Session 1 : Énergie

	Nom et Prénom	Titre de la présentation	Institution
1	Carlos Ceballos Alvarez 9:45-10:00	Influence of Graphene Oxide on Mechanical and Morphological properties of Nafion® Membranes	École de Technologie Supérieure (ETS)
2	Arindam Saha 10:00-10:15	π-Donor ligands to the rescue: influence of the metal-ligand covalency on photophysical properties.	Université de Montréal (UdeM)
3	Aida Amini 10:15-10:30	Investigating Pulsed Laser Annealing of Hafnia-Zirconia Using a Dynamic Transmission Electron Microscope	Institut National de Recherche Scientifique (INRS)
4	Brittany Pelletier-Villeneuve 10:30-10:45	Lithium-ion batteries electrolyte salts concentration profiles using a laboratory source	Université du Québec à Montréal (UQAM)
5	Joseph Daniel Chiong 10:45-11:00	Titania Nanotube Semiconductor Arrays for Copper(I)-Bis(diimine) Sensitized Photoelectrodes.	Concordia University (Concordia)

Break : 11:00-11:15

Session 2 : Énergie et Nanosciences

6	Christopher Copeman 11:15-11:30	Metal–Organic Frameworks for the Adsorptive Removal of Oxyanions in Nuclear Power Plants	Concordia University (Concordia)
7	Victoria Lapointe 11:30-11:45	Effects of Doping on the Self-Assembly of $CsPbX_3$ Perovskite Supercrystals	Concordia University (Concordia)
8	Samaneh Salek 11:45-12:00	Single particle electrocatalysis using Scanning Electrochemical Cell microscopy (SECCM)	Université du Québec à Montréal (UQAM)
9	Pedro Mena-Giraldo 12:00-12:15	The versatility of micromotors: a perspective for new research in Quebec	Concordia University (Concordia)

Lunch : 12:15-13:00

13:00-13:45 Plenary speaker :

Dr. Valentina Guccini

Exploring the Structure-Property Relationship of Soft Matter to Enhance their Performance

Uppsala University

Department of Chemistry – Ångström Laboratory Uppsala University, Uppsala, Sweden

valentina.guccini@kemi.uu.se

Cellulose nanofibers and nanocrystals (CNFs and CNCs), collectively referred to as nanocellulose, are bio-derived nanomaterials characterized by remarkable chemical and physical versatility. They exhibit high intrinsic mechanical properties, water affinity and biocompatibility. Additionally, their colloidal suspensions self-assemble into liquid crystalline phases, resulting in materials with intriguing optical properties such as structural colors. Due to this diversity and versatility, nanocellulose-based materials have been implemented in a wide range of applications.

In my research, I study the structure-property relationships of nanocellulose-based materials with respect to their building blocks and fabrication methods, aiming to tailor their physical and chemical properties towards specific functionalities. In my contribution, I will present this approach demonstrated by my research on fossil-free energy applications (e.g. fuel cells and lithium-ion batteries) and photosynthetic biohybrids for biotechnological processes, such as water remediation and carbon dioxide bioconversion. Furthermore, I will share my experience conducting interdisciplinary research at the intersection of materials chemistry, microbiology and art, as well as in affirming my identity as a researcher

Session 3 : Nanosciences et Développement durable

	Nom et Prénom	**Titre de présentation**	**Institution**
10	Jaspal Singh 13:45-14:00	Insight exploration of efficient charge transfer in boosting photocatalytic of Ag-WS_2 plasmonic nanohybrids toward textile and pharmaceutical waste	Université du Québec à Trois-Rivières (UQTR)
11	Israt Ali 14:00-14:15	In situ Electron Energy Loss Spectroscopy (EELS) Studies of Laserinduced Graphene Oxide Reduction in a Dynamic Transmission Electron Microscope (DTEM)	Institut National de Recherche Scientifique (INRS)
12	Camilo Garcia Henao 14:15-14:30	Routes to improve persistent luminescence in $NaLuF_4$ nanoparticles.	Concordia University (Concordia)
13	Mehdi Shamekhi 14:30-14:45	Computational Investigation of Potential-Dependent Competition of NRR and HER via Grand Canonical Ensemble DFT	Concordia University (Concordia)

Break : 14:45-15:00

Session 4 : Auto-assemblage Moléculaire et biomédical

	Nom et Prénom	Titre de présentation	Institution
14	Léo Boivin 15:00-15:15	Tuning the Photosensitization Activity of Fluorenone-Based Materials	Université de Sherbrooke (UdeS)
15	Gabrielle Mandl 15:15-15:30	On the Development of Praseodymium-Doped Radioluminescent Nanoparticles and Their Use In X-Ray Mediated Photodynamic Therapy Of Glioblastoma Cells	Concordia University (Concordia)
16	Samila León Chaviano 15:30-15:45	MRI-assisted Monitoring and Explantation of Alginate Microbeads Encapsulating Insulin-producing Cells along with Magnetic Nanoparticles	Université Laval (ULaval)
17	Sirirat Khemasiri 15:45-16:00	The Development of Aptasensors for Costimulatory Protein Receptors Detection	Université du Québec à Montréal (UQAM)
18	Elaheh Asgari 16:00-16:15	First-Ever Integration of Ionic Liquid Crystal Elastomers (iLCEs) For biomedical Microelectromechanical (MEMS) Sensors	École de Technologie Supérieure (ETS)

Break : 16:15-16:30

Session 5 : Polymères

	Nom et Prénom	Titre de présentation	Institution
19	Ramzi Zidani 16:30-16:45	Préparation et caractérisation de mélanges polymère:photosensibilisateur	Université de Montréal (UdeM)
20	Marie-Lynn Al-Hawat 16:45-17:00	Development of a polymersome blood ammonia assay coupled with a portable near-infrared fluorometer	Université de Montréal (UdeM)
21	Maxime Goulet 17:00-17:15	Caractérisation locale des phases dans les polymères semicristallins imprimés	Université de Montréal (UdeM)
22	Tristan Perodeau 17:15-17:30	Towards a better understanding of the polymer – salt coordination phenomenon in solid polymer electrolyte	Université de Montréal (UdeM)
23	Ehsan Hamzehpoor 17:30-17:45	Azatriangulene-based Conductive C=C Linked Covalent Organic Frameworks with Near-Infrared Emission	University of British Columbia

17:45-18:00 Invited speaker:

Dr. Olivier Rynne

Volt-Age, Concordia University

Poster session: 18:00-19:45

Liste des intervenants par présentation Affiche

Énergie

	Nom et Prénom	Titre de présentation	Institution
1	Elizabeth Lamothe	Synthesis and characterization of AMidine OXide (AMOX) ligands with photoactive anthracene core and their associated metal complexes	Université de Montréal (UdeM)
2	Aaron Gabriel Nunez Avila	Towards insoluble diphenoquinones for a use in organic batteries	Université de Montréal (UdeM)
3	Oubaha Ilyes	Homoleptic cobalt(III) bisguanidylpyridine complexes for photocatalytic and photoredox processes	Université de Montréal (UdeM)
4	Qihang Yu	An active bifunctional natural dye for high-areal-capacity all-solid-state batteries.	Concordia University (Concordia)
5	Joseph F. Ricardo-Noordberg	Molecular Copper(I)-Sensitized Photoanodes for Alcohol Oxidation under Ambient Conditions	Concordia University (Concordia)
6	Orlando Ortiz	Synthesis of radical-based fluorophores for stimuli responsive devices: a proof of concept	Université de Montréal (UdeM)
7	Orlando Ortiz	Photostable open-shelled fluorophores for near-infrared organic light-emitting diodes: a proof of concept	Université de Montréal (UdeM)
8	Ameer Nizami	Modeling Metal Nitrides for Thin-Films in Lithium-Sulfur Batteries on GPU and CPUs	Concordia University (Concordia)
9	Zhao Yang	Self-Healing Multi-Functional Coating of Sulfur Cathodes for High-Performance Li-S Batteries from Liquid-State to Solid-State	Concordia University (Concordia)
10	Vivian Alexandra	Synthesis of Formamidines as Precursors for N,N'-Disubstituted Amidine N-Oxide Ligands for Transition Metal Complexes	Université du Québec à Trois-Rivières (UQTR)
11	Rupinder Kaur	Electroactive Polymer coatings of Perylene derivatives for energy storage devices	Université de Montréal (UdeM)

12	Ilies Seddiki	DFT calculation for selecting redox active biosourced material as a cathode for organic batteries	Université de Montréal (UdeM)
13	Donia DRIDI	Enhanced photocatalytic performance of Intercalated 2D BiOBr nanosheets into 3D knobs-like Bi2WO6 for the degradation of antibiotics and textile pollutants	Université du Québec à Trois-Rivières (UQTR)
14	Mohammad Masaeli	High-entropy hydride for Fast and Reversible Hydrogen Storage at Room Temperature	Université du Québec à Trois-Rivières (UQTR)
15	Maryam Alihosseini	In-situ study of surface modification on TI3C2 as a catalyst for hydrogen evolution reaction	Université du Québec à Montréal (UQAM)
16	Anna Thinphang-nga	Self-Healing Poly(Hindered Urea) Polymer Network as Coating Layer on Carbon/Sulfur Composite in High-Performance LithiumSulfur Batteries	Concordia University (Concordia)

Développement durable

	Nom et Prénom	**Titre de présentation**	**Institution**
17	Ahmed Azrrar	Phosphorylation des écorces des feuillus et des résineux avec l'ester de phosphate	Université du Québec à Trois-Rivières (UQTR)
18	Cristina Pomilio	Characterization of Fe-Metal Coordination Complexes for Enhanced Redox-Flow Battery Applications	Concordia University (Concordia)

Auto-assemblage Moléculaire et biomédical

	Nom et Prénom	**Titre de présentation**	**Institution**
19	Mahdokht Akbari Taemeh	Development of a 3D-printed cell-laden hydrogel phantom for improvement of precision in eye cancer brachytherapy	Université Laval (ULaval)
20	Raquel Espino-López	Development of Hydrogel-Based Eye Models for Enhanced the Ocular Ultrasound Training	Université Laval (ULaval)
21	Anne-Frédéric Laurin	Perfusable pancreatic tissues fabrication using a sacrificial embedded writing approach	McGill University (McGill)
22	Nishadi Lokuge	PVA e-spun nanofibrous mats modified with carbon nanodots for wound dressing: synthesis, characterization, and fluorescence analysis	Concordia University (Concordia)
23	Souheib Zekraoui	Development of Biocompatible Therapeutic Objects with Radiopaque properties by Fused Filament Fabrication (FFF) 3D Printing	Université Laval (ULaval)

24	Myriam Lessard	Quantification de la structure de matériaux moléculaires	Université de Montréal (UdeM)

Polymères

	Nom et Prénom	Titre de présentation	Institution
25	Sacha Porlier	Electrochromic and Electrofluorochromic Properties of Conjugated Copolymers Carried Over to the Solid-State for Applications in Chromic Devices	Université de Montréal (UdeM)
26	Ghazal Minoofar	Weathering Properties of Silicone-Epoxy Coatings for Enhancing Wind Turbine Efficiency in Cold Climates: Effect of Different Silicone Intermediates	Université du Québec à Chicoutimi (UQAC)
27	Sofia Nieves Casillas-Popova	Exploration of boronic ester chemistry to develop pH-responsive degradable crosslinked electrospun nanofibers for controlled drug release wound dressing	Concordia University (Concordia)
28	Rachid AMRHAR	Époxydation des huiles usagées	Université du Québec à Trois-Rivières (UQTR)
29	Gabriel Mercier	Synthesis and characterization of a new terpyridine ligand and corresponding ruthenium complexe for artificial photosynthesis	Université de Montréal (UdeM)
30	Fateme Eslampanah	Developing silicone acrylic coating: A step forward in ice mitigation for wind turbines	Université du Québec à Chicoutimi (UQAC)

Awards – Closing remarks 19:45-20:00

Abstracts' Talks

1.- Influence of Graphene Oxide on Mechanical and Morphological

properties of Nafion® Membranes

Carlos Ceballos-Alvarez[1], Maziar Jafari[3], Mohamed Siaj[3], Samaneh Shahgaldi[2] and Ricardo Izquierdo[1]
1. École de Technologie Supérieure - Département de génie électrique; 1100 Notre-Dame Street West, H3C 1K3, Montreal, Québec, Canada.
2. Université du Québec à Trois-Rivières-Institute de Recherche sur l'Hydrogene, 3351, Boul. des Forges C.P.500, G9A 5H7 Trois-Rivières, Québec, Canada.
3. Université du Québec à Montréal - Département de Chimie, 2101 rue Jeanne-Mance, H2X 2J6, Montréal, Québec, Canada.
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This study explored the influence of graphene oxide (GO) on the morphological and mechanical properties of Nafion® 115 membranes with the objective of enhancing the mechanical properties of the most widely employed membrane in Proton Exchange Membrane Water Electrolyzers (PEMWE) applications. The membrane surface was modified by ultrasonically spraying a GO solution, and different annealing temperatures were tested. Scanning Electron Microscopy (SEM) cross-sectional images revealed that annealing the composite membranes was sufficient to favor an interaction between the graphene oxide and the surface of the Nafion® membranes. The GO covering only 35% of the membrane surface increased the composite's wettability from hydrophobic (105.2°) to a highly hydrophilic angle (84.4°) while slightly reducing membrane swelling. Tensile tests depicted an increase in both strain levels and tensile loads before breaking. The samples with GO presented remarkable mechanical properties when the annealing time and temperature increased, while the Nafion® control samples failed at elongations of 95% and 98%. Their counterparts with GO on the surface achieved elongations of 248% and 191% when annealed at 80°C and 110°C respectively, demonstrating that the presence of GO mechanically stabilizes the membranes under tension. In exchange, the presence of GO altered the smoothness of the membrane surface, going from an average of 1.4 nm before the printing to values ranging from 8.4 to 10.2 nm depending on the annealing conditions, which could affect the quality of the subsequent catalyst layer printing. Overall, the polymer's electrical insulation was unaffected, making the Nafion®-GO blend a more robust material than those traditionally used.

2.- Donor ligands to the rescue: influence of the metal-ligand covalency on photophysical properties.

Arindam Saha[$], Georges Turner[$], Mihaela Cibian[#], Fausto Puntoriero[+], Francesco Natasi[+],
Sebastiano Campagna[+] and Garry S. Hanan[$]*
$ Département de Chimie, Université de Montréal
 # Département de biochimie, chimie, physique et science forensique, Université du Québec à Trois-Rivières
+ Department of Chemical, Biological, Pharmaceutical and Environmental Science, Università degli Studi di Messina

The development of photoactive transition metal complexes has traditionally focused on second- and third-row transition metal ions, such as ruthenium, iridium, and platinum, due to their favorable photophysical properties. However, these metals are scarce, expensive, and pose environmental concerns, prompting a shift towards first-row transition metal ions as more sustainable alternatives. First-row transition metal complexes (e.g., those based on iron, copper, cobalt, nickel, and zinc) offer several advantages, including abundance, lower cost, and reduced environmental impact. Despite these benefits, these metal complexes often exhibit less desirable photophysical characteristics, such as shorter excited-state lifetimes and lower photostability. Overcoming these challenges through ligand design, coordination geometry optimization, and tuning electronic properties is crucial to unlocking the potential of these metals for applications in solar energy conversion, photocatalysis, and light-emitting devices. Herein, we present a novel class of Co(III)-amidine N-oxide complexes exhibiting weak low energy LMCT absorptions beyond 500 nm. High lying π-orbitals on the ligand scaffold lead to this novel photophysical properties wherein the complexes refuse to obey Kasha and Vavilov rules. The nanosecond excited-state lifetimes of these complexes pave the way to new avenues for π-donor ligand sites in the enhancement of optoelectronic properties of complexes of abundant transition metal ions.

1. Rau, S.; Pfeffer, M. G.; Staehle, R. Metal Complexes for Photohydrogenation and Hydrogen Evolution. *Chemical Photocatalysis* **2020**, 301–32
2. Förster, C.; Heinze, K. Photophysics and Photochemistry with Earth-Abundant Metals – Fundamentals and Concepts. *Chemical Society Reviews* **2020**, 49 (4), 1057–1070.
3. Wegeberg, C.; Wenger, O. S. Luminescent First-Row Transition Metal Complexes. *Journal of the American Chemical Society Au* **2021**, 1 (11), 1860–1876.

3.- Investigating Pulsed Laser Annealing of Hafnia-Zirconia Using a Dynamic Transmission Electron Microscope

Aida Amini[1], *Kenneth Beyerlein*[1*], *Katharina Kohlmann*[1], *Sebastian Obernberger*[1], *Andreas Ruediger*[1]
1 Institut national de la recherche scientifique (INRS), Energy Materials and telecommunication, Varennes, QC, Canada.
** Corresponding author: Kenneth.Beyerlein@inrs.ca*

Understanding the transient phenomena such as phase transitions in polymorphic materials is crucial for advancements in materials science, impacting the development of innovative materials and devices. This study focuses on the phase transition induced by pulsed laser annealing (PLA) in $Hf_{0.5}Zr_{0.5}O_2$ (HZO), a promising candidate for ferroelectric applications due to its ability to exhibit a non-centrosymmetric orthorhombic phase, which is responsible for the ferroelectricity in this material. The objective is to examine in-situ the quantitative ferroelectric phase formation due to PLA, along with analyzing the effects of laser energy density and HZO film thickness on it. This aims to identify optimized laser parameters for achieving the desired ferroelectric crystal structure. This study involves the analysis of selected area electron diffraction (SAED) patterns which is a potent characterization tool for quantitative phase determination of the ferroelectric phase in HZO. The dynamic transmission electron microscope (DTEM) at INRS can perform in-situ PLA and electron diffraction studies, which have not previously been reported for HZO. The DTEM is a novel TEM instrument which is coupled with a drive laser (pump laser) that interacts with the sample, initiating an irreversible transformation in the material which can be captured in situ. Our experimental setup utilized the second harmonic of a Nd:YAG laser, coupled within the DTEM to initiate in-situ PLA, providing local observation of the structural transformations in HZO thin films. By adjusting the laser energy density, the study aimed to optimize the conditions for the crystallization of the ferroelectric phase. The results of the SAED studies indicate a clear crystallization and formation of the orthorhombic phase at a laser energy density of 287 mJ/cm^2, for 8nm HZO, where the characteristic electron diffraction peak corresponding to the orthorhombic/tetragonal phase, o(111)/t(101), was significantly observed, indicating successful phase transformation. Additionally, the study examines the influence of HZO film thickness on the orthorhombic phase formation, providing insights into the tailored application of PLA for achieving desired ferroelectric properties. In summary, this research sheds light on the critical parameters influencing the ferroelectric phase formation in HZO, providing new insights into the crystallization of HZO thin films by laser annealing. The findings demonstrate the ability to control phase formation through PLA, which is a promising low thermal-budget end-of-the-line processing step to fabricate ferroelectric devices.

4.- Lithium-ion batteries electrolyte salts concentration profiles using a laboratory source

Brittany Pelletier-Villeneuve, Bastian Krueger, Jonathan Adsetts, Marie-Claude Ricard, Steen Schougaard
Département de chimie, Université du Québec à Montréal
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The development of high-power lithium batteries is seriously limited by the understanding of the formation of electrolyte salts concentration gradient. This limiting factor, though critical at high charging rate, is difficult to study effectively and to model accurately. Often, their study is limited to the concentration in the separator or require the use of a synchrotron source which is a very limited resource. In here, we used a laboratory source to track the electrolyte salt concentration gradient in *operando* through the entire electrode-separator-electrode stack by X-ray fluorescence (XRF). The heatmaps plot of salt concentration as a function of position and time showed excellent temporal and spatial resolution. These results show the performance of a laboratory source to be similar to previous synchrotron-based measurements. The cross section of electrochemical cell can be fully scanned in 184 seconds with a beam of 5 µm and step size of 15.5µm. The measurements were done over a period of 24h and multiple charging rate were studied.

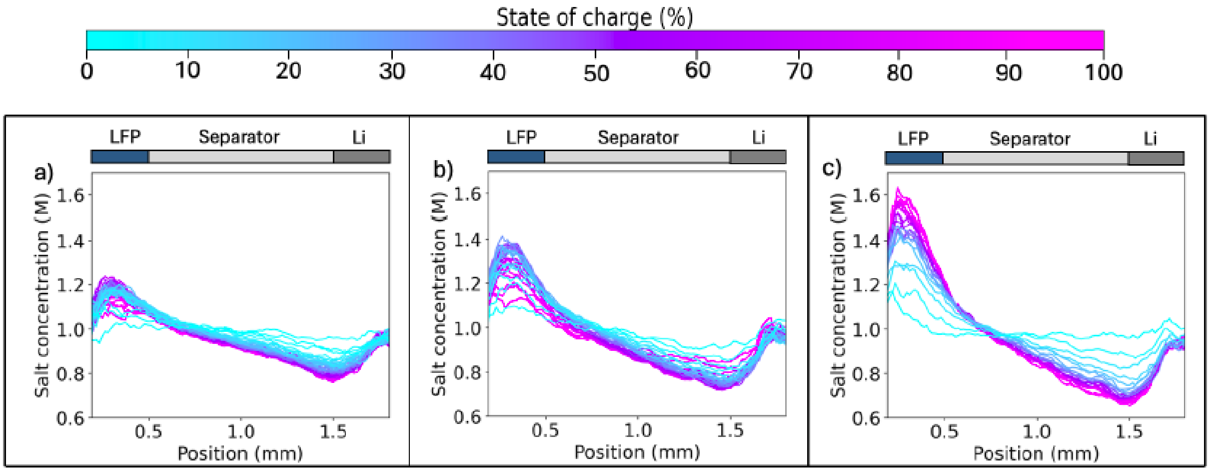

Figure 1 - Electrolyte salt gradient concentration during charge at a) c/3, b) c/2 and c) c/1.5

5.- Titania Nanotube Semiconductor Arrays for Copper(I)-Bis(diimine) Sensitized Photoelectrodes.

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The use of chemical bonds to store solar energy is a way to advance current sustainability goals and address intermittent limitations. The approach of interest to drive these processes is to use a bespoke semiconductor surface implemented in a photoelectrode to absorb light and generate charge carriers that can drive redox reactions such as the direct oxidation of adsorbed species on the photoanode. To minimize the recombination of photogenerated electron-hole pairs, molecular donor-chromophore-acceptor (D-C-A) systems can be used to sensitize wide bandgap semiconductors for visible light absorption and to generate (high energy) long-living charge separated states. Presented here is a highly ordered and oriented array of TiO_2 1-dimensional nanostructure purpose-grown using a self-organizing electrochemical anodization approach (SOA) and functionalized with a Cu(I)-based chromophore. The resulting photoanode, Figure 1, is investigated against a water oxidation catalyst (e.g., [Cp*Ir(pyalk)OH], pyalk = 2-(pyridine-2-yl)propan-2-ol) for the ability to generate oxidizing equivalents that can subsequently drive follow-on oxidation reactions.

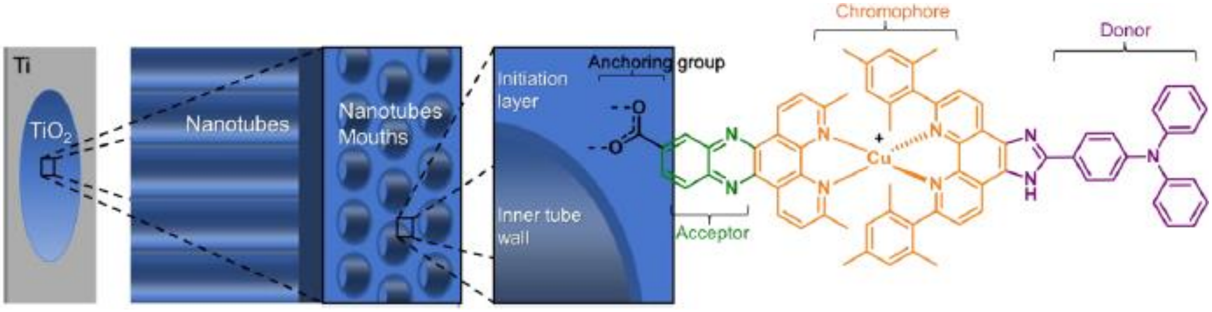

Figure 1. Proposed photoanode architecture presented in this work.

6.- Metal–Organic Frameworks for the Adsorptive Removal of Oxyanions in Nuclear Power Plants

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Nuclear power represents 10% of global electricity production and 28% of low carbon electricity generation. To keep power plants running safely and efficiently, the water used must be ultrapure, to prevent corrosion or interference in the nuclear reaction. Oxyanions of various elements are common contaminants in water used in the generation of electricity at nuclear power plants. Zirconium-based metal–organic frameworks (MOFs) have been previously shown in the literature to capture a variety of oxyanions by adsorption on nodal open metal sites, typically binding in an $\eta_2\mu_2$ fashion. Herein, adsorption of oxyanions on Zr_6-based MOFs will be discussed, including the kinetics of adsorption, maximum uptake capacity, and characterization of the adsorption mechanism as well as the effect of harsh conditions present in power generation environments on the MOF adsorption characteristics and material stability.

7.- Effects of Doping on the Self-Assembly of $CsPbX_3$ Perovskite Supercrystals

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Supercrystal formation afforded by the self-assembly of cesium lead halide (CsPbX3) perovskite nanocrystals has been a phenomenon of interest due to the high three-dimensional structural order required and the resulting properties. The high structural order is influenced by the surface chemistry and particle morphology of the starting nanocrystal building blocks. Ion doping into metal halide perovskite nanocrystals has also been investigated as these dopants have been found to improve their optoelectronic and morphological properties while also imparting other characteristics not originally present in the metal halide perovskites. In this work, we investigate the structural and photophysical effects of dopants on cesium lead halide perovskite supercrystals through absorbance and photoluminescence spectroscopies, photoluminescence quantum yields, powder X-ray diffraction, and electron microscopy.

8.- Single particle electrocatalysis using Scanning Electrochemical Cell microscopy (SECCM)

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Scanning electrochemical cell microscopy (SECCM) is a method that measures electrochemical fluxes at the micro and nanoscale. In this method, a nanopipette filled with electrolyte and a quasi-reference counter electrode is used to create a confined electrochemical cell between the tip of the pipette and an electrode surface [1]. Due to its high sensitivity, SECCM has been used to study functional materials at the single particle level for a variety of electrocatalytic reactions.[2] The oxygen reduction reaction (ORR) is a critical process in renewable energy conversion technologies, such as low-temperature fuel cellsand metal-air batteries[3]. For the ORR, SECCM provides a setup with a three-phase boundary that includes the solid electrode, liquid electrolyte, and atmosphere (air) [4]. In this work a multimicroscopy approach of scanning electrochemical cell microscopy combined with scanning electron microscopy to study the influence of particle size on the electrocatalytic current of individual particles toward the oxygen reduction reaction (ORR) and Hydrogen Evolution Reaction (HER).

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9.- The versatility of micromotors: a perspective for new research in Quebec

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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. The micromotors are mainly classified by their propulsion mechanisms, such as self-diffusiophoretic, magnetic, and difussiophoresis, which can be divided into two principal groups: chemical- and free-fuel systems. The first group presents a finite motion depending on the time the fuel is consumed, and the second group is based on the use of external fields, such as magnetic fields, sound waves, and light. Furthermore, the versatility of micromotors can be demonstrated by the use of proteins, metals, hydrogels, organic materials, and polymers for biomedical, environmental, and many other applications.[1]

Here, we explain the versatility of motion production and the application of micromotors with tree systems based on chemical- and free-fuel micromotors. Firstly, self-propelled micromotors were developed with platinum and magnetic nanoparticles embedded in a matrix of modified chitosan, which can propel the micromotor for O_2 bubbles by a catalytic reaction in the presence of H_2O_2 and external motion control with the use of a magnetic field. In order to increase the enzymatic activity of immobilized enzymes on the motors for enhanced substrate and pollutant degradation.[2]

In contrast, near-infrared (NIR)-activated micromotors were made, composed of a chitosan biopolymer, magnetite, and lanthanide upconverting nanoparticles (UCNPs), and the curcumin photosensitizer. Under 976 nm excitation, magnetite nanoparticles generate a temperature gradient to activate the photophoretic motion, enabling the movement from cold to hot regions. Meanwhile, the UCNPs produce visible light used for micromotor tracking and triggering reactive oxygen species generation for pollutant degradation.[3]

Micromotors are characterized by producing motion in water solutions. To translate the frontier of micromotors from water to air matrix, we developed micromotors based on ZnO dandelions (microdrone-likes) with gold and UCNPs on their surface. These can produce convection movement by photophoresis mechanism under NIR irradiation, overcoming gravity with the potential for gas photocatalysis.

Together, these systems provide a versatile approach to achieving motion in water and air while taking advantage of micromotors' many potential applications. Capobianco's lab pioneers developing micromotors in Quebec, venturing into and showing a niche to explore in different research areas.

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10.- Insight exploration of efficient charge transfer in boosting photocatalytic of Ag-WS_2 plasmonic nanohybrids toward textile and pharmaceutical waste

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Plasmonic nanoparticles functionalized two-dimensional layered nanostructures have proven to be advanced materials in environmental remediation applications and have aroused great attention. In this work, Ag nanoparticles functionalized a few layers of WS2 nanosheets, which were prepared through liquid-phase exfoliation and hydrothermal methods, are studied for photocatalytic applications. Field emission scanning electron microscopy and transmission electron microscopy studies affirm the attachments of spherical Ag nanoparticles with an average size of 42 nm, which are uniformly attached on the surface of 2D- nanosheets of WS2. X-ray diffraction results inferred the presence of Ag nanoparticles with WS_2 nanostructures while Raman spectroscopy results manifest the significant shift due to the different loading of Ag nanoparticles over WS_2 nanosheets. Optical absorption spectroscopy and photoluminescence imply the effective bandgap narrowing and efficient charge separation in Ag-WS_2 nanohybrids as compared to pure WS_2 nanosheets. Optimum Ag-WS_2 nanohybrids (0.5 mg/mL) show enhanced photocatalytic behavior as compared to other prepared samples and decomposed 10µM of MB, 10µM of MO, and 1mg/mL of OTC-HCl solution in 60, 40, and 60 minutes respectively which has not been reported yet. The enhanced photo-degradation nature of Ag-WS_2 nanohybrids can be attributed to the effective charge transfer among Ag nanoparticles and WS_2 nanosheets which is further explored by first principle density functional theory. Although few reports are available that demonstrate the photocatalytic profile of plasmonic-WS_2, precise optimization, insight charge transfer dynamics and their direct co-relation for efficient charge transfer mechanisms still need to be explored.

Keywords: plasmonic, photocatalyst, WS_2, Ag NPs, OTC-HCl

11.- In situ Electron Energy Loss Spectroscopy (EELS) Studies of Laserinduced Graphene Oxide Reduction in a Dynamic Transmission Electron Microscope (DTEM)

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Reduced graphene oxide (rGO) is crucial for applications in energy storage and sensors due to its high electrical conductivity and large surface area. Additionally, its tunable chemical and physical properties make it a versatile material for catalysis and biomedical applications. rGO can be obtained from graphene oxide (GO) by many methods, including wet chemical reduction, thermal reduction, and photoreduction. Photoreduction of graphene oxide to rGO offers precise control over reduction areas and degrees, allowing for patterned and localized reduction without hazardous chemicals. Unlike chemical reduction, it avoids introducing unwanted impurities, and compared to thermal reduction, it requires lower energy and operates at ambient temperatures, making it more eco-friendly and energy efficient. Additionally, photoreduction enables real-time process monitoring and modulation of reduction parameters. However, a detailed study to understand the real mechanism of laser-induced photoreduction of GO is not well explored. We conducted in situ experiments using a dynamic transmission electron microscope (DTEM) watching the photoreduction process of GO sheets. The DTEM at INRS-EMT is based on a JEOL 2100Plus and has been modified to couple laser light into the column through an optical port and focus it onto the sample. We used this configuration to track the reduction in oxygen concentration in the sample upon irradiation by nanosecond laser light pulses. The GO sample was prepared using a modified Hummer's method and drop cast on a lacey carbon grid. The second harmonic from a Nd:YAG nanosecond pulsed laser (wavelength = 532 nm, repetition rate = 10 Hz, pulse duration = 11 ns) was aligned into the microscope and focused to a spot size of 100 m on the sample. Laser pulse energy densities ranging from 3.18 to 15.9 mJ/cm² were systematically applied to investigate their impact on the reduction process. We utilized electron energy loss spectroscopy (EELS) to quantify the change in oxygen reduction with a collection angle of 12.7 mrad. Multiple EELS spectra of Carbon and Oxygen K-edges were collected before and after laser irradiation to determine relative composition atomic percentages. Further, the log ratio method was used to determine the changes in the thickness of graphene oxide. In this presentation, we will showcase the trends observed while measuring the reduction of oxygen concentration and sample thickness as a function of laser fluence. We will also demonstrate how these quantities evolve as a function of laser exposure time which allows us to measure the kinetics of the GO photoreduction process. We will discuss the optimal laser parameters to produce high-quality rGO by photoreduction while minimizing material ablation. This information is important for the growing graphene manufacturing and application industries. Furthermore, this presentation exemplifies the kind of information that can be obtained by in situ laser irradiation TEM experiments.

12.- Routes to improve persistent luminescence in $NaLuF_4$ nanoparticles

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Persistent luminescence is the phenomenon where a luminescent material keeps glowing after the excitation source is turned off, it is a type of transient energy storage. Persistent luminescent nanoparticles can be convenient for several applications where the need for constant light excitation is a limitation; however, these materials are limited to the afterglow duration and intensity. Er-based persistent luminescence is rarely explored but represents an interesting choice of activator because of its strong and narrow emissions in the green and red regions. As this phenomenon depends on the release of energy from traps within the bandgap to produce luminescence, We explored the use of Li(I), K(I) and Fe(III) as a means to generate defects and produce new trapping states in NaLuF4:Er. The morphological characterization of the developed materials was carried out using TEM and XRD, and their optical properties were studied using emission spectroscopy (radioluminescence and persistent luminescence). An example is shown in the Figure 1, below.

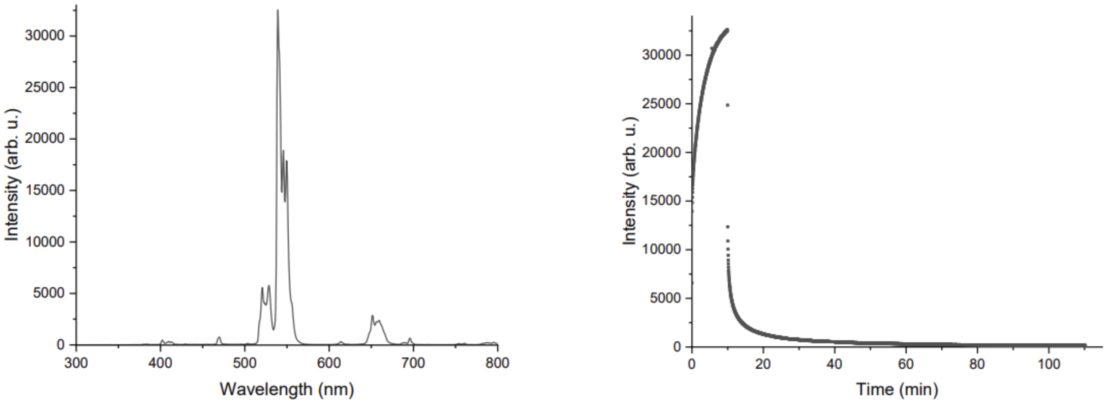

Figure 1. Radioluminescence spectra (left) and persistent luminescence kinetics (right) of $NaLuF_4$:Er nanoparticles

13.- Computational Investigation of Potential-Dependent Competition of NRR and HER via Grand Canonical Ensemble DFT

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Electrochemical reactions take place at the solid-electrolyte interface, however, modeling of these processes at the atomic scale is challenging and may require techniques beyond conventional models. Charge neutrality is essential for density functional theory (DFT) calculations and the computational hydrogen electrode, a standard quantum chemistry approach in the field, neglects the effect of potential experienced by the electrode material in a proton-coupled electron transfer step in an electrochemical reaction. On the other hand, grand canonical ensemble DFT (GC-DFT) allows the treatment of a system at fixed electrode potential by fixing the Fermi level and varying the number of electrons in the simulation box. Accordingly, we evaluate adsorption free energies of the nitrogen reduction reaction (NRR) and the hydrogen evolution reaction (HER) intermediates on transition metal surfaces at constant electrode potential. The HER is found to be more favourable than the NRR with increase in the electrode potential, a feature that is not predicted by standard DFT, and rationalizes the premature decrease in NRR activity observed experimentally. This highlights the importance of accounting for the electrode potential in computational investigations of the thermodynamics and kinetics of electrochemical reactions.

14.- Tuning the Photosensitization Activity of Fluorenone-Based Materials

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Through synthetic modifications, 9-fluorenone was derived into 2,7-bis(propylthio)-9-fluorenone (L7), 2,7-bis(4'-methylthiophenyl)-9-fluorenone (L8), and 2,7-bis(methylthio)-9-fluorenone (L9) as ligands for the self-assembly of UDS-7, UDS-8, and UDS-9 as coordination polymers with rhomboid Cu_2I_2 as secondary building units. A systematic photophysical study of both the ligands and the polymers allow for the elucidation of a structure-activity relationship towards singlet oxygen 1Δg photosensitization, detected by its phosphorescence at λem ~ 1275 nm. Clear and marked deviations from the results expected by literature are observed by the appearance of a clearly ligand-centered photophysical system (1,3LC) instead of the classic metal halide-to-ligand charge transfer (1,3MXLCT). This is attributed to the novel utilization of chromophoric ligands in conjunction with a chromophoric node, and critical photophysical interactions between both photoactive systems are extracted and discussed. All in all, the photosensitization of singlet oxygen 1Δg at the solid-gas interface can be of use for several applications, such as the elimination of Botrytis cinerea, which is the subject of ongoing experimentation.

15.- On the Development of Praseodymium-Doped Radioluminescent Nanoparticles and Their Use In X-Ray Mediated Photodynamic Therapy Of Glioblastoma Cells

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Despite decades of research, improvements in glioblastoma prognosis remain limited. The current standard treatment involves fluorescence-guided surgical resection, followed by radiotherapy and chemotherapy. This surgery uses 5-aminolevulinic acid (5-ALA) to induce the accumulation of fluorescent protoporphyrin IX (PPIX) with high specificity in malignant cells. Notably, 5-ALA is also a widely used agent in photodynamic therapy (PDT), where visible light activates a photosensitizer to produce reactive oxygen species that kill cells. However, PDT's efficacy is constrained by limited tissue penetration of UV and visible light. Nanomedicine offers a promising solution to this limitation, enabling PDT via luminescent nanoparticles that can be excited by X-rays, a method known as X-ray mediated photodynamic therapy (X-PDT). In this study, we developed $NaLuF_4:Pr^{3+}$ radioluminescent nanoparticles for X-PDT. The emission spectrum of Pr^{3+} aligns well with the absorption spectrum of PPIX. We established a reproducible synthetic route for uniform $NaLuF_4:Pr^{3+}$ nanoparticles suitable for cell uptake and performed in-depth characterization of their spectroscopic properties prior to conducting in vitro studies. The nanoparticles were optimized to excite PPIX and tested in the U251 human glioblastoma cell line. We assessed their therapeutic effects with and without 5-ALA to determine both radiosensitization and X-PDT efficacy. Three nanoparticle concentrations and four radiation doses, including those relevant for intraoperative radiotherapy, were studied. The impact on cell stress, death, damage, senescence, and proliferation was evaluated, showing promising proof-of-concept results. Our experimental design was guided by current clinical practices, laying a strong foundation for using Pr^{3+}-doped nanoparticles in XPDT with endogenous PPIX during intraoperative radiotherapy.

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16.-MRI-assisted Monitoring and Explantation of Alginate Microbeads Encapsulating Insulin-producing Cells along with Magnetic Nanoparticles

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Introduction: Hydrogel encapsulation of pancreatic islets is a promising approach for protecting cells from immune responses in type-1 diabetes treatment (T1D). However, postimplantation monitoring and retrievability in case of failure of encapsulated cells are crucial. While Magnetic Resonance Imaging (MRI) offers high-resolution soft tissue imaging, it requires a contrast agent for effective visualization. Ultrasmall superparamagnetic iron oxide nanoparticles (USPION) have emerged as a potential alternative to gadolinium-based compounds, providing "positive" contrast enhancement in T1-weighted MRI scans. This study aims to demonstrate that polyethyleneglycol (PEG)-stabilized USPION (USPION-PEG) can be successfully implemented for MRI visualization of encapsulated insulin-producing cells within alginate microbeads implanted in vivo in diabetic mice.

Materials & Methods: USPION-PEG were synthesized through thermal decomposition followed by phosphate-PEG(5K)-COOH ligand exchange and characterized. USPION-PEG were incorporated to alginate microbeads during the cell encapsulation by emulsification (water-mineral oil) and internal gelation method. Biocompatibility and functionality (glucose levels) were monitored in vitro (14 days), as well as in vivo (up to 10 weeks) including a complete T1-weighted imaging tracking procedure. Results & Discussion: USPION-PEG (TEM: 4.8±0.6 nm, DLS: 35±4 nm) were successfully synthesized and characterized, demonstrating their effectiveness as positive contrast agent. Nanoparticles were retained within microbeads for 3 months showing their capacity of contour delineation in T1-weighted MRI. Also, nanoparticles presence did not affect cell survival and insulin-producing capacity. MRI visibility of alginate-USPION microbeads was successfully demonstrated in vivo with graft monitored over a 10-week period. These encapsulated cell implants also demonstrated to lower blood glucose up to normoglycaemia in diabetic mice within 2-4 weeks, and an MRI-assisted surgical explantation was successfully conducted to completely retrieve the microbeads.

Conclusion: This study demonstrated the potential of USPION as an effective positive contrast agent for MRI monitoring of islet-containing hydrogel microbeads implanted in vivo, as well as for facilitating MRI-assisted surgical extraction interventions in the context of T1D.

17.- The Development of Aptasensors for Costimulatory Protein Receptors Detection

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Rheumatoid Arthritis (RA) is a widespread autoimmune disease diagnosed using various biomarkers. However, these biomarkers have limitations, making early diagnosis through alternative molecules particularly challenging. Recently, costimulatory proteins associated with the CD28-B7 pathway have gained attention due to their significant roles in the immune system. This study aims to create a reliable, sensitive, and cost-effective aptasensor for detecting these proteins. We are utilizing conventional in-vitro exponential enrichment (SELEX) for aptamer selection, followed by the development of a DNA-based biosensor using electrochemical impedance spectroscopy (EIS). The optimized sensors are intended to detect the CD28-B7 protein family in biological matrices. The study is divided into three sub-projects focused on the following protein targets: CTLA-4, CD28, and CD60. Currently, aptamers obtained after the 14th SELEX cycle have been sent for sequencing, while the binding affinity of aptamers for CTLA-4 is also being evaluated.

18.- First-Ever Integration of Ionic Liquid Crystal Elastomers (iLCEs) For biomedical Microelectromechanical (MEMS) Sensors

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Traditional MEMS technologies, often relying on silicon or ceramics, face limitations in flexibility and high-voltage actuation, hindering their application in biomedical fields. This research introduces ionic liquid crystal elastomers (iLCEs) as a promising polymeric material for overcoming these challenges. iLCEs offer a unique combination of flexibility, self-healing properties, and low-power operation, making them ideal for the development of miniaturized, high-performance MEMS actuators and sensors. A novel MEMS fabrication process for iLCE devices is introduced in this Ph.D. research. The process flow is shown schematically in Figure 1. By leveraging the exceptional properties of iLCEs, this process enables the creation of flexible, sensitive, and scalable MEMS components. The ultimate goal of this research is to develop the first MEMS pressure sensor specifically designed for biomedical applications, paving the way for advancements in healthcare technology.

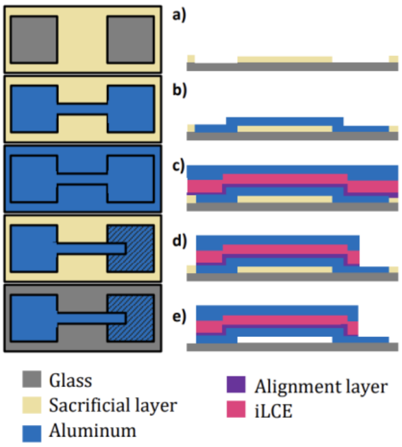

Figure 1. A schematic representation of the manufacturing steps involved in integrating the iLCE into flexible MEMS structures.

19.- Préparation et caractérisation de mélanges polymère : photosensibilisateur.

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La fonctionnalisation de la surface d'un objet en 3D permet d'accéder à diverses propriétés intéressantes, telles que l'inactivation photodynamique (IPD). L'IPD est une méthode d'élimination des bactéries et des virus utilisant l'oxygène singulet comme élément cytotoxique, produit avec un photosensibilisateur. Notre projet repose sur l'hypothèse d'incorporer ce photosensibilisateur dans l'objet en 3D (c'est-à-dire dans la formulation utilisée pour l'impression) au lieu de fonctionnalisé la surface de l'objet déjà imprimé. Dans ce contexte, nous explorons la corrélation entre la forme et les propriétés d'un matériau en termes de production d'oxygène singulet en imprimant un polymère thermodurcissable, comme le polydiméthylsiloxane (PDMS), contenant des photosensibilisateurs tels que le bleu de méthylène. Le mélange est imprimé à l'aide de l'impression directe de formulation (DIW). Tout d'abord, les propriétés rhéologiques de la formulation sont étudiées pour mieux comprendre la réticulation du thermodurcissable. De plus, des mesures de profilométrie ont été utilisées pour caractériser la fidélité d'impression des échantillons imprimés en 3D. Ensuite, le taux apparent de production d'oxygène singulet est évalué de manière indirecte pour évaluer l'impact de différents rapports surface/volume des échantillons imprimés en 3D. Ces résultats nous aident à concevoir de manière rationnelle des architectures imprimées en 3D avec un rapport surface/volume optimal qui pourraient être utiles dans le contexte de l'IPD.

20.- Development of a polymersome blood ammonia assay coupled with a portable near-infrared fluorometer

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PURPOSE: Ammonia is an endogenous metabolite that has crucial roles in pH-homeostasis and protein metabolism[1]. It is a key biomarker in inborn and acquired liver disease. At high levels, ammonia exerts neurotoxic effects[2]. As clinical point-of-care blood-ammonia assays are lacking[3], we developed a polymersome formulation for point-of-care sensing using a portable fluorometer.

METHODS: Polymersomes were prepared by dissolving Ps-b-PEG polymers, followed by addition into an isotonic citric acid solution containing a pH-sensitive near-infrared (NIR) fluorescent dye: IRDYE680RD[4]. After emulsification and solvent evaporation, purification was achieved using columns, replacing the external phase with an isotonic sodium chloride-containing phosphate buffer (pH 7.4). Mouse blood was obtained from cardiac puncture. The polymersomes solution and blood were spiked with ammonium chloride standards up to 0.5 mM. As typically used in capillary blood assays, merely 3 µL of whole blood was needed.

RESULTS: Initially, the fluorescence of polymersomes was assessed using a plate reader, covering a clinically relevant range of ammonia concentrations up to 500 µM. A highly linear response ($R^2 = 0.9948$) was observed overtime with a concentration-dependent increase. Then, the fluorescence was tested with a portable fluorometer, revealing a concentration-dependent increase in both buffer and blood.

CONCLUSION: The portable fluorometer effectively detected a pH-dependent fluorescence increase of the pH-sensitive NIR-dye. Combined with the polymersome formulation and the NIR-dye, this assay required merely three microliters of blood, offering promising potential for point-of-care blood ammonia diagnostics. These encouraging results underscore the need for further development and clinical translation of this innovative approach to blood-ammonia testing.

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21.- Caractérisation locale des phases dans les polymères semicristallins imprimés

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La fabrication additive, également connue sous le nom d'impression 3D, consiste à déposer du matériau ou un mélange de matériaux de manière robotisée en suivant des mouvements cartésiens dans les directions X, Y et Z. Ces mouvements sont pré-calculés selon une conception assistée par ordinateur (CAO) et confèrent à l'impression 3D une polyvalence en termes de forme et de matériau. Cette technique de fabrication ouvre une nouvelle voie vers l'étude des relations structure – traitement – propriétés des matériaux, tels que les polymères. L'adoption généralisée et l'utilisation accrue de l'impression ont donné lieu à de nouveaux défis, car la demande croissante accélère le rythme auquel les imprimantes doivent fonctionner. Par conséquent, des problèmes tels que la délamination et la réduction de l'adhésion entre les couches sont apparus. Ces problèmes revêtent une importance notable, entraînant la production de produits finaux plus faibles en termes, entre autres, de propriétés mécaniques. L'une des solutions actuelles consiste à réduire les vitesses d'impression, bien que cette approche soit loin d'être idéale en termes de productivité. Ici, une compréhension plus approfondie de la cinétique de cristallisation des polymères et de l'enchevêtrement des chaînes entre les couches offre un éclairage plus précis sur les mécanismes macromoléculaires qui régissent le domaine de l'impression 3D. Pour établir ces relations, diverses techniques de caractérisation avancées sont employées. La rhéologie est utilisée pour étudier les comportements thixotropiques et d'écoulement, simulant les forces de cisaillement inhérentes à l'impression 3D. De plus, une combinaison de calorimétrie différentielle à balayage (DSC) et de techniques spectroscopiques est utilisée pour suivre la cristallisation qui se produit après l'extrusion du polymère pendant le processus d'impression. En fin de compte, le travail présenté ici offre des perspectives qui peuvent conduire à une performance optimisée et à une polyvalence dans la fabrication additive de polymères.

22.- Towards a better understanding of the polymer – salt coordination phenomenon in solid polymer electrolyte

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The development of solid polymer electrolyte for different electrochemical applications such as energy storage devices enables a safer and denser energy storage solution to the ones currently available. Fundamental understanding of ionic transport through interaction strength and polymer chain relaxation in the solid and melted states is necessary to develop better electrolytes. In this work, we developed and applied a characterisation method through multiple techniques allowing us to interpret the impact of the salt coordination on the ionic transport of a solid polymer electrolyte's The polycaprolactone (PCL) / lithium bis(trifluomethane)sulfonimide (LiTFSI) system studied was analyzed by differential scanning calorimetry (DSC), variable temperature infrared spectroscopy (FT-IR), electrochemical impedance spectroscopy (EIS) and oscillatory rheology. Polyester electrolytes being less reported than their polyether counterparts, the phase diagram of the PCL / LiTFSI system was constructed from DSC results. The concentration gradient was then analysed by various techniques to obtain a better understanding of coordination throughout the gradient. Standard FT-IR spectroscopy allowed to probe the coordination environment of the lithium salt as a function of concentration while variable temperature FT-IR enabled a quantitative evaluation of an interaction strength between the lithium cation and the carbonyl moiety of PCL. Ionic conductivities of the prepared electrolytes were evaluated and linked with interaction strength. Finally, the use of oscillatory rheology enabled the determination of relaxation times linked with the molecular structure of the system. Comparative analysis of the results obtained allowed a fundamental understanding of the impact of coordination strength on ionic transport in the solid and melted states.

23.- Azatriangulene-based Conductive C=C Linked Covalent Organic Frameworks with Near-Infrared Emission

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Zhenzhe Zhang,[a] *Mahdi Salehi,*[b] *Robin S. Stein,*[a] *Jorge Ramos-Sanchez,*[a] *Arnaud W.*
Laramée,[c] *Gonzalo Cosa,*[a] *Christian Pellerin,*[c] *Ali Seifitokaldani,*[b] *Rustam Z. Khaliullin,*[a]
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We synthesized two near-infrared (NIR) emissive π-conjugated covalent organic frameworks (COFs) pTANG1 and pTANG2 using Knoevenagel condensation of trioxaazatriangulenetricarbaldehyde (TATANG) with benzene- and biphenyldiacetonitriles, respectively. Donor-acceptor interactions result in small bandgaps (~1.6 eV) and near-infrared (NIR) emission in these COFs (λmax = 789 nm for pTANG1). pTANG1 can absorb up to 9 molecules of water per unit cell which is accompanied by a marked quenching of the NIR emission, suggesting applications as humidity sensors. p-Doping with magic blue significantly increases the electrical conductivities of the COFs by up to 8 orders of magnitude, with the room temperature conductivity of pTANG1 reaching 0.65 S cm-1, the highest among reported C=C linked COFs

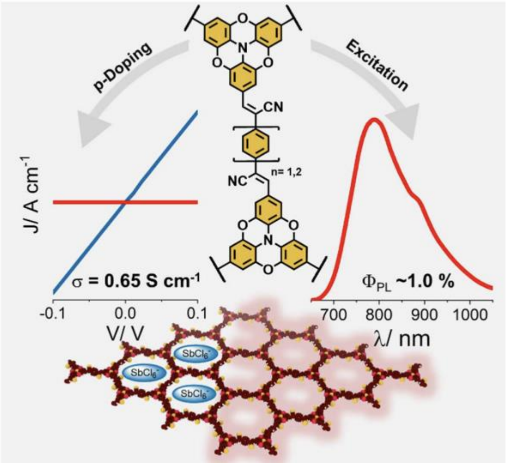

Figure 1. Graphical Abstract

Abstracts' Posters

Session 1 : Énergie

1.- Synthesis and characterization of AMidine OXide (AMOX) ligands with photoactive anthracene core and their associated metal complexes

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The photophysical and structural properties of amidine oxide (AMOX) ligands and complexes make them interesting candidates as components of photosensitizers and/or catalysts, in the optics of an artificial photosynthetic system. The ligands were synthesized by N-oxidation of amidines containing anthracene on the central carbon by m-CPBA. The complexes were then formed from salts of Ni(II) and Zn(II). Both the ligands and the complexes were characterized by NMR, IR and UV-vis spectroscopy, and mass spectrometry. The crystal structures of both the ligands and the complexes were also elucidated by X-ray diffraction analysis. An example is shown in Figure 1, below.

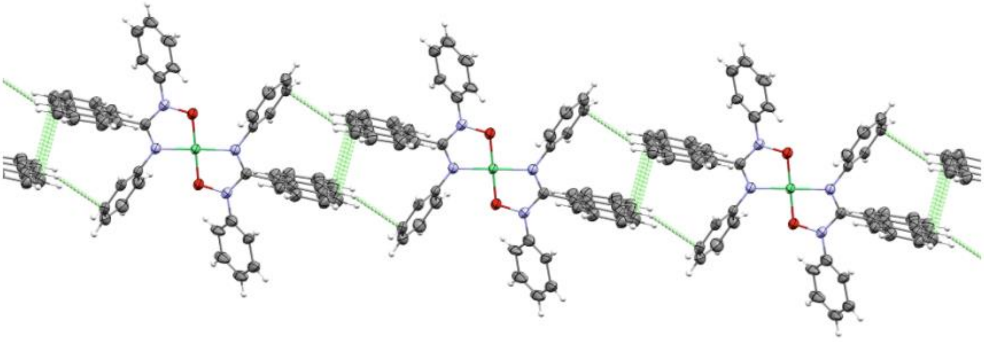

Figure 1. The solid-state structure of one of the AMOX ligands presented in this work.

2.- Towards insoluble diphenoquinones for a use in organic batteries

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Accelerating the exploitation of wind and solar energy is essential to slow down climate change. Because these energy sources are intermittent, they must be used in conjunction with energy storage solutions that can be deployed at very large scales. Currently, lithium-ion batteries (LIBs) are highly competitive for certain applications, but since they use oxides of heavy metals such as cobalt or nickel, their large-scale exploitation is not sustainable. Zinc-ion batteries (ZIBs) offer a promising alternative due to the abundance of zinc and its compatibility with aqueous electrolytes, making them safer and less polluting. However, a major obstacle remains: the absence of cathode materials capable of reversibly intercalating Zn^{2+} ions. Organic molecules, notably quinones, are being investigated for their potential as cathode materials for ZIBs, as they offer flexible structures for reversible incorporation of bulky ions and good redox activity.

Diphenoquinones (DPQs) are an extended version of benzoquinones and were recently proposed as promising active materials for battery applications due to their lower solubility, reversible redox process, and higher reduction potential. This work explores the application of 3,3’,5,5’-tetramethoxy-4,4’-diphenoquinone in ZIBs, examining its performance in two types of electrolytes with varying pH levels. The study analyzes the effect of these conditions on the resulting capacity across different C-rates and assesses stability over 100 cycles.

3.- Homoleptic cobalt(III) bisguanidylpyridine complexes for photocatalytic and photoredox processes

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There is a great need to replace precious metals in photochemical reactions. In this regard we prepared room-temperature luminescent CoIII(dGPy)$_2$(X)$_3$ (dGPy = 2,6-bis(1,5,7-triazabicyclo[4.4.0]dec-5-ene)pyridine , X = BF4 - or PF6 -) complexes that show LMCT (Ligand to Metal Charge Transfer) and LLCT (Ligand to Ligand Charge Transfer) transitions in the relatively low-energy UV region (λabs≈360–400 nm) and quasi-reversible reductions (E1/2(red)= −0.58 V vs. SCE) in their electrochemistry. A blue emission from the excited state of CoIII(dGPy)$_2$(X)$_3$ can be linked to the large bite angle and strong σ donation of the guanidine moieties. The combination of these effects helps separate the emissive 3LMCT state and the non-emissive 3MC state. Herein we present a new photoredox catalyst for the regioselective mono trifluoromethylation of polyarene but also for the photosynthesis of H_2.

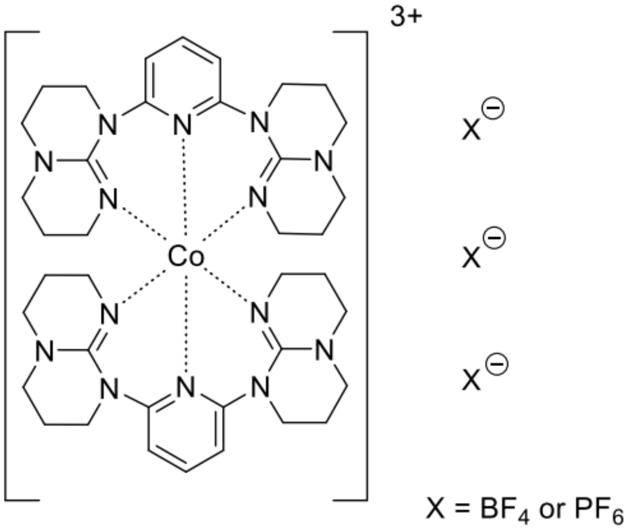

Figure 1: Structure of the complex Co(dGPy)$_2$(X)$_3$.

4.- An active bifunctional natural dye for high-areal-capacity all-solid-state batteries

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Sustainable and cost-effective organic electrode materials (OEMs) are promising candidates for nextgeneration lithium-ion batteries (LIBs) but are currently hindered by the severe shuttle effect. While emerging all-solid-state batteries (ASSBs) offer a fundamental solution, their current areal capacity and cycling stability are limited by the chemical or mechanical incompatibility between OEMs and inorganic solid electrolytes (SEs), falling short of practical requirements. Here, we report a bifunctional indigo natural dye that serves as both an active material and an efficient solid molecular catalyst in sulfidebased ASSBs to resolve the compatibility challenges between OEMs and inorganic SEs. Contrary to the belief that chemical reactions between OEMs and sulfide SEs are detrimental, our study shows that the reversible reaction between indigo and Li6PS5Cl (LPSC) SE catalyzes their synergistic redox processes during charge-discharge cycles, thereby resulting in a high reversible capacity of 583 mAh g1 at 0.1 C, a high areal capacity of 3.84 mAh cm^{-2} and excellent cycling stability at room temperature. Our findings demonstrate that incorporating bifunctional OEMs into sulfide-based ASSBs is a promising strategy to overcome current bottlenecks in practical applications. Figure 1 shows the working mechanism of indigo natural dye as both the active material and the molecular catalyst in sulfide-based ASSBs.

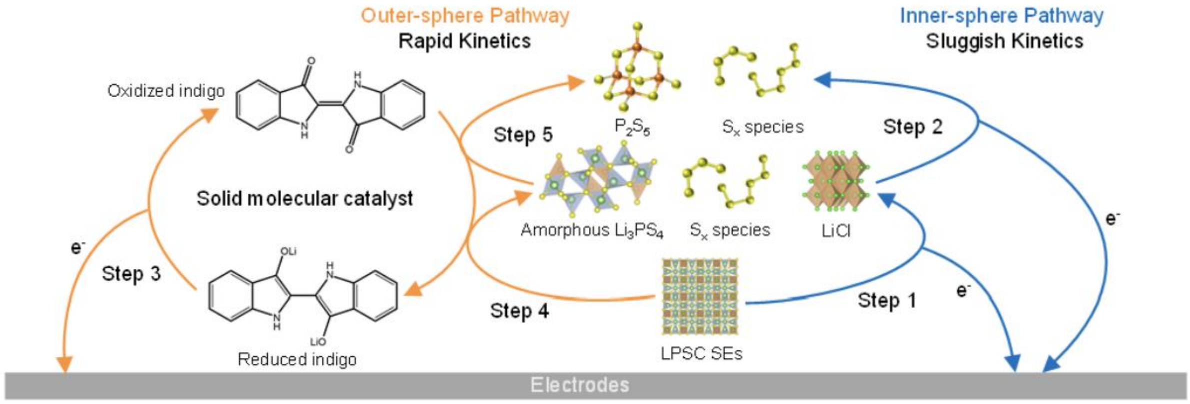

Figure 1. Schematic illustration of the outer-sphere redox pathway (catalyzed by the indigo molecular catalyst) and the typical inner-sphere redox pathway (electrochemical reaction) of LPSC SE.

5.- Molecular Copper(I)-Sensitized Photoanodes for Alcohol Oxidation under Ambient Conditions

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Dye-sensitized photoelectrochemical cells can enable the production of molecules currently accessible through energetically demanding syntheses. Copper(I)-based dyes represent electronically tunable charge transfer and separation systems that can be utilized in such transformations. In this presentation, we explore a Cu(I)-bisdiimine donor-chromophore-acceptor dye with an absorbance in the visible part of the solar spectrum composed of a phenothiazine electron donor, and dipyrido[3,2-a:2′,3′-c] phenazine electron acceptor. This complex is incorporated onto a zinc oxide nanowire semiconductor surface effectively forming a photoanode that is characterized spectroscopically and electrochemically. We investigate the photo-oxidation of hydroquinone, and the photosensitization of 2,2,6,6- tetramethylpiperidine-1-oxyl and N-hydroxyphthalimide for the oxidation of furfuryl alcohol to furfuraldehyde, resulting in near quantitative conversions, with poor selectivity to the alcohol. This opens the door to a non-selective heterogeneous sensitizer, capable of sensitizing or photocatalyzing a variety of oxidation reactions, provided there is appropriate redox leveling.

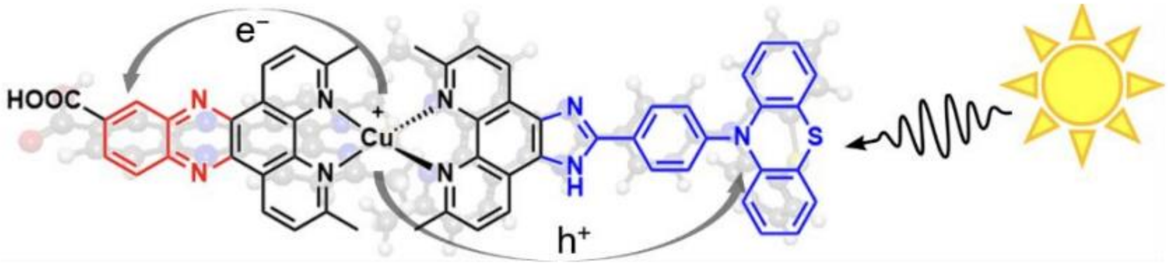

Figure 1. The proposed molecular structure of the donor-Cu(I)-acceptor visible light photosensitizer overlaid on the DFT optimized structure showing the proposed electron transfer and separation processes occurring on visible light irradiation.

6.- Synthesis of radical-based fluorophores for stimuli responsive devices: a proof of concept

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Developing displays that have reduced blue emission has gained interest during the last decades.1 This is to prevent eye discomfort to users during prolonged use. Electrochromic devices (ECD) are a viable solution to ocular discomfort because of their outdoor readability and no blue emission. The advantage of such devices is the color is generated either by reflected or transmitted light, rather than by emission as with convention displays.2 The operation of ECDs is therefore not reliance on blue emission.

Radicals are open-shell molecules with an unpaired electron located on the singly occupied molecular orbital (SOMO). Their ground and the lowest excited states have a doublet multiplicity.3 Thus, reversible full-color tunability would be possible by an electrochemical redox process. Replacing traditionally used closed-shell emitters with neutral organic radicals would be advantageous for thin films devices, especially in ECDs.

In this work, we detail the synthesis of radical fluorophores that have covalently attached electron-rich core and a carbon-centered organic radical. Preliminary results regarding the potential application of these materials as electrochromic layers for ECD will also be presented.

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7.- Photostable open-shelled fluorophores for near-infrared organic light-emitting diodes: a proof of concept

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Closed-shell organic materials that emit in the visible have been widely investigated in the last decades.[1] In this context, near-infrared organic light-emitting diodes (NIR OLEDs) hold significant interest owing to their extensive applicability across various technological domains such as biosensing, optical imaging, photodynamic therapy, and ensuring security in personal identification and surveillance systems.[2]

Spin-statistics dictates that 25% singlet and 75% triplet states are formed when closed-shell molecules are electrically excitation by electron injection into the lowest occupied molecular orbital (LUMO) and abstraction from the highest occupied molecular orbital (HOMO). Of interest for emitting applications is the singlet excitons because of their spin-allowed radiative decay.[3] Hence, the internal quantum efficiency (IQE) of closed-shell emitters is limited to 25%.

Radicals are open-shell molecules. They consist of an unpaired electron that located on the singly occupied molecular orbital (SOMO). Owing to this, their ground and lowest excited states have a doublet multiplicity.[4] Thus, upon electrical and optical excitation doublet excited states radiatively decay to the ground state. This **opens the possibility of achieving a theoretical IQE of 100%**.[5] Within the context of NIR OLEDs, it is advantageous to replace traditionally used closed-shell molecules with thin films of neutral radicals. Besides, organic radicals achieve high photoluminescence quantum yield (PLQY) in the NIR range due to their unique electronic structure, bypassing traditional energy gap law constraints.[6]
In this work, we detail the synthesis of novel photostable radical fluorophores that have covalently attached electron-rich core and a carbon-centered organic radical. Preliminary results regarding the potential application of these materials as emitters for NIR OLEDs will also be presented.

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8.- Modeling Metal Nitrides for Thin-Films in Lithium-Sulfur Batteries on GPU and CPUs

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As current battery technologies near their limits, lithium-sulfur batteries offer promise but face key challenges: low material utilization, cathode degradation, and incomplete polysulfide conversion, which can corrode the anode. Nano-scale deposition of metal nitride (MNx, M = Ti, V, Zr, etc.) layers on graphene-sulfur cathodes may enhance conductivity and cycling performance. Given the vast number of metal candidates, density-functional theory (DFT) screening is crucial for identifying optimal materials. This study uses DFT to assess metal nitride coatings by evaluating their surface adsorption strength with lithium polysulfides (Li_2S, Li_2S_2, Li_2S_4, etc.), ensuring it exceeds the DOL/DME electrolyte's adsorption energy (~0.99 eV). We also analyze the electronic band structure before and after adsorption, looking for a high density of states near the Fermi level, which improves conductivity. Additionally, free energy profiles of the sulfur reduction reaction (SRR) are studied, focusing on the Li_2S_2 to Li_2S step, the SRR's rate-limiting step. Viable candidates will exhibit exothermic or near-neutral energy transitions. The study also compares computational efficiency using CPUs and GPUs, offering insightsinto faster modeling. The results aim to guide the development of experimentally viable lithium-sulfur batteries and next-generation interfaces for energy storage.

9.- Self-Healing Multi-Functional Coating of Sulfur Cathodes for High-Performance Li-S Batteries from Liquid-State to Solid-State

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The development of liquid-state lithium-sulfur (Li-S) batteries is plagued by serious polysulfide shuttling, sluggish redox reaction kinetics, and low sulfur utilization. In this work, a multifunctional polymer designed as a sulfur/carbon coating layer with self-healability and polar groups is designed and prepared for Li-S batteries to achieve improved electrochemical performance. The dynamic poly(hindered urea) (PHU) polymer coating layer uniformly covered on the surface of the sulfur/carbon (S/C) composites acts as a physical barrier for the dissolution of lithium polysulfide (LiPSs) from the cathode to the lithium metal anode, which accumulates LiPSs on the cathode side and protects the lithium anode from corrosion. In addition, the dynamical and reversible self-healing hindered urea bonds (HUBs) endow the PHU coating layer with the ability to maintain structural integrity and stability even after numerous volume expansions and shrinkages of the S/C electrodes. More importantly, the polar groups carried by the PHU polymer exerted a strong adsorption effect on LiPSs, thus further hindering the shuttling of LiPSs. Consequently, the Li-S batteries using PHU coating layer exhibit impressive cycle stability (maintaining 82.8% capacity retention after 150 cycles at 0.5 C), and outstanding rate performance (capacity retention of 623.9 mAh g^{-1} at 2 C). Furthermore, even under a high sulfur loading of 8.47 mg cm^{-1}, a high areal-specific capacity of 6.4 mAh cm^{-2} is still delivered. Moreover, the PHU coating was also utilized in solid-state Li-S batteries (SSLSBs) to decrease the electrolyte decomposition, impede the large volume change, and enhance the solid-to-solid three-phase interfacial contact. The PHU-based batteries exhibited improved long cycling performance even under high current density.

10.- Synthesis of Formamidines as Precursors for N,N'-Disubstituted Amidine N-Oxide Ligands for Transition Metal Complexes

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The synthesis of transition metal complexes has attracted great interest due to their unique properties in catalysis, redox processes, and the importance of their fundamental study in coordination chemistry.[1] Transition metals, such as cobalt, exhibit flexible electronic configurations and a great ability to form coordinated bonds with ligands, allowing them to adopt various geometries and oxidation states. These properties are particularly useful in homogeneous catalysis, bond activation processes and the generation of solar fuels (e.g., artificial photosynthesis).[2] In this context, the use of N,N'-disubstituted N-hydroxamidines/ amidine N-oxides (AMOXs) as chelating ligands for the synthesis of complexes has been explored.[3] These ligands are highly tunable and capable of forming stable chelate rings with metal ions, due to their structural and electronic flexibility. Formamidines, in turn, can be transformed into AMOXs through oxidation processes. They stand out by their structural and chemical versatility, allowing them to be easily modified and functionalized, making them ideal precursors for the targeted AMOXs.

Therefore, this study focuses on the synthesis of formamidines, carried out by microwave activation. This method allowed optimized reactions, achieving higher yields compared to traditional heating, while also significantly reducing reaction times, the number of experimental steps, and the formation of byproducts.[4] The characterization of these intermediates was performed using spectroscopic techniques, confirming their structure and purity, thereby establishing a solid foundation for future stages of the project.

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11.- Electroactive Polymer coatings of Perylene derivatives for energy storage devices

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Energy is the most important problem faced by our society nowadays. The global demand of energy is increasing day by day with growing human population. Electricity from sunlight can meet global energy needs. Non-polluting sources of electricity such as solar cells have garnered 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 cannot be produced during intermittent light and dark periods. A traditional photovoltaic battery system involves operating a photovoltaic (PV) and battery as two independent units that are electrically connected by wires. This makes the traditional PV battery system bulky, requiring space for storing and loss of energy through external wires. A viable solution for storing the electricity captured from the sun is a photorechargeable electric energy storage system. 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. However, to address the issue of portability of electricity generation and storage, the individual light harvesting and energy storage components needs to be merge. This will result into photo charging a battery at molecular level. In this work, we detail the synthesis of a molecular dye that can both harvest sunlight and convert the energy for storage in a battery. The synthesized dye will be used for developing electroactive coatings on conventional redox active rechargeable battery components. The study of photo-physical properties of these polymers will also be presented.

12.- DFT calculation for selecting redox active biosourced material as a cathode for organic batteries

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Currently, humanity is increasingly dependent on energy derived from both fossil resources (fuels, gas) and renewable sources (electricity). To mitigate climate change driven by the excessive use of fossil fuels, it is essential to develop more sustainable solutions for electricity production. One of the major challenges in recent decades has been the storage of this electrical energy in batteries. The primary components of these batteries, cathode and electrolyte, are the focus of extensive research. The cathodes currently in use are entirely inorganic and contain metals that are difficult to extract, such as lithium and cobalt [1]. The extraction methods for these minerals have detrimental impacts on ecosystems and adversely affect the living conditions of workers. However, exclusively organic cathodes are emerging, which offer superior properties compared to inorganic cathodes. Organic cathodes, composed of benzoquinone [2, 3] and phenazine [4] units, demonstrate excellent electrochemical characteristics, including prolonged cycling lifetimes, increased electron storage capacity, and enhanced specific capacities. Optimizing their structure to increase the number of redoxactive units is crucial for improving their performance as cathodes. Quantum modeling using Density Functional Theory (DFT) enhances the likellihood of discovering new molecules suitable for cathodes. In this context, a computational method developed by Z. Li et al. [5] has been reported; however, this study remains limited in scope. To deepen our understanding, several computational parameters will be examined, including solvent polarity, the conformational aspects of hydrogen and lithium bonds, and the specific computational functions employed. Ultimately, if a computational methodology that accurately reflects reality can be established, it will be possible to significantly reduce development time and pave the way for new molecules.

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13.- Enhanced photocatalytic performance of Intercalated 2D BiOBr nanosheets into 3D knob-like Bi_2WO_6 for the degradation of antibiotics and textile pollutants

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Semiconductor metal-oxide based heterostructues photocatalyst aroused huge interest for field of water detoxification applications. We report the hydrothermal fabrication of 3D/2D Bi_2WO_6/BiOBr efficient photocatalyst and their employment for water detoxification application. The morphological and structural characteristics of the resulting Bi_2WO_6/BiOBr nanocomposite were comprehensively investigated using scanning electron microscopy (SEM), X-Ray diffraction (XRD), and Raman spectroscopy. SEM analysis provided insights into the surface morphology and structure of the composite material, revealing its intricate architecture at the micro and nano scales. XRD and Raman studies assures the formation of Bi_2WO_6/BiOBr heterostructures Remarkably, the degradation efficiency of the 3D/2D Bi_2WO_6/BiOBr heterostructures was found to be exceptionally high, achieving degradation rates of 99.37% for Rhodamine B (RhB) dye pollutant and 68.67% for Ciprofloxacin within a remarkably short duration of 20minutes and 30 minutes respectively. The improved photodecomposition activity Bi2WO6/BiOBr remarkable degradation performance highlights the potential of the synthesized nanocomposite material for applications in wastewater treatment and environmental remediation.

Keywords: Heterostructures, photocatalyst, Bi_2WO_6, BiOBr, Ciprofloxacin

14.- High-entropy hydride for Fast and Reversible Hydrogen Storage at Room Temperature

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High-entropy hydrides have garnered significant attention as potential materials for fast and reversible hydrogen storage at room temperature. In this study, we investigate the hydrogen storage properties of TiZrVHfNb high-entropy alloys, augmented with Fe as a transition metal. Alloys of compositions TiZrVHfNb1−xFex where x = 0, 0.2, 0.4, 0.6, 0.8, 1 at.% were synthesized and characterized for their microstructure evolution and hydrogen storage capabilities. results reveal that the TiZrVHfNb1−xFex alloys consist of a hexagonal C14 Laves phase and a Body-centered Cubic (BCC) phase for x=0, with the fraction of the C14 Laves phase increasing with higher iron content. Notably, alloys with x>0.7 exhibit enhanced hydrogenation kinetics and activation at room temperature, attributed to the rise in the Valence Electron Concentration (VEC) of the C14 Laves phase, leading to reduced hydrogen binding energy and improved hydrogenation kinetics. Furthermore, reversible phase transitions involving the BCC phase and metal C14 Laves phase demonstrate the potential of these alloys for cyclic hydrogen storage.

15.- In-situ study of surface modification on TI_3C_2 as a catalyst for hydrogen evolution reaction

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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 Mn+1XnTx where M is a transition metal, X is carbon or nitrogen and Tx is surface terminations, such as -O, -OH, -F or -Cl. MXenes are synthesized by selective etching of A layers from a MAX phase precursor (Mn+1AXn), 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 applications [2]. However, poor stability in oxidating environments and restacking limit their performance. It has been shown that modification of surface termination Tx and defect engineering are promising avenues to enhance the electrocatalytic activity of MXenes[3]. In this work, the titanium carbide (Ti_3C_2Tx) 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_2Tx 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.

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16.- Self-Healing Poly(Hindered Urea) Polymer Network as Coating Layer on Carbon/Sulfur Composite in High-Performance Lithium Sulfur Batteries

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Development of covalent adaptive networks (CANs) has been significantly explored as a promising platform toward applications requiring self-healing and reprocessability, such as biomedical, electronic, aerospace, and coatings functions. Of typical dynamic CANs integrated with disulfide, imine, and boronic ester, hindered urea bond (HUB) undergoes reversible exchange under catalyst-free conditions and mild temperatures. Recently, we have explored dynamic hindered urea chemistry to develop robust a poly(hindered urea) network material for the development of high-performance Li-S batteries aiming to solve the intrinsic challenges of Li-S batteries, including polysulfide shuttling, slow redox reaction kinetics, and cathode cracking due to volume expansion. This presentation describes the fabrication of a self-healable PHU crosslinked with HUBs through step-growth polymerization with two steps, including the preparation of a pre-polyurea consisting of hexamethylene diisocyanate and poly(dimethylsiloxane) diamine, and followed by the addition reaction of a tetra-functional secondary amine with bulky t-butylamino group (called T-NH) as a dynamic crosslinker. The fabricated PHU was proven to be homogenous and possessed high thermal stability and excellent mechanical properties. Being formulated with C/S composite, the self-healable sulfur cathode as PHU@C/S cathodes exhibit favorable cycle stability and maintenance of capacity retention. This work demonstrates the simple design of polymeric network in electrochemical applications as a promising strategy for the development of high-performance Li-S batteries and advanced HUB-based materials with excellent self-healing and reprocessability.

Session 2 : Développement durable

17.- Phosphorylation des écorces des feuillus et des résineux avec l’ester de phosphate

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La phosphorylation est une méthode de modification chimique qui sert à introduire des groupements phosphate à la structure chimique de la matière traitée. Différents agents de phosphorylation comme l’acide phosphorique, le phosphate de diammonium et l’ester de phosphate ont été utilisés pour la phosphorylation des fibres lignocellulosiques dans l’objectif d’élaborer des matériaux retardateurs de flamme. Cependant, à ce jour, les écorces n’ont jamais été phosphorylées. Cette étude se propose donc d’évaluer l’efficacité de l’ester de phosphate pour phosphoryler les écorces de feuillus et de résineux dans le but de développer une méthode de freinage de la propagation des flammes et ainsi contribuer à la protection des forêts contre les incendies. Les écorces de six espèces (Peuplier faux-tremble, Peuplier baumier, Bouleau à papier, Thuya occidental, Epinette blanche et Sapin baumier) de la forêt d’enseignement et de recherche du lac Duparquet ont été récoltées, broyées et phosphorylées avec l’ester de phosphate en présence d’urée dans un four sous vide. La caractérisation des échantillons a été réalisée par spectroscopie infrarouge à transformée de Fourier (FTIR), microscopie électronique à balayage (MEB) et spectrométrie à dispersion d’énergie (EDX). Les résultats de l’analyse EDX confirme la présence du phosphore sur la surface des écorces après phosphorylation. Un taux de 3,2 % est obtenu pour l’écorce du Peuplier baumier et de 3,3 % pour l’écorce du Thuya occidental. L’analyse FTIR montre le greffage des groupements phosphates sur tous les écorces modifiées par l’apparition des bandes caractéristiques de la liaison P=O et la liaison P-O-C. Les résultats obtenus sont encourageants pour approfondir les résultats dans le sens d’ignifugation des écorces par le bai de la phosphorylation.

18.- Characterization of Fe-Metal Coordination Complexes for Enhanced Redox-Flow Battery Applications

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The world is in need of reliable and renewable energy alternatives to fossil fuels. However, since most renewable energies do not supply continuous power, it is important to have clean energy storage methods. Electrochemical energy storage technologies such as redox-flow batteries are of interest because they offer a cheap and sustainable energy source option.1,2 Redox-flow batteries are comprised of multiple components, such as electrolyte solutions, half-cells, a membrane, electrodes, pumps, and a power source. Of particular focus are the chemical components responsible for the redox activity in the battery. To date, various electrolyte solutions composed of metal-ligand coordination complexes dissolved in salt solutions, have been explored. However, the key is that the electrolytes must be electrochemically compatible in order to be employed together in the battery. Herein, we investigate the synthesis and characterization of iron 2+ and 3+ coordination complexes, as electrolytes in redox-flow batteries. Preliminary characterization of these iron-based complexes include infrared and optical spectroscopies, optical microscopy, Pourbaix analyses, and ground state electrochemistry.

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Session 3 : Auto-assemblage Moléculaire et biomédical

19.- Development of a 3D-printed cell-laden hydrogel phantom for improvement of precision in eye cancer brachytherapy

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Background and purpose: Uveal melanoma (UM, eye cancer), the second most common type of melanoma, is usually treated by brachytherapy (BT) (placement of radioactive objects in or at the tumor). UM is characterized by strong radiosensitivity differences between sub-populations of cells, leading to heterogeneous responses to BT. Radiobiologists assist medical physicists in studying these differences, and help them in the integration of radiobiological characteristics into dose planning for higher precision in BT. However, radiobiologists lack biological phantoms designed to reproduce cancer tumor geometry. This project aimed at developing 3D-printed eye-shaped cell-laden hydrogel phantoms for enhancing UV BT precision through radiobiological studies.

Methods: Collagen-methacrylate (Col-MA; for printability and cell viability), precrosslinked-alginate (preX-ALG; ALG:D-glucono-δ-lactone:$CaCO_3$ (3:1:1 volume ratio); for printability), Matrigel™ (for cell viability) and UV cells of three different types/radiosensitivities (Mel270, Mµ2, 92.1), were carefully mixed (proprietary methodology). Hydrogel viscosity was measured by rheometry. A crosslinking strategy was developed using CaCl2 (for ALG) and exposure to UVA (for Col-MA). Cell viability was assessed on non-printed and printed hydrogels (Cellink BioX-printer) using the Live/Dead cell assay kit at days (0, 1, 4) for UM lines and choroidal stromal fibroblasts (CSF). Finally, eye-shaped phantoms were 3D-printed on hemispherical supports (for oxygen and nutrient supply), and cell viability was evaluated at days (0, 1, 2).

Results: Rheological measurements allowed balancing hydrogel viscosity for optimal 3D printing, whereas crosslinking led to a stable hydrogel formulation for >2 days (minimal duration of BT) in cell culture medium Cell viability in the hydrogel exceeded 90% for all cell types, with and without 3D-printing, (>95.2% was reached in the eye-shaped phantom).
Conclusions: These 3D-printed cell-containing hydrogel phantoms will be used by radiobiologists in the design of clonogenic assays aiming at enhancing the precision of dose planning by medical physics BT procedures (cancers: eye, breast, prostate, gynecological, esophagus, etc.).

Keywords: Biological phantoms, biological models for radiation therapy, 3D bioprinting

20.- Development of Hydrogel-Based Eye Models for Enhanced the Ocular Ultrasound Training

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Ocular ultrasound is a critical imaging modality for the screening, diagnosis, and monitoring of various ocular pathologies, including intraocular tumors. This minimally invasive technique is widely accessible across Quebec hospitals. However, the absence of specialized teaching models limits training opportunities for both practicing and future ophthalmologists. Realistic simulation models are essential to enhance hands-on learning and improve proficiency in this field.

This project utilizes a mold-based technique with three-dimensional (3D) printing, chosen for its precision and flexibility in replicating anatomical structures. Eye molds were fabricated using polylactic acid (PLA) to create a 24 mm diameter model, reflecting the average size of an adult eye. These models were design to mimic the sclera, optic nerve and aqueous humor.

To accurately replicate the behavior of ocular tissues, two formulations of alginate-based hydrogels (2% and 4%) were developed and evaluated. The study examined the impact of varying alginate concentrations and cross-linking protocols using calcium ions (Ca2+) to optimize the mechanical properties of the hydrogels. Temperature control and calcium ion supplementation were applied to enhance the structural integrity and durability of the models, ensuring they mimic the biomechanical characteristics of the tissues. Preliminary results indicate that adjustments in alginate concentration and molding procedures significantly influence the models' mechanical properties and stability. Future work will focus on testing ultrasound-guided intraocular injections to further validate the models.

This project offers a cost-effective solution to bridge gaps in ophthalmology training by integrating this biomaterials-based tools into programs, improving diagnostic skills, patient care, and practice opportunities for ophthalmologists.

21.- Perfusable pancreatic tissues fabrication using a sacrificial embedded writing approach

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Type 1 diabetes (T1D) destroys insulin-producing beta cells, and islet transplantation offers a viable alternative to insulin therapy. However, islet loss after transplantation highlights the need for improved vascularization. We introduce a new method for creating vascularized pancreatic tissues using embedded writing techniques, avoiding the need for self-supporting bioinks or long build times. We utilized partially gelled alginate with suitable rheological properties as a support matrix for embedded writing. The self-healing properties of various partially gelled alginate formulations were evaluated by measuring their yield stress, ranging from 11.0 ± 0.6 to 51.0 ± 3.5 Pa. Pluronic F127 filaments were printed into the partially gelled alginate matrix using embedded 3D printing. The constructs were then gelled in a calcium bath and cooled to liquefy the Pluronic sacrificial material, resulting in perfusable constructs with multi-branched internal flow networks. Using the embedded 3D printing method, we generated thick, centimeter-scale, cell-laden, perfusable hydrogel constructs with up to five internal channels. After two days of perfusion, MIN6 cell lines maintained viability within a 600 ± 85 μm radius around each channel. Pluripotent stem cells (H1) were differentiated into islet-like clusters (PSC-islets) with viable C-peptide positive cells for over 25 days of perfusion. A glucose concentration change increased the insulin response. In this work, we also explored the use of an alginate-fibrin composite gel matrix, which successfully supported human umbilical vein endothelial cell (HUVEC) network formation and viability. Future work will integrate collagen as a support matrix, enhancing it with microvascular networks to improve nutrient and oxygen perfusion and better replicate natural vasculature. This biofabrication technique creates perfusable, human-scale pancreatic tissues for transplantation or studying oxygenation and 3D environment effects on cell fate.

22.- PVA e-spun nanofibrous mats modified with carbon nanodots for wound dressing: synthesis, characterization, and fluorescence analysis

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Considering advances in treatment processes, pathogenic bacterial contamination remains an important concern for human health and safety. The use of nanoparticles as imaging and detection agents has demonstrated their enormous promise for infectious disease management. Among nanoparticles, fluorescent carbon nanodots (CNDs) have generated considerable scientific interest due to their unique physicochemical qualities such as superior biocompatibility, low toxicity, adjustable photoluminescence, and high quantum yield. Further their modifiable surface groups can be functionalized to serve a wide range of therapeutic applications. Their small size allows them to be easily incorporated into flexible materials used for wound dressings, such as polyvinyl alcohol (PVA) nanofibers. CNDs are becoming superior candidates for imaging and detection of pathogenic bacteria. The fluorescent properties of CNDs allow for simple quantification of their release from such materials through fluorescence spectroscopy. The release of CNDs can be affected by changes in pH.

In this study, 0.1% w/w CND-embedded PVA nanofibrous mats were fabricated through electro-spinning (e-spinning) of an in-situ preparation of CND-PVA solution. The fibers were then crosslinked with 1,4-benzenediboronic acid (DBA) through the formation of boronic ester bonds and qualitatively assessed through FTIR-ATR and SEM analysis. Both showed the evidence of effective crosslinking through the appearance of bands representing the presence of boronic ester linkages on the FTIR spectra and through the appearance of more closely compact fibers in cross-linked mats relative to uncrosslinked mats. A degradation study was performed on crosslinked mats to assess their degree of degradation at different pHs in a given time. Spectroscopic techniques were utilized to determine the CND release kinetics from the fibers at different pH levels. The general trend showed that the release of CND was rapid under basic and acidic conditions. Further, our study extends to exploring the applications of CNDs in imaging, detecting, and eliminating pathogenic bacteria to be a potentially promising antimicrobial agent.

23.- Development of Biocompatible Therapeutic Objects with Radiopaque properties by Fused Filament Fabrication (FFF) 3D printing

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Background and purpose: 3D printing of radiopaque polymers is an important challenge in the field of radioactive implants for personnalised brachytherapy (BT; internal radiotherapy). Polyetheretherketone (PEEK; chemically and mechanically resistant), is widely used in orthopedy and implantology. However, plaque BT requires the embedding of radioisotopes into a material that provides both radiolucent and/or radiopaque properties, depending on geometrical design. Radiopacity can be modulated by the addition of a dense component into the polymer matrix, without compromising its 3D- printing capacity. Here, novel radiopaque filaments were developed allowing the 3D printing of radiological devices by fused filament fabrication (FFF).

Materials & Methods: A proprietary method allowed the development of PEEK matrices with high volume fractions (10-20 % v/v) of high-Z radiopaque metals (here: tungsten (W)), prior to their extrusion into mm-sized filaments. The homogeneous distribution of W in the filaments was confirmed by electron microscopy, X-ray fluorescence, and elemental analysis. Filament printability was evaluated at different temperatures using a FFF 3D printer (Apium P220), whereas radiopacity was assessed with a µCT scanner (GE eXplore Locus) using objects of various thicknesses. The viability of primary human choroid fibroblast (CSF) cells in contact with W-loaded PEEK objects was evaluated at days (0, 1, 4).

Results: Radiopaque PEEK filaments achieving <10% v/v in tungsten exhibited a uniform distribution of W particles (SEM, XRF). Optimal 3D printing parameters were identified, and X-ray attenuation properties were measured via radiographic imaging. 3Dprinted objects of a dimension ≤ 1 mm demonstrated a high radiation-blocking capacity when CT-scanned at 40 kVp achieving ~94% efficiency with a 7.57 cm−1 attenuation coefficient. The scanned objects were defect-free and non- porous. The cytotoxicity of CSF cells grown at the surface were viable (>92% for 4 days; implementation time of a BT plaque).

Conclusion: This study demonstrates the possibility of 3D printing radiopaque polymer devices using high-Z materials contents PEEK filaments. This technology lays the groundwork for producing robust 3D-printed radiopaque polymer parts, with potential medical, aerospace, and nuclear applications.

Keywords: fused filament fabrication (FFF), polymers additive manufacturing, composite materials, radiotherapy, polyetheretherketone, radiopaque materials, radiation shielding.

24.- Quantification de la structure de matériaux moléculaires

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Les verres moléculaires, des petites molécules organiques pouvant adopter une phase amorphe, sont des matériaux émergents dans plusieurs domaines tels que les industries alimentaire et pharmaceutique et l'optoélectronique. En effet, la phase amorphe possède des propriétés intéressantes qui sont absentes dans la phase cristalline, comme sa malléabilité et sa transparence. Cette phase de la matière est toutefois métastable et les verres moléculaires ont tendance à cristalliser à long terme. Dans ce contexte, le trempage (*dip-coating*) est une technique qui permettrait de préparer des films minces et ultraminces de verres moléculaires plus résistants à la cristallisation.

Dans ce travail, nous avons étudié la stabilité amorphe de films d'un verre connu pour être cinétiquement stable, possiblement grâce à des ponts H. Les films ont été préparés en vue d'obtenir différentes épaisseurs, soit en variant la vitesse de retrait du substrat, la volatilité du solvant et sa capacité à faire des ponts H ou interactions π-π avec le verre. L'application d'un modèle chimiométrique *Purity* sur les spectres infrarouges (IR) des films de verre a révélé une augmentation des ponts H avec l'épaisseur des films, mesurée par ellipsométrie spectroscopique (SE), et l'atteinte d'un plateau aux épaisseurs élevées.

D'un autre côté, à épaisseur constante, la formation des ponts H au sein des films de verre a été favorisée selon une tendance générale par les solvants qui forment le plus de ponts H avec le verre. Cependant, les solvants qui interagissent par ponts H à un degré modéré seulement ont généré le moins de ponts H, possiblement parce qu'ils réduisent la mobilité du verre pendant l'évaporation, ce qui empêcherait un réarrangement subséquent des ponts H au sein du verre. Finalement, la formation des ponts H a également été favorisée par les solvants moins volatils.

Session 5 : Polymères

25.- Electrochromic and Electrofluorochromic Properties of Conjugated Copolymers Carried Over to the Solid-State for Applications in Chromic Devices

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Electrochromic materials (ECM) hold exceptional promises in a variety of technological applications including smart windows, flexible/multi-colored electronic devices, sensors and energy storage. Their intrinsic properties allow reversible tuning of their color and optical properties such as transmittance, reflection and absorbance with applied potential. In recent years, conjugated polymers have gathered substantial attention as electrochromes. Their large □-system backbones coupled with fine tweaking of their substituents result in comparable optical, conductive and electronic properties to inorganic ECMs with the advantage of offering a wider color palette in addition to a higher degree of tunability. One such insertion to the backbone are electroactive fluorophores which exhibit reversible changes in emission with an external electrical stimulus, known as electrofluorochromism. Current applications are mostly in displays, information encryption and biosensors. Thus, materials that can both behave electrochromicly and electrofluorochromicly are of interest because of their potential dual role within electrochromic devices (ECD).

Organic electrochromes have been widely studied as monomers in solution and display outstanding properties, but literature suggests that transferring their performance to the solid state within ECDs is challenging. This is in part because the monomers need to be polymerised in thin films insoluble to the electrolyte used and immobilized on an electrode all while preserving electrochromic (EC) and electrofluorochromic (EFC) activities.

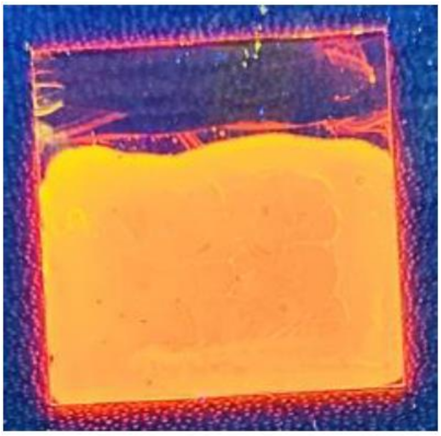

Figure. Immobilized polymer film on ITO that retains its fluorescence in the solid state

It will be shown that a donor-acceptor conjugated monomer retains its electrochromic and electrofluorochromic properties after photopolymerization on ITO as a copolymer using a cross-linker polymer. In addition, the parameters of its incorporation within a chromic device will also be discussed.

26.- Weathering Properties of Silicone-Epoxy Coatings for Enhancing Wind Turbine Efficiency in Cold Climates: Effect of Different Silicone Intermediates

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Ice accumulation on wind turbine blades poses a significant challenge to turbine performance and safety, and these issues have led to extensive research on developing effective anti-icing methods. Polymer-based such as silicone-epoxy icephobic coatings have emerged as promising solutions given their passive nature and low energy requirements. However, creating efficient icephobic coatings that withstand environmental wear, possess robust mechanical strength, and anti-icing properties, and resist UV exposure is a challenging endeavor. Here, we fabricated a durable silicone-epoxy icephobic coating to enhance turbine efficiency in cold climates with two different silicone intermediate resins and compared their icephobicity.

27.- Exploration of boronic ester chemistry to develop pH-responsive degradable crosslinked electrospun nanofibers for controlled drug release wound dressing

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The most recent advances for the efficient treatment of chronic wound treatment involves the application of nanostructured based materials as cutting-edge wound dressings based on nanostructured materials. For instance, poly(vinyl alcohol) (PVA)-based electro-spun (e-spun) nanofibers have been extensively investigated due to PVA remarkable electrospinnability, high water-absorbing capacity, and good biocompatibility, as well as FDA approval for biological purposes. Since PVA is highly soluble in water, to ensure their dimensional stability in aqueous environment, PVA nanofibers need to be chemically crosslinked. However, chemical crosslinking motifs based on carbamate, ester, and even acid-responsive degradable acetal bonds (with glutaraldehyde) show several limitations including non-degradability, uncontrolled release, and cytotoxicity.

To stabilize PVA e-spun nanofibers, boronic ester (BE) chemistry emerges as an alternative method because of their biocompatibility and reactivity. The formation of boronic ester bonds may occur rapidly when diols react with boronic acids at room temperature. BE chemistry is appealing for the fabrication of degradable stimuli-responsive drug delivery systems because BE bonds may degrade under exposition to enzymes, pH changes, oxidizing agents (e.g. in the presence of hydrogen peroxide), and high diol concentrations (e.g. glucose).

This research describes our proof-of-concept approach exploring BE chemistry in the fabrication of effective pH-degradable BE-crosslinked e-spun PVA nanofibers. With a choice of a commercially- available phenyldiboronic acid as a difunctional crosslinker our comprehensive characterization of crosslinking, pH-responsive degradation, encapsulation and controlled drug molecule release as well as antimicrobial properties confirms that our approach allows for the fabrication of dimensionally-stable boronic ester-crosslinked PVA e-spun nanofibers degradable in acidic and alkali pHs, which are promising for smart wound dressings.

Further, this presentation shows the versatility of our approach with design and synthesis of novel diboronic acid crosslinkers integrated with desired functionality (e.g. pH-degradable imine bonds) for the fabrication of multifunctional degradable e-spun nanofibers.

28.- Époxydation des huiles usagées

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L'époxydation des huiles végétales est une réaction clé dans la modification chimique des huiles, conduisant à des produits à valeur ajoutée utilisés dans divers secteurs industriels, notamment les plastiques, les adhésifs et les revêtements. Dans le cadre de cette recherche, nous nous sommes concentrés sur l'époxydation des huiles alimentaires usagées, une source renouvelable souvent considérée comme un déchet. Cette étude vise non seulement à valoriser ces huiles usagées mais aussi à promouvoir des pratiques durables en chimie verte. Les huiles végétales sont constituées principalement de triglycérides, comportant des acides gras insaturés. L'époxydation de ces acides gras permet d'introduire des groupes époxydes, rendant les huiles plus réactives et adaptées à diverses applications industrielles. La littérature rapporte plusieurs méthodes d'époxydation, parmi lesquelles la méthode conventionnelle utilisant l'acide acétique, l'acide sulfurique comme catalyseur, et le peroxyde d'hydrogène (H2O2) comme agent oxydant est bien documentée pour son efficacité et sa simplicité. Nous avons suivi un protocole rigoureux pour purifier les huiles alimentaires usagées avant de les soumettre à l'époxydation. La méthode utilisée implique les réactifs suivants : huile purifiée, acide acétique, acide sulfurique (comme catalyseur) et peroxyde d'hydrogène à 30%. Les huiles purifiées ont été époxydées dans des conditions contrôlées, et les produits obtenus ont été analysés par diverses techniques spectroscopiques et chromatographiques. Les analyses IRTF ont montré la disparition du pic à 3010 cm−1, caractéristique des liaisons C=C, indiquant ainsi la consommation de ces doubles liaisons lors de l'époxydation. Les analyses RMN 1H et 13C ont confirmé la présence des groupes époxydes, et les tests GC-MS ont permis d'identifier les principaux acides gras présents dans les huiles usagées, à savoir l'oléique, le palmitique, le linoléique, et le stéarique. Un plan d'expérience factoriel, en modifiant la température, le temps de réaction, et le ratio de peroxyde d'hydrogène, a permis d'optimiser les conditions de réaction, atteignant ainsi un rendement de conversion des époxydes des acides gras de 95%. Notre recherche sur l'époxydation des huiles alimentaires usagées a démontré l'efficacité d'une méthode de purification et d'époxydation. Les analyses IRTF, RMN 1H et 13C, et GC-MS ont confirmé la transformation des huiles et identifié les principaux acides gras. Grâce à un plan d'expérience factoriel, nous avons optimisé les conditions de réaction pour atteindre un rendement de 95 %. Cette valorisation des huiles usagées ouvre la voie à des applications industrielles durables. Cette étude démontre que les huiles alimentaires usagées peuvent être efficacement époxydées en utilisant une méthode conventionnelle. Les résultats obtenus soulignent l'importance de la purification préalable des huiles et de l'optimisation des conditions de réaction pour atteindre des taux de conversion élevés. Cette approche non seulement valorise les déchets huileux mais contribue également à la chimie durable et à la réduction de l'empreinte carbone des procédés industriels.

Mots-clés : Époxydation, Huiles alimentaires usagées, Chimie verte, IRTF, RMN, GC-MS, Valorisation des déchets.

29.- Synthesis and characterization of a new terpyridine ligand and corresponding ruthenium complexe for artificial photosynthesis

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``For decades ruthenium polypyridyl complexes have attracted considerable interest thanks to their useful optical properties, e.g., visible light absorption and long-lived excited states, and ease of incorporation into artificial light-harvesting systems. We report herein the synthesis of a novel tridentate ligand (tris 4,4',4''-(4'''-pyridyl)-2,2':6',2''-terpyridine, labeled py3tpy) and its corresponding homoleptic ruthenium (II) complex through high temperature microwave synthesis. This last is a suitable photosensitizer (PS) as it shows hydrogen photoproduction with a sustained activity over more than seven days under green light with a final TON over 345 $mol_{H2}.molPS^{-1}$.

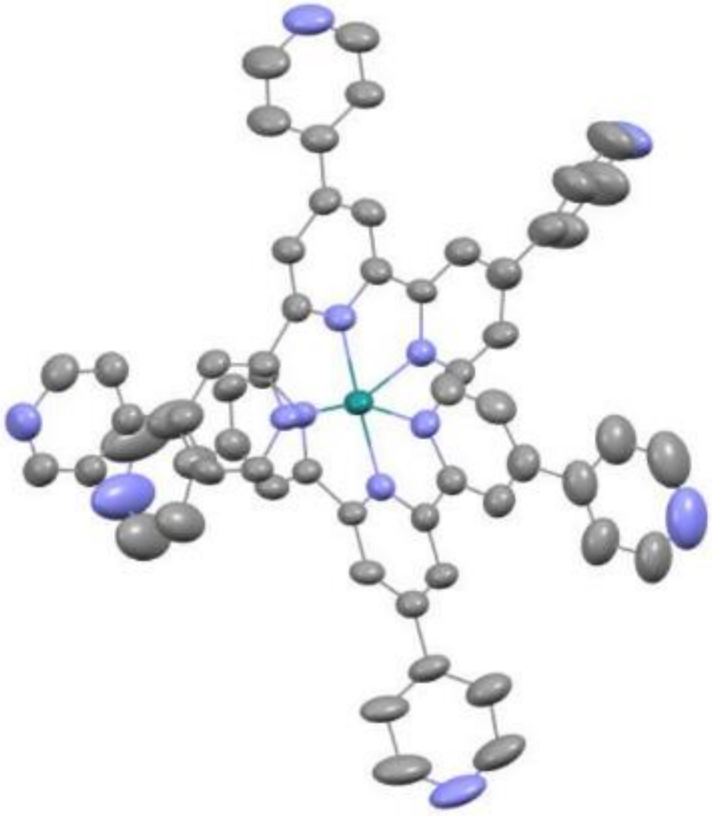

Figure 1. Ortep representation of the [Ru(py3tpy)2](PF6)2 complex with ellipsoids drawn at 50% probability level. Solvent and counter-anion molecules are omitted for clarity.

30.- Developing silicone acrylic coating:

A step forward in ice mitigation for wind turbines

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This study presents a novel silicone-acrylic resin coating designed to improve the ice-phobic properties of wind turbine blades and enhance efficiency in cold climates. By blending silicone polymers with acrylic resins, the hybrid coating combines strong ice repellency with improved weathering resistance. Performance evaluations demonstrate its effectiveness in reducing ice accumulation, offering a promising solution for operational efficiency in adverse weather conditions