

2023

CQMF/QCAM

7^e Colloque annuel
sur la recherche
des **matériaux**
fonctionnels

MAI 14-16 MAY 2023

Hôtel le Victorin, Victoriaville

7th **Advanced Materials**
Annual Meeting



CQMF LES INTER-MATÉRIAUX
QCAM NETWORKING MATERIALS

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Remerciements / Acknowledgements

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Petr Fiurasek (QCAM)

Directeur / Director: Mohamed Siaj (UQAM)

Codirecteur / Co-director: Fiorenzo Vetrone (INRS)

Comité étudiant / Student committee

Nous remercions les commanditaires de leur généreux appui à notre colloque annuel. Grâce à eux, nous sommes en mesure de vous offrir un programme stimulant et enrichissant.

Nous sommes donc heureux de vous accueillir à cette fête des matériaux fonctionnels et le comité organisateur espère que ce colloque vous sera agréable.

We thank the sponsors for their generous support of our annual meeting. They have allowed us to offer you an exciting and rewarding program.

We are therefore pleased to welcome you to this celebration of advanced materials and the organizing committee hopes that you will enjoy this meeting.





Quoi de mieux que de se retrouver tous ensemble au colloque annuel du CQMF en ce 15 mai, la date de la Journée Internationale des Familles? Car vous êtes chez vous au CQMF, votre famille scientifique!

There is nothing better than getting together at the QCAM annual meeting on 15 May, the International Day of Families! Because you are at home at QCAM, your scientific family!



Horaire

Dimanche, 14 mai – Président : Rafik Naccache

17h00	Arrivée des participants de Montréal et UQTR
17h15	Réception Inscription
17h45	Arthabaska Souper
18h30	Victoria A/B Mot d'ouverture – Mohamed Siaj
18h45	Victoria A/B Conférence plénière : Bin Liu - Université Nationale de Singapore
19h45	Victoria A/B Jacopo Profili - Université Laval
20h15	Victoria A/B Philippe Dauphin Ducharme - Université de Sherbrooke
20h45	Hall Réception de bienvenue et exposition

Lundi, 15 mai – Présidente : Dongling Ma

8h45	Hall A/B Accueil
9h00	Victoria A/B Conférence plénière : Peter Nordlander - Université Rice
10h00	Victoria A/B Mihaela Cibian - Université du Québec à Trois-Rivières
10h30	Hall Pause-Café
11h00	Victoria A/B Changhong Cao - Université McGill
11h30	Victoria A/B Conférence plénière : Will Chueh - Université Stanford
12h30	Salle à manger Dîner

Ateliers et Séances thématiques - 4 sessions

13h00	Victoria B Au-delà du CV	Victoria D EDI – Inclusion des étudiants Internationaux		
	A. Soldera / A. Laramée	A. Wustrow/B.Shahreza	Y.Chen/E.Orgiu	T. van de Ven/M.Shagar
	Victoria B Polymères	Victoria D Énergie	Colibri 2/3 Nano	Suzor-Côté Dév.Dur.
14h00	Rozita Sadeghzadeh	Mohammad Masaali	Nadi Braidy	Pierre Bambier
14h15	Nora Chelfouh	Alex Hebert	Lucille Kuster	Michelle Pains Duarte
14h30	Arnaud Laramée	Babak Shahreza	Loïc Demoulin	Issa Malam Mahamadou
14h45	Saba Goharshenasmoghadam	Nooshin Zeinali Galabi	Maziar Jafari	Kevin Daoust
15h00	Weiguang Qiu	Aisha Hamilton	Khalid Nowaz Anindya	Ahmad Al Shboul
15h15	Pause-café			
15h45	Jérémy Baribeault	Allison Wustrow	Yiwen Chen	Rhea Guha
16h00	Meng Liu	Francia Ravalison	Zuchong Yang	Peipei Liu
16h15	Xinshi Chen	Zhao Yang	Lindimar Borges De Avila Jr	Theo van de Ven
16h30	Abdenour Chenni	Erica Tomassi	Wanting He	Ahmed Ayari
16h45	Armand Soldera	Ameer Nizami	Zhiyuan Peng	Elie Haddad
17h00	Victoria B Assemblée générale annuelle des membres			
17h00	Victoria D Assemblée générale du comité étudiant			
18h00	Hall Session d'affiches scientifiques - cocktail dînatoire avec service et bar			
18h-19h30	Visite des communications par affiche - chiffres IMPAIRS			
19h30-21h	Visite des communications par affiche - chiffres PAIRS			
22h00	Ajournement			

Mardi, 16 mai – Président : Will Skene

8h50	Victoria A/B	Bienvenue aux participants
9h00	Victoria A/B	Conférence plénière : Emilie Genin - Université Bordeaux
10h00	Victoria A/B	Nhat Truong Nguyen - Université Concordia
10h30		Pause-Café
11h00	Victoria A/B	Conférence plénière : Theresa Reineke - Université de Minnesota
12h00	Victoria A/B	Kulbir Ghuman - Institut national de la recherche scientifique
12h30	Salle à manger	Dîner

Séances thématiques - 3 sessions

13h-14h30	Visite INOVEM (Cégep de Victoriaville)		
	Victoria B Auto-assemblage	Victoria D Énergie	Colibri 2/3 Bio
	Louis Cuccia	Eric McCalla	Fiorenzo Vetrone
13h15	Mostafa Eesaee	Peikui Wang	Erfan Rahbarimehr
13h30	Bin Li	Qihang Yu	Ruiqi Yang
13h45	Mostafa Shagar	Karimi Azari	Mathieu Frenette
14h00	Élodie d'Astous	Samaneh Salek	Souheib Zekraoui
14h15	Tuan Doan	Jeremy Dawkins	Miao Liu
14h30	Hudson de Aguiar Bicalho	Anoir Hamdi	Rouslan Svintsitski
14h45	Pedro Donnarumma	Ethan Anderson	Adryanne Clermont-Paquette
15h00	Victoria A/B		

Schedule

Sunday, May 14 – Chair: Rafik Naccache

5:00pm	Arrival of participants from Montreal and UQTR
5:15pm	Reception Registration
5:45pm	Arthabaska Dinner
6:30pm	Victoria A/B Opening remarks – Mohamed Siaj
6:45pm	Victoria A/B Plenary talk: Bin Liu - National University of Singapore
7:45pm	Victoria A/B Jacopo Profili - Université Laval
8:15pm	Victoria A/B Philippe Dauphin Ducharme - Université de Sherbrooke
8:45pm	Hall Welcome reception and Exhibition

Monday, May 15 – Chair: Dongling Ma

8:45am	Hall A/B Registration
9:00am	Victoria A/B Plenary talk: Peter Nordlander – Rice University
10:00am	Victoria A/B Mihaela Cibian - Université du Québec à Trois-Rivières
10:30am	Hall Coffee break
11:00am	Victoria A/B Changhong Cao - McGill
11:30am	Victoria A/B Plenary talk: Will Chueh – Stanford University
12:30pm	Dining room Lunch

Workshops and 4 scientific sessions

1:00pm Chairs	Victoria B Beyond the CV	Victoria D	EDI - Inclusion of International students	
	A. Soldera / A. Laramée	A. Wustrow/B.Shahreza	Y.Chen/E.Orgiu	T. van de Ven/M.Shagar
2:00pm	Victoria B Polymers	Victoria D Energy	Colibri 2/3 Nano	Suzor-Côté Sus.Dev.
	Rozita Sadeghzadeh	Mohammad Masaeli	Nadi Braidy	Pierre Bambier
2:15pm	Nora Chelfouh	Alex Hebert	Lucille Kuster	Michelle Pains Duarte
2:30pm	Arnaud Laramée	Babak Shahreza	Loïc Demoulin	Issa Malam Mahamadou
2:45pm	Saba Goharshenasmoghadam	Nooshin Zeinali Galabi	Maziar Jafari	Kevin Daoust
3:00pm	Weiguang Qiu	Aisha Hamilton	Khalid Nowaz Anindya	Ahmad Al Shboul
3:15pm	Coffee break			
3:45pm	Jérémy Baribeault	Allison Wustrow	Yiwen Chen	Rhea Guha
4:00pm	Meng Liu	Francia Ravalison	Zuchong Yang	Peipei Liu
4:15pm	Xinshi Chen	Zhao Yang	Lindiomar Borges De Avila Jr	Theo van de Ven
4:30pm	Abdenour Chenni	Erica Tomassi	Wanting He	Ahmed Ayari
4:45pm	Armand Soldera	Ameer Nizami	Zhiyuan Peng	Elie Haddad
5:00pm	Victoria B Annual general meeting of members			
5:00pm	Victoria D General assembly of students			
6:00pm	Hall Poster Session, Reception and Exhibition			
6-7:30pm	Visit of posters: ODD numbers			
7:30-9pm	Visit of posters: EVEN numbers			
10:00pm	Adjournment			

Tuesday, May 16 – Chair: Will Skene

8:50am	Hall A/B	Registration
9:00am	Victoria A/B	Plenary talk: Emilie Genin - Université Bordeaux
10:00am	Victoria A/B	Nhat Truong Nguyen – Concordia University
10:30am		Coffee break
11:00am	Victoria A/B	Plenary talk: Theresa Reineke - University of Minnesota
12:00pm	Victoria A/B	Kulbir Ghuman - Institut national de la recherche scientifique
12:30pm	Dinning room	Lunch

3 Scientific sessions

1-2:30pm	Visit to INOVEM (Cégep de Victoriaville)		
Chairs	Louis Cuccia	Eric McCalla	Fiorenzo Vetrone
	Victoria B Self-Assembly	Victoria D Energy	Colibri 2/3 Bio
1:15pm	Mostafa Eesaee	Peikui Wang	Erfan Rahbarimehr
1:30pm	Bin Li	Qihang Yu	Ruiqi Yang
1:45pm	Mostafa Shagar	Karimi Azari	Mathieu Frenette
2:00pm	Élodie d'Astous	Samaneh Salek	Souheib Zekraoui
2:15pm	Tuan Doan	Jeremy Dawkins	Miao Liu
2:30pm	Hudson de Aguiar Bicalho	Anoir Hamdi	Rouslan Svintsitski
2:45pm	Pedro Donnarumma	Ethan Anderson	Adryanne Clermont-Paquette
3:00pm	Victoria A/B	Coffee break	
3:30pm	Victoria A/B	Award ceremony sponsored by SFR and closing remarks – Mohamed Siaj	
4:15pm		Bus departure	

Poster # Affiche

#	Prénom First Name	Nom Last Name	Institution	Nom du direct.eur.rice Supervisor
1	Aaron Gabriel	Nunez Avila	Université de Montréal (UdeM)	James D. Wuest
2	Adela	Abidi	Université du Québec à Trois-Rivières (UQTR)	Mihaela Cibian
3	Adryanne	Clermont-Paquette	Concordia University	Rafik Naccache
4	Alizée	Debiais	Université de Montréal (UdeM)	Dominic Rochefort
5	Amna	Khierallah	Université du Québec à Trois-Rivières (UQTR)	
6	Azam	Usefian Babukani	École de Technologie Supérieure (ETS)	Ricardo Izquierdo
7	Caroline	Dubois	Université de Montréal (UdeM)	Jean-François Masson
8	Cephas	Amoah	Université de Montréal (UdeM)	Will Skene
9	Chris	Copeman	Concordia University	Ashlee Howarth
10	Cloé	Maranda	Université Laval (ULaval)	Élodie Boisselier
11	Diane	Rawach	Institut National de Recherche Scientifique (INRS)	Shuhui Sun
12	Élodie	d'Astous	Université de Sherbrooke (UdeS)	P. Dauphin Ducharme
13	Eric	Dionne	Université de Montréal (UdeM)	Autre/Other
14	Faranak	Hosseini	Université du Québec à Trois-Rivières (UQTR)	Jacques Huot
15	Fazia	Mechai	École de Technologie Supérieure (ETS)	
16	Francia	Ravalison	Université du Québec à Trois-Rivières (UQTR)	Jacques Huot
17	Gabrielle	Raîche-Marcoux	Université Laval (ULaval)	Élodie Boisselier
18	Ghizelane	Lebar	Université du Québec à Montréal (UQAM)	Mohamed Siaj
19	Gregory	Amato	Concordia University	Louis Cuccia
20	Guy	Prevot	Université de Sherbrooke (UdeS)	P. Dauphin Ducharme
21	Gym Clerc	Lentsolo Yalli	Université Laval (ULaval)	Véronic Landry
22	Haiyan	Wu	Université de Montréal (UdeM)	
23	Hannah A.	Williams	Université de Montréal (UdeM)	Jean-François Masson
24	Hannah	Wiebe	McGill University (McGill)	
25	Hichem	Gamraoui	Université du Québec à Montréal (UQAM)	Mohamed Siaj
26	Ignacio	Lopez	Université du Québec à Trois-Rivières (UQTR)	Jacques Huot
27	Ilias	El Alaoui-ElBalrhiti	Université de Sherbrooke (UdeS)	Nadi Braidy
28	Issa	Malam Mahamadou	Université du Québec à Montréal (UQAM)	Mohamed Siaj

Poster # Affiche

#	Prénom First Name	Nom Last Name	Institution	Nom du direct.eur.rice Supervisor
29	James	McGettrick	Swansea University, Pays de Galles, UK	
30	Johann	Sosoe	Université de Montréal (UdeM)	James D. Wuest
31	Joseph	Chiong	Concordia University	Marek Majewski
32	Juan Carlos	Ceballos Alvarez	École de Technologie Supérieure (ETS)	Ricardo Izquierdo
33	Kalvin	Durand	Université Laval (ULaval)	Denis Rodrigue
34	Karuna	Malik	Concordia University	John Oh
35	Kenneth	Beyerlein	Institut National de Recherche Scientifique (INRS)	
36	Khaled	Rhili	Université du Québec à Montréal (UQAM)	Mohamed Sijaj
37	Laurier	Gauvin	McGill University (McGill)	Corinne Hoesli
38	Louis	Caussin	Université de Montréal (UdeM)	Will Skene
39	Louise	Gourdelier	Université de Montréal (UdeM)	Antonella Badia
40	Luc Aurelien	Fotue	Université du Québec à Trois-Rivières (UQTR)	Mihaela Cibian
41	Mahdokht	Akbari Taemeh	Université Laval (ULaval)	Marc-André Fortin
42	Manon	Faral	Université de Montréal (UdeM)	Mickaël Dollé
43	Maram	Sandouka	Université du Québec à Montréal (UQAM)	Mohamed Sijaj
44	Maryam	Afkari	Université de Sherbrooke (UdeS)	Jerome Claverie
45	Marzieh	Abdolhosseini	McGill University (McGill)	Eric McCalla
46	Maxime	Goulet	Université de Montréal (UdeM)	Audrey Laventure
47	Meghan	McNeil	Université de Montréal (UdeM)	Audrey Laventure
48	Mingrui	Guo	McGill University (McGill)	Marta Cerruti
49	Minh Dat	Nguyen	Université de Sherbrooke (UdeS)	P. Dauphin Ducharme
50	Mohammad	Bakhtiari	Université du Québec à Chicoutimi (UQAC)	Gelareh Momen
51	Mohan Raj	Anthony Raj	Université de Montréal (UdeM)	Will Skene
52	Nan	Jia	Université Laval (ULaval)	Jesse Greener
53	Natalia	Vargas Perdomo	Concordia University	Louis Cuccia
54	Nicola	Teolis	Université de Montréal (UdeM)	Christian Pellerin
55	Nicolas	Fontaine	Université de Sherbrooke (UdeS)	P. Dauphin Ducharme
56	Niloofer	Zamanian	Université de Sherbrooke (UdeS)	Yue Zhao

Poster # Affiche

#	Prénom First Name	Nom Last Name	Institution	Nom du direct.eur.rice Supervisor
57	Norbert	Villeneuve	Université de Montréal (UdeM)	James D. Wuest
58	Olivier	Roy	Université de Montréal (UdeM)	Christian Pellerin
59	Orlando	Ortiz	Université de Montréal (UdeM)	Will Skene
60	Pan	Wang	Institut National de Recherche Scientifique (INRS)	Shuhui Sun
61	Patricia	Moraille	Université de Montréal (UdeM)	
62	Patrick	Ayotte	Université de Sherbrooke (UdeS)	
63	Paul	Camus	Université de Sherbrooke (UdeS)	Nadi Braidy
64	Pierre-Philippe	Roy	Université de Sherbrooke (UdeS)	Yves Dory
65	Poh Ying	Fong	Concordia University	Louis Cuccia
66	Priyanka	Bhatt	Université du Québec à Trois-Rivières (UQTR)	Jacques Huot
67	Ramzi	Zidani	Université de Montréal (UdeM)	
68	Raphaël	Vincent-Dubé	Université de Montréal (UdeM)	Christian Pellerin
69	Rouslan	Svintsitski	3DCERAM Sinto	
70	Samaneh	Keshavarzi	Université du Québec à Chicoutimi (UQAC)	Gelareh Momen
71	Samila	Leon Chaviano	Université Laval (ULaval)	Marc-André Fortin
72	Saqib	Ali	Université Laval (ULaval)	Jesse Greener
73	Sara	Tiferras	Université de Sherbrooke (UdeS)	Nadi Braidy
74	Sierra	Cranmer-Smith	McGill University (McGill)	Theo van de Ven
75	Simon	Sprocq	Polytechnique Montréal	Alain Rochefort
76	Sixiang	Liu	Institut National de Recherche Scientifique (INRS)	Shuhui Sun
77	Taki	Aissou	Université de Sherbrooke (UdeS)	Nadi Braidy
78	Taylor	Fisher	Concordia University	Ashlee Howarth
79	Thomas	Boulanger	Université de Montréal (UdeM)	Dominic Rochefort
80	Tianyang	Deng	Université Laval (ULaval)	Jesse Greener
81	Will	Skene	Université de Montréal (UdeM)	
82	Xiaofeng	Zheng	Université de Sherbrooke (UdeS)	Yue Zhao
83	Yaru	Ma	Université de Sherbrooke (UdeS)	Yue Zhao
84	Yilu	Su	Université du Québec à Montréal (UQAM)	Mohamed Sij
85	Yiwei	Jiang	McGill University (McGill)	Theo van de Ven
86	Zeping	Liu	Université de Sherbrooke (UdeS)	Yue Zhao

Conférences plénières / Plenary lectures

ACCELERATING BIOMEDICAL RESEARCH THROUGH MATERIALS INNOVATION



Bin Liu

National University of Singapore, Singapore

ABSTRACT

Recent years have witnessed the fast growth of fluorogens with aggregation-induced emission characteristics (AIEgens) in biomedical research. The weak emission of AIEgens as molecular species and their bright luminescence as nanoscopic aggregates distinguish them from conventional organic luminophores and inorganic nanoparticles, making them wonderful candidates for many high-tech applications. In this talk, we summarize our recent AIE work in the development of new fluorescent bioprobes for biosensing and imaging. The simple design and fluorescence turn-on feature of the molecular AIE bioprobes offer direct visualization of specific analytes and biological processes in aqueous media with higher sensitivity and better accuracy than traditional fluorescence turn-off probes. The AIE dot probes with different formulations and surface functionalities show advanced features over quantum dots and small molecule dyes in non-invasive cancer cell detection, long-term cell tracing, and vascular imaging. In addition, our recent discovery that AIEgens with high brightness and efficient reactive oxygen species generation in the aggregate state further expanded their applications to image-guided cancer surgery and therapy. Recently, we combined accurate prediction of material performance via first-principal calculations and Bayesian optimization-based active learning to realize a self-improving discovery system for high-performance photosensitizers, which can significantly accelerate materials innovation for biomedical research.

BIO - LIU

Dr. Bin Liu is currently Distinguished Professor of the National University of Singapore (NUS). She is a foreign member of the US National Academy of Engineering, and a Fellow of Singapore National Academy of Sciences and the Academy of Engineering Singapore. She received B.S. degree from Nanjing University and Ph.D. degree from NUS before her postdoctoral training at the University of California, Santa Barbara. She joined NUS in late 2005 and was promoted to Dean's Chair Professor in 2014 and Provost's Chair Professor in 2017.

Liu's research is focused on organic nanomaterials for energy and biomedical applications. She is among the World's Most Influential Minds and Top 1% Highly Cited Researchers in Materials Science and Chemistry 2014-2022. Liu has received many prestigious awards, and the recent ones include ACS Nano Lectureship Award 2019, Kabiller Young Investigator's Award and the RSC Centenary Prize and Medal 2021. Liu is passionate about nurturing the next generation research leaders and encouraging more women to pursue careers in science, engineering, and nanotechnology.

PLASMON-ENHANCED PHOTOCATALYSIS FOR GREEN CHEMISTRY



Peter Nordlander

Rice University, Houston, TX, USA

ABSTRACT

Plasmons can serve as efficient generators of hot electrons and holes that can be exploited in light harvesting applications. The physical mechanism for plasmon-induced hot carrier generation is plasmon decay. Plasmons can decay either radiatively or non-radiatively with a branching ratio that can be controlled by tuning the radiance of the plasmon mode. Non-radiative plasmon decay is a quantum mechanical process in which one plasmon quantum is transferred to the conduction electrons of the nanostructure by creating an electron-hole pair, i.e., excitation of an electron below the Fermi level of the metal into a state above the Fermi level but below the vacuum level. These hot carriers interact with all charge carriers in the system and eventually transfer their energy into phonons (heat). In my talk, I will discuss the time-dependent relaxation of plasmon-induced hot carriers including electron-electron scattering, fluorescence, and electron-phonon coupling ^[1-2] and show that the hot carrier lifetimes can exceed several picoseconds. I will also discuss recent applications of plasmon-induced hot carrier generation such as plasmon-enhanced photocatalysis, and how photocatalytic efficiencies can be enhanced and quantified by placing catalytic reactors in the nearfield of a plasmonic antenna in Antenna/Reactor geometries ^[3-8].

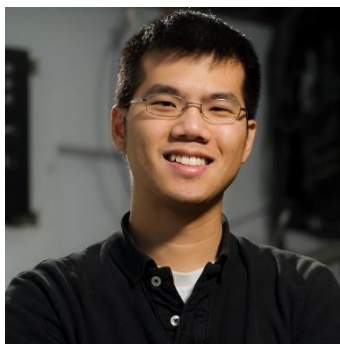
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BIO - NORDLANDER

Prof. Peter Nordlander (<http://nordlander.rice.edu>, ResearcherID: A-2560-2008; ORCID: 0000-0002-1633-2937) obtained his PhD degree in Theoretical Physics at Chalmers University of Technology in Gothenburg in Sweden in 1985. After postdoctoral positions at IBM Thomas J. Watson Research Center at Yorktown Heights (USA) and AT&T Bell Laboratories at Murray Hill (USA) and at Rutgers University, he joined the faculty at Rice University in 1989 and is currently Wiess Chair of Natural Sciences and Professor of Physics and Astronomy, Professor of Electrical and Computer Engineering and Professor of Materials Science and Nanoengineering. He has been a Visiting Professor at University of Paris, at the Institute of Physics at the Chinese Academy of Sciences, a C.N. Yang Professor at the Chinese University of Hong Kong, at Peking University, and a Prominent Overseas Visiting Professor in the Department of Physics at Wuhan University. His research background is in theoretical condensed matter and nanoscience. His current research is focused on the theoretical and computational modeling of Plasmonics and Nanophotonics phenomena. He is an associate editor of ACS Nano. He is a fellow of APS, AAAS, SPIE, OSA, and MRS and is the recipient of the 1999 Charles Duncan Award for Outstanding Academic Achievement (Rice), the 2013 Willis E. Lamb Award for Laser Science and Quantum Optics, the 2014 Frank Isakson Prize for Optical Effects in Solids, the 2015 R. W. Wood Prize for Optics, the 2019 Hershel M. Rich Invention Award (Rice), the Hans Fischer Senior Fellowship in 2022-2025, and the 2022 Eni Energy Transition Prize. He has published more than 350 refereed articles, given more than 400 invited presentations at international conferences and workshops, has been cited more than 60,000 times with a Web of Science h-index above 130, and has been a Thomson-Reuters Highly Cited Researcher in Physics, Chemistry, or Materials Science since 2013.

DYNAMIC ELECTROCHEMICAL PHENOMENA AT THE MESOSCALE



William Chueh

Stanford University, Stanford, CA, USA

ABSTRACT

Classically, the electrode-electrolyte interface is considered the heart of electrochemistry. More recently, the use of electrochemistry to drive bulk ion insertion (e.g., Li) has powered the battery revolution. As such, electrochemical ion insertion is also extensively studied as a bulk phenomena, which also has applications in advanced computing (e.g., ionic memory devices) and dynamic tuning of functional materials (e.g., electrochromics). Bridging the length-scale gap between interfaces and bulk is the fascinating mesoscale (tens to hundreds of nanometers). It is an under-investigated length scale in electrochemistry, yet it is the length of particles, the building block of porous electrodes. In this talk, I will provide an overview of emergent electrochemical phenomena at the mesoscale, focusing on how lithium intercalation take place in a many-particle ensemble. Breakthroughs in operando microscopy techniques have led to unexpected observations such as mosaic inter-particle phase separation, metastable solid-solution and fictitious phase separation. These behaviors can be rationalized by carefully considering the competition between bulk and interfacial free energy, as well as between reaction and diffusion kinetics. With these fundamental insights at hand, we can finally explain mesoscale phenomena in terms of fundamental thermodynamics and kinetics rather than in terms of unexplained heterogeneities, providing practical design rules on engineering more uniform electrochemical devices.

BIO - CHUEH

Will Chueh is an Associate Professor in the Department of Materials Science and Engineering, a Senior Fellow of the Precourt Institute for Energy at Stanford University, and a faculty scientist at SLAC National Accelerator Laboratory. He leads a group of more than thirty researchers tackling the challenge of decarbonizing various energy transformation pathways, and co-directs Stanford's StorageX Initiative that builds academic-industrial partnerships to accelerate the electrification of transportation and the penetration of intermittent renewable electricity in energy systems. He received his BS in applied physics, and his MS and PhD in materials science from Caltech. Prior to joining Stanford in 2012, he was a Distinguished Truman Fellow at Sandia National Laboratories. Chueh has received numerous honors, including the MRS Outstanding Young Investigator Award (2018), Volkswagen/BASF Science Award Electrochemistry (2016), Camille Dreyfus Teacher-Scholar Award (2016), Sloan Research Fellowship (2016), NSF CAREER Award (2015), Solid State Ionics Young Scientist Award (2013), Caltech Demetriades-Tsafka-Kokkalis Prize in Energy (2012), and the American Ceramics Society Diamond Award (2008). In 2012, he was named as one of the "Top 35 Innovators Under the Age of 35" by MIT's Technology Review.

PHOTOACTIVE AND FLUORESCENT MOLECULAR TOOLS WITH APPLICATIONS SPANNING BIOLOGY AND DATA STORAGE



Emilie Genin

Université de Bordeaux, France

ABSTRACT

The use of light as an external stimulus is particularly attractive for many applications in biology and in materials science. Thus, fluorescent or photoactive molecular systems are very popular in these fields. In this context, we have implemented the organic synthesis of fluorescent molecules and their grafting onto surfaces to design systems used either for the detection of molecules of therapeutic interest (neurotransmitters, sugars) or as theranostics tools as well as platforms allowing the oriented covalent immobilization of biomolecules with direct visualization of the process. A complementary research project deals with the synthesis of photoresponsive NLO switches and their immobilization on surfaces for applications in data storage.

BIO

Dr. Emilie Genin (ORCID: 0000-0002-5536-1933) studied at the Ecole Normale Supérieure in Paris and obtained her PhD (awarded by the French Chemical Society – Sigma-Aldrich prize) at the Ecole Nationale Supérieure de Chimie in Paris in 2006, working on organic synthesis and metal catalyzed reactions dedicated to green chemistry. During her post-doctoral internship at CEA Saclay, she was then involved in an interdisciplinary project at the interface between organic synthesis, luminescent nanomaterials (QDs) and biology. She is currently Associate Professor at the University of Bordeaux and is member of the Institute of Molecular Sciences. Since 2007, she has participated in several interdisciplinary and international research projects and has gained a strong expertise spanning multi-step organic synthesis (of chromophores, peptides, etc.) and the functionalization / elaboration of (nano) materials. She previously coordinated five research projects and participated in several other national and European projects. She is a co-author of about fifty publications and has been an expert for several committees. Her research activities are centered on the development of photoactive and fluorescent molecular systems for applications in biology and materials sciences.

PARALLEL SYNTHESIS, CHARACTERIZATION, AND MACHINE LEARNING YIELDS EFFICIENT POLYMER VEHICLES FOR CRISPR GENE EDITING AND PLASMID DNA PAYLOADS



Theresa M. Reineke

University of Minnesota, Minneapolis, MN, USA

ABSTRACT

The field of nucleic acid therapeutics, which aims to treat patients by modulating gene expression, has come to fruition, and has landed several landmark FDA approvals. Cationic polymers are tailorable alternatives to engineered lipids and viruses for the delivery of nucleic acid payloads. The clinical translation of chemical vehicles hinges on facile exploration of the broad chemical design space and deriving structure-function relationships governing performance with diverse payloads and cell types, which can significantly alter performance. In this work, we demonstrate a parallel workflow coupled with machine learning to discover successful candidates for delivering Cas9 ribonucleoprotein (RNP), plasmid (pDNA) and combination payloads. A diverse library of copolymers have been synthesized via ROMP and RAFT polymerization methods offering systematic variations in physicochemical properties and trends for encapsulating RNP and pDNA payloads. This multiparametric polymer library was then examined in parallel through a variety of physical and biological characterization techniques. This workflow allowed rapid discovery of successful architectures that outperform commercial reagents, achieving nearly 60% editing efficiency via non-homologous end-joining as well as similar pDNA delivery efficiency. Structure-function correlations underlying cellular internalization, editing efficiency, gene expression, and cellular toxicity of the polymer-payload formulations were probed through machine learning approaches. This allowed us to uncover the physicochemical basis of delivery performance, offering discovery of divergent requirements for successful delivery of RNP and plasmid payloads. This work demonstrates that combinatorial synthesis and high-throughput characterization methodologies coupled with data science approaches enables the rapid discovery polymeric vehicle structures-property relationships and promising formulations that would have otherwise remained inaccessible to chemical intuition.

BIO - REINEKE

Theresa M. Reineke is the Prager Chair in Macromolecular Science and Distinguished McKnight University Professor in the Department of Chemistry at The University of Minnesota. She also holds graduate faculty appointments in the Departments of Chemical Engineering/Materials Science and Pharmaceuticals. She received a B.S. Degree from the University of Wisconsin-Eau Claire, a M.S. Degree from Arizona State University, and a Ph.D. from The University of Michigan. She then received a National Institutes of Health Postdoctoral Fellowship to further her research background at the California Institute of Technology prior to beginning her independent faculty career. Her research group is focused on enabling fundamental and applied technology advancements of polymers in the fields of gene therapy and genome editing, drug delivery, and sustainability. She has published over 170 peer-reviewed manuscripts, has numerous patents, and manages a large group of researchers funded by several corporate, private foundation, and national funding agency grants. Reineke has received several awards, including the 2009 National Institutes of Health Director's New Innovator Award, 2012 Outstanding New Investigator Award from the American Society of Gene and Cell Therapy, 2017 Carl S. Marvel Creative Polymer Chemistry Award from the American Chemical Society Division of Polymer Chemistry, 2018 was awarded the DuPont Nutrition and Health Sciences Excellence Medal, and most recently the 2022 Arthur C. Cope Scholar Award from the American Chemical Society. She has also served as Associate Editor of ACS MacroLetters and Chemical Science and in 2023 became Editor-in Chief of Bioconjugate Chemistry. She also currently serves on the Editorial Advisory Boards of the peer-reviewed journals Biomacromolecules, Bioconjugate Chemistry, Polymer Chemistry, and ACS Applied Polymer Materials.

Conférences invitées / Invited lectures

ORGANOSILICON COATINGS MADE BY A COLD PLASMA PROCESSES AT ATMOSPHERIC PRESSURE FOR ELECTROCHEMICAL APPLICATIONS

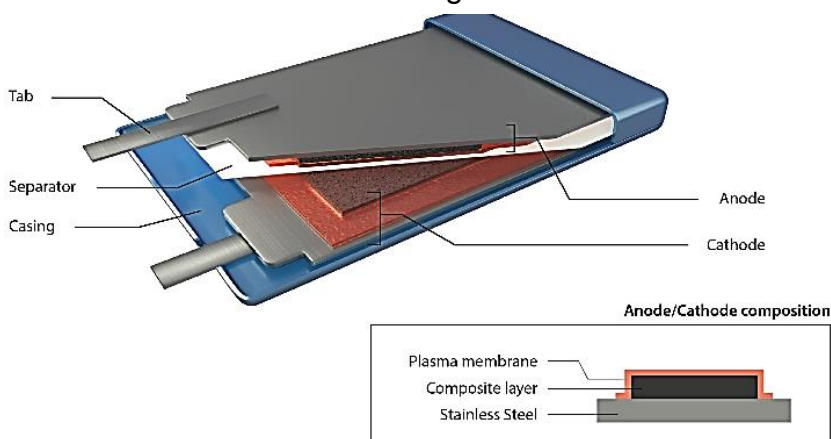


Jacopo Profili

Université Laval, Québec, QC, Canada

ABSTRACT

Cell manufacturing is estimated to account for up to 40% of battery-industry and the related market will grow 14.1% in the next five years (108.4 B\$ in 2019). In this context, high-power and stationary large-scale energy storage systems, such as lithium-ion batteries (LiBs), will be essential to make electricity quickly accessible to the power grid. This is particularly true when it comes to power plants located in remote areas or the use of renewable energy sources. Despite their advantages, commercial LiBs are today limited by their environmental and safety hazards. These limitations lead researchers around the world to discover and employ new technologies for safe recycling operations and a better control of the cycling processes. Currently, works are focused on the development of new advanced materials, composite design as well as advanced interfacial layers. In this context, surface modification by cold plasma is one of the most promising solutions to control and modify charge transport mechanisms at the interfaces. Although, the synthesis of nano-layers made by plasma at atmospheric pressure has already received a lot of interest, their use to modify electrochemical devices, such as electrochemical cells remain limited. In this work, the synthesis of organosilicon coatings on composite conductive layers by atmospheric pressure DBD is studied in detail. The influence of different organosilicon molecules has been analyzed to highlight the effect of the growth mode as well as chemical functionalities on the operation of the final electrochemical device. The physical and chemical modifications of plasma on the conductive layer as well as the water stability of the coatings were investigated by ATR-FTIR, XRD, SEM and contact angle.



BIO - PROFILI

Jacopo Profili is a young international researcher working and combining three topics: nanomaterials, environment and plasma.

His main goal is to develop new materials for energy technologies and sustainable applications, by using alternative advanced plasma processes with minimal impact on the environment.

His academic career has helped him build an international network of researchers known for their expertise in plasma, and also from industry, specifically relating to the industrial supply chain related to his research.

Profili is also founder of KALEGO, a company specialising in the creation of highly innovative surfaces from applying plasma to atmospheric pressure. Co-inventor of an anti-fog process for medical endoscopy, he has spent 10 years in the academic domain. Today, he is responsible for aspects related to innovation and technology for his company.

Versatile and trilingual, Profili has been able to execute numerous international industrial research projects. With a strong will to give back to the community, Profili founded in 2022 the Collectif des entrepreneur(e)s scientifiques et innovant(e)s du Québec (CESIQc). This non-profit organization has the mission to represent scientific entrepreneurs to facilitate development, commercialisation and the adoption of innovations. His energy and dynamism are part of the fabric he brings to his undertakings on a daily basis.

ELECTROCHEMICAL DNA-BASED BIOSENSORS FOR MOLECULAR MONITORING IN COMPLEX MATRICES AND IN THE BODY



Philippe Dauphin-Ducharme

Université de Sherbrooke, Sherbrooke, QC, Canada

ABSTRACT

Achieving continuous, real-time monitoring of a wide range of molecules directly in finger-pricked sized volumes of undiluted whole blood or directly in the living body would represent a significant feat in solving the paradigm of personalized medicine. At the moment, only two molecules can be monitored in this fashion: glucose and oxygen, thanks to the commercialization of the glucometer and the pulse oximeter. This limited offering of technologies ultimately impacts how we deliver and prescribe therapeutics to patients.

Motivated by this goal, we are developing electrochemical DNA-based biosensors. Our biosensors are comprised of a DNA strand modified with a redox active host (i.e., cyclobis(paraquat-p-phenylene)) or a redox reporter (i.e., methylene blue) attached directly on gold electrodes coated with a self-assembled monolayer of alkanethiols. Upon binding to the molecular target, because these biosensors rely on a biology-inspired principle (i.e., conformational rearrangement) and an electrochemical signaling mechanism, they readily deploy in undiluted whole blood or saliva. Due to the rapid binding kinetics, they also afford continuous real-time monitoring, a property we show by threading these biosensors in catheters for molecular measurements in the body.

All these advances in developing electrochemical DNA-based biosensors are aimed toward developing new analytical tools for personalized medicine to improve our understanding of drug pharmacokinetics.

BIO – DAUPHIN-DUCHARME

Dr. Philippe Dauphin-Ducharme a complété son baccalauréat en chimie à l'Université de Montréal. Par la suite, il entreprend un doctorat en chimie des matériaux à l'université McGill sous la supervision du Prof. Janine Mauzeroll où il se spécialisera dans le développement de techniques de microscopie électrochimiques à balayage afin de suivre la corrosion d'alliages légers envisagés pour réduire le poids de véhicules. Grâce à une collaboration avec la Prof. Hanadi Sleiman sur un projet d'électrochimie de l'ADN, il décide de poursuivre au post-doctorat à l'University of California at Santa Barbara sous la supervision de Prof. Kevin Plaxco, où il participera au développement de nouveaux biocapteurs électrochimiques à base d'ADN. Embauché en tant que professeur adjoint en janvier 2020, Dr. Dauphin-Ducharme a récemment démarré son groupe de recherche indépendant à l'Université de Sherbrooke au sein du département de chimie. Son groupe se spécialise sur le développement de nouveaux biocapteurs électrochimiques, incluant ceux fabriqués à base d'ADN afin de faire le suivi en continu de molécules directement dans des matrices complexes ou dans le corps.

SOLAR FUELS – FROM FICTION TO REALITY



Mihaela Cibian

Université du Québec à Trois-Rivières, Trois-Rivières, QC, Canada

ABSTRACT

Solar fuels as products of artificial photosynthesis (AP) systems is discussed. Based on the operating principles of natural photosynthesis, AP is defined in the large sense of converting solar energy into chemical energy stored in chemical bonds (e.g., producing hydrogen – as green fuel, from water; producing value-added chemicals from carbon dioxide (CO₂) and water) by using sunlight, light harvesters and catalysts.^[1] The field of AP has evolved from the study of isolated components to systems integration and devices. However, despite important advances, AP systems are still at the prototype level and more basic research is needed, in order to adequately tune the numerous parameters involved in complete solar-to-fuel systems.^[1-4]

Herein, an overview of the evolution of the AP solar fuel field is presented, with emphasis on the successes and the milestones achieved as well as the perspectives and the challenges to come. The role of AP solar fuels in the energy transition is also discussed.

[1] Faraday Discuss. 2019, 215; [2] Reisner et al., Chem. Rev. 2019, 119, 2752; [3] Sun et al., Chem. Soc. Rev. 2019, 48, 2216; [4] Segev et al., J. Phys. D: Appl. Phys. 2022, 55, 323003.

BIO

Mihaela CIBIAN obtained her PhD in Chemistry (Inorganic/ Coordination Chemistry) from Université de Montréal (2016). She continued her research career as a FRQNT postdoctoral fellow at Kyushu University in Japan (2017-2019), working on projects related to photocatalytic systems for carbon dioxide reduction and hydrogen production. From 2019, Mihaela CIBIAN is Assistant Professor at the Department of Chemistry, Biochemistry and Physics at l'Université du Québec à Trois-Rivières (UQTR) and a researcher at the Hydrogen Research Institute (HRI). Her field of interest is artificial photosynthesis with focus on solar fuels.

EXPERIMENTAL INVESTIGATION OF THE MULTI-SCALE MECHANICS OF ULTRATHIN FILMS AND MECHANICS-GUIDED ASSEMBLY OF FUNCTIONAL STRUCTURES



Changhong Cao

McGill University, Montréal, QC, Canada

ABSTRACT

Continued advances in engineering technologies with increased complexity, enhanced performance and new capabilities, demand novel material systems with unprecedented properties as well as novel manufacturing approaches to accelerate the transfer of lab-scale inventions to the marketplace. Advanced materials, such as nanotubes and nanofilms, were demonstrated to be promising candidates for various applications including energy storage, electronics and transportation vehicles. Before advanced materials-based inventions can be widely applied to everyday life, their mechanical stability needs to be investigated, validated and engineered because it determines their long-term viability in all their applications. Also, by understanding the mechanical behaviors of advanced materials, novel material systems with tailored mechanical properties can be rationally designed for targeted applications. In this talk, I will use graphene oxide as a representative material to showcase the experimental explorations of its multiscale mechanical behaviors from sub-nanometer scale to microscale as well as development of printing technologies for the assembly of functional structures.

BIO

Dr. Changhong Cao is an Assistant Professor in the Department of Mechanical Engineering at McGill University. He received his Ph.D. in Mechanical Engineering from the University of Toronto and worked as a postdoctoral fellow in the Department of Mechanical Engineering at MIT before joining McGill. His current main research interests include the development of novel printing technologies (2D and 3D), synthesis and multi-scale characterizations of low-dimensional materials and their composites, MEMS development for multi-physics studies of thin films, as well as mechano-electrochemical studies of energy materials.

PHOTOCATALYSTS FOR CO₂ CONVERSION



Nhat Truong Nguyen

Concordia University, Montréal, QC, Canada

ABSTRACT

Developing catalysts for the CO₂ conversion processes is critical to a sustainable future. In particular, photocatalysts operated under solar light irradiation have attracted significant attention due to their ability to use renewable energy. Herein, we develop a ternary heterostructured catalyst based on titanium nitride, titanium oxide, and indium oxide for improved photocatalytic reverse water gas shift reaction performance. It was found that the order of the individual constituent plays a vital role in the catalytic activity. Specifically, TiN – a metallic material – can effectively absorb a broad spectrum of sunlight and provide a photothermal driving force for the reaction. Simultaneously, the TiO₂ intermediate layer supplies photogenerated electrons and holes transferred to the active sites on indium oxide nanoparticles where the reaction occurs. The ternary catalyst exhibits a conversion rate outperforming that of its individual components or any binary compositions.

BIO

Nhat Truong Nguyen is an assistant professor at the Department of Chemical and Materials Engineering, Concordia University, Canada. He received his Ph.D. degree in Materials Engineering at the University of Erlangen-Nuremberg under the supervision of Prof. Patrik Schmuki in 2017. Prior to joining Concordia University, he was a postdoctoral researcher at the University of Toronto with Prof. Geoffrey Ozin. Nguyen's research group is focused on the design of advanced catalysts for renewable energy applications.

DESIGNING DEFECTS AND DISORDER IN ENERGY MATERIALS



Kulbir Kaur Ghuman

Institut national de la recherche (INRS), Varennes, QC, Canada

ABSTRACT

Addressing climate change is one of the most daunting challenges that humanity faces in this century. This significant challenge faced by our global society could be solved if we can find sustainable, efficient, and affordable materials required for clean energy technologies. The functionality of the materials used for energy applications is critically determined by the physical properties of small active regions such as dopants, dislocations, interfaces, grain boundaries, etc. The capability to manipulate and utilize the inevitable disorder in materials, whether due to the finite-dimensional defects (such as vacancies, dopants, grain boundaries) or due to the complete atomic randomness (as in amorphous materials), can bring innovation in designing energy materials. With the increase in computational material science capabilities, it is now possible to understand the complexity present in materials due to various defects resulting in pathways required for optimizing their efficiencies. In this talk, I will provide a critical overview of such computational advancements specifically for designing realistic materials with various types of defects. I will discuss the traditional approaches (implemented via tools such as density functional theory, and molecular dynamics) as well as modern approaches such as machine learning that exist for understanding the impact of defects and disorder present in polycrystalline materials, thereby identifying the future opportunities for energy materials design and discovery.

BIO

Kulbir Kaur Ghuman is an early-career researcher, recently appointed as Assistant Professor at Institut national de la recherche scientifique, Centre Énergie Matériaux Télécommunications (INRS-EMT) and a Tier-2 Canada Research Chair in 'Computational Materials Design for Energy and Environmental Applications'. Before joining INRS-EMT she worked as a postdoctoral fellow at University of Toronto (2013-2016) and Kyushu University, Japan (2017-2019). Her current laboratory, Insilico Matters Laboratory (IML), is equipped with advanced software and computational infrastructure, dedicated to understanding the theoretical underpinnings of the behaviour of complex materials and chemical reactions. She has established several novel structure-property relationships and mechanisms for optimizing fuel cell materials and designing efficient catalysts imperative for mitigating climate change. Currently, she is also spearheading a recently established consortium 'Computational Energy Materials Design Infrastructure (CEMDI)' at INRS-EMT that aspires to foster innovation in the area of energy materials research via collaboration and advanced computational techniques.

Ateliers / Workshops

ACCUEIL ET INCLUSION DES ÉTUDIANTS INTERNATIONAUX; UNE RESPONSABILITÉ PARTAGÉE



Suzie Yeo

Autrement d'ici, QC, Canada

RÉSUMÉ

- 1) La charge mentale de l'étudiant international et son impact sur l'adaptation et la réussite des études ;
- 2) Comprendre le processus d'adaptation, le choc culturel et les zones sensibles de la rencontre entre les cultures.
- 3) La responsabilité du milieu dans l'accompagnement des étudiants internationaux; un premier pas ;
- 4) Savoir reconnaître les symptômes du choc culturel et proposer les stratégies adéquates pour soutenir les étudiants.

BIO

Depuis son enfance, Suzie Yeo est animée par les questions d'inclusion et de diversité. Toute jeune, elle voulait déjà contribuer à créer plus de solidarité et de justice pour les personnes issues de groupes sous représentés.

Véritable passionnée des relations humaines, elle cumule plusieurs diplômes universitaires dans les domaines des sciences de l'éducation, de la formation des adultes en milieu de travail, de la coopération interculturelle, de l'intervention psychosociale et de l'intervention en milieu multiethnique. Ayant à cœur le rapprochement culturel et de saines relations en milieu diversifié, elle a fondé « [Autrement d'ici](#) », dont la mission est de développer les compétences interculturelles de professionnel·le·s et de citoyen·ne·s québécois·es de secteurs variés. Suzie est non seulement poussée par une vision inclusive du monde de demain en dirigeant Autrement d'ici, mais elle s'implique également au sein de sa collectivité afin de susciter la réflexion et l'ouverture envers les personnes issues de la diversité ethnoculturelle et des Premières Nations. Elle a également enseigné en milieu universitaire la communication interculturelle. Suzie est définitivement une entrepreneure sociale axée sur le changement, l'espoir et les dynamiques humaines positives!

BEYOND THE CV



Gad Sabbatier

2nd Lab, Axelys, Québec, QC, Canada

ABSTRACT

Understand recruitment and build an application package to an impactful employment
The CV is the key to the job interview, however, as any key, a CV opens only one door. So, it is necessary to understand job market players and the recruitment process in putting ourselves in the recruiter's shoes; understand their jargon, their challenges, and constraints. During this workshop, participants will think about CV building tactics that think outside the box. Participants will be able to elaborate and adjust their nonacademic CV to pique the curiosity of employers and construct a successful application that will open the doors outside academia. Goal: Build a successful application

BIO

Gad Sabbatier obtained a PhD in a joint-PhD program in materials and metallurgy engineering from Université Laval and in mechanical engineering from the University of Haute-Alsace in 2015 in the field of biomaterials. Gad then worked as a researcher at Queen's University and then at McGill University in collaborative research contracts with companies. He then joined SOVAR and Axelys, an organization for the development and innovation transfer from Quebec's public research institutions. With a Certificate in Educational Leadership from Queen's University, Gad is an outstanding trainer with 15 years of experience. He has a keen understanding of the challenges of transitioning from academia to non-academic careers through his personal experience, his position as co-founder of the 2nd lab, and for having mentored 80+ graduate students and post-doctoral researchers to impact careers for society.

Séances thématiques / parallel sessions

BIO-BASED BARRIER COATING MATERIALS FOR PACKAGING PAPER

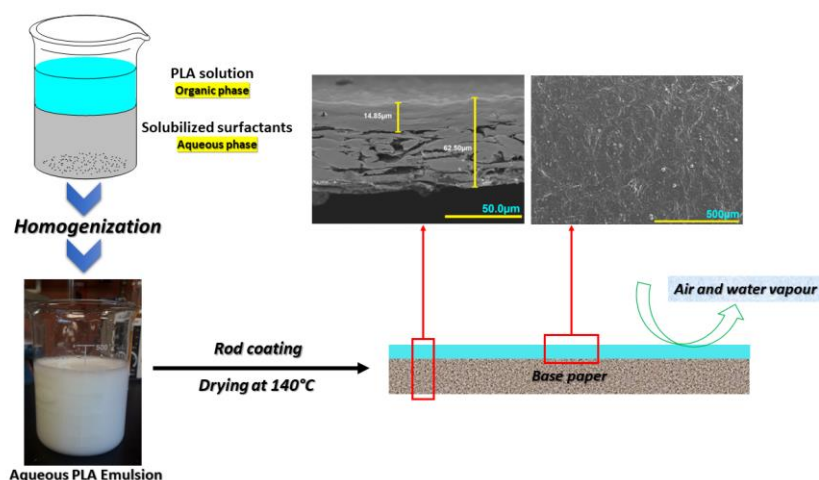
Abdenour CHENNI¹., Bruno CHABOT²., Simon BARNABÉ²., Julien BLEY³., Phuong NGUYEN-TRI¹

- 1- Laboratory of Advanced Materials for Energy and Environment, Université du Québec à Trois-Rivières, 3351 boul. des Forges, C.P. 500, Trois-Rivières, QC G9A 5H7, Canada.
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ABSTRACT

THERE HAS BEEN A GROWING CURIOSITY IN USING SUSTAINABLE AND NATURALLY DEGRADABLE MATERIALS AS AN ALTERNATIVE TO NON-RENEWABLE SUBSTANCES, MOSTLY IN THE FIELD OF PACKAGING MATERIALS. THESE MATERIALS SHOULD IDEALLY COME FROM RENEWABLE RESOURCES. THIS WORK DISCUSSES THE DEVELOPMENT OF NEW STABLE WATER-BASED POLYLACTIC ACID (PLA) EMULSIONS WITH A HIGH-WATER CONTENT THAT WAS SUCCESSFULLY PREPARED USING TWO FOOD-GRADE SURFACTANTS COMBINED WITH HIGH-SHEAR MECHANICAL MIXING AND ULTRASONIC TREATMENT. PLA PARTICLE SIZES WERE FOUND TO BE VARIED FROM MICROMETRIC TO NANOMETRIC FOR STABLE EMULSIONS DEPENDING ON THE PREPARATION CONDITIONS, AS CONFIRMED BY DIGITAL MICROSCOPIES AND DYNAMIC LIGHT SCATTERING (DLS) ANALYSIS. IN ORDER TO APPLY THE PREPARED EMULSIONS AS COATINGS ON PAPER, XANTHAN GUM (XG) WAS USED AS A FOOD-GRADE THICKENING AGENT TO REGULATE THE APPARENT VISCOSITY. THICKENED PLA EMULSIONS WITH DIFFERENT AMOUNTS OF XANTHAN GUM (XG) HAVE BEEN SHOWN TO DISPLAY A SHEAR-THINNING BEHAVIOR IN THE WHOLE INVESTIGATED CONCENTRATIONS UP TO 2 (WT.%) UNDER CONTROLLED SHEAR CONDITIONS, WITH APPARENT VISCOSITY VALUES DEPENDENT ON XG CONCENTRATIONS. THE BARRIER PROPERTIES OF PLA-COATED PAPER SHOWED THAT THE BASE PAPER'S BARRIER PROPERTIES WERE SIGNIFICANTLY INCREASED WITH THE INCREASE IN PLA COATING THICKNESS. THE DATA FROM AIR AND WATER VAPOUR PERMEABILITY ANALYSIS REVEALED THAT OUR PLA COATING IN WEIGHTS RANGING FROM 10 TO 15 (G/M²) IS SUITABLE TO OBTAIN SUPERIOR OVERALL BARRIER PROPERTIES COMBINED WITH A SMOOTH SURFACE THAT IS ESSENTIALLY NEEDED FOR THE FABRICATION OF COATED PAPER PRODUCTS IN THE PAPER INDUSTRY.



A PROMISING NEW OPTICAL NANOPROBE FOR CELLULAR IMAGING: AMINE PASSIVATED FLUORESCENT CARBON DOTS

ADRYANNE CLERMONT-PAQUETTE

Adryanne Clermont-Paquette ^{1,2,3}, Alisa Piekny ³, Rafik Naccache ^{1,2}

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YOUR ABSTRACT / VOTRE RÉSUMÉ

Carbon dots (CDs) have garnered significant attention in the past decade owing to their fascinating luminescent properties and potential use in cell and tissue imaging, as well as for the study of biological processes. These quasi-spherical amorphous carbon-based nanomaterials can be tailored to emit light from the UV-NIR regions of the spectrum while offering low cytotoxicity and good biocompatibility. These properties then influence their cellular uptake, cytotoxicity, and sub-cellular localization. The physico-optical and -chemical properties of CDs are determined by the precursors, methods of preparation, and reaction conditions.

In this work, CDs synthesized from citric acid and five different amine passivating agents were characterized to reveal their properties, and determine how these properties affect their uptake and localization in cultured human cells (HFF-1; human male foreskin fibroblasts, and HeLa; human female cervical carcinoma). All CDs exhibited fluorescence with a corresponding max λ_{ex} at 350 nm and max λ_{em} at 450 nm. We found that these quasi-spherical amine passivated CDs ranged in size from 1.3 to 2.7 nm, and had similar functional groups such as carboxyl, amines and amides. There was an increase in surface charge from -21 mv to +8 mv that correlated with the increase in amine passivation. All of the CDs had low cytotoxicity in both HFF-1 and HeLa cells, with an increase in uptake that correlated with an increase in their surface charge. While all of the CDs localized to the lysosomes, suggesting entry and trafficking via the endomembrane system, there was a difference in their enrichment; some (with the most amine-passivation) most strongly co-localized with lysosomes in both cell lines. Interestingly, CDs with amphiphilic properties also localized in the cytosol likely due to passive uptake. These findings indicate that CDs could be designed to have diverse optical properties and subcellular localization, which could be explored for applications as bioimaging nanotools, and delivery agents.

PRINTED FLEXIBLE HYDROGEN SULFIDE GAS SENSOR: AN INNOVATIVE APPROACH FOR SMART SUPPLY CHAIN AND CIRCULAR ECONOMY IN THE MEAT INDUSTRY

Al Shboul, Ahmad

Ahmad Al Shboul, Ricardo Izquierdo

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The food industry is facing a significant challenge in reducing meat waste, as households in Canada alone discard 138,000 tonnes of meat annually, accounting for 6% of all food waste and 45% of the meat supply chain. Meat freshness indicators/sensors can detect accurately meat freshness, reducing meat waste. This approach helps determine the actual expiry date, which prevents reaching the meat spoilage level. Moreover, the use of these indicators can lead to a circular economy by re-produce meat into ready-to-eat products or converting meat waste to valuable products such as biofuels and animal feed. Incorporating freshness indicators in packaging empowers meat managers/consumers to make informed decisions about meat products, improving supply chain management efficiency, or the "smart supply chain."

Hydrogen sulfide gas sensors with unique properties have emerged as a promising solution to detect accurately and efficiently the freshness of meat. We have developed a new generation of printed and flexible hydrogen sulfide sensors, using indium oxide-based nanocomposites¹⁻³. Our innovative fabrication technique involves the simple blending of sensor components and a low drying temperature, eliminating the need for costly and time-consuming processes. Our work highlights the sensor components' significance in manipulating sensor performance, anti-humidity properties, and sensing mechanisms.

Our proposed sensor has exceptional sensing performance, detecting low H₂S concentrations below 100 ppb at ambient conditions and a high anti-humidity property up to relative humidity (RH) 100%, enabling them to retain sensitivity to H₂S in moist environments. Moreover, these sensors possess exceptional chemical and mechanical durability in harsh environments that simulate storage conditions. Moreover, our sensors demonstrated an excellent response to determining meat freshness when tested with various types of meat products to ensure their performance. Given these compelling qualities and low cost, the sensors have the potential for meat packaging applications.

(1) Al Shboul, A. M.; Ketabi, M.; Mechael, S. S.; Nyayachavadi, A.; Rondeau-Gagné, S.; Izquierdo, R. Hydrogen Sulfide Gas Detection in Ppb Levels at Room Temperature with a Printed, Flexible, Disposable In 2 O 3 NPs-Based Sensor for IoT Food Packaging Applications. *Adv. Mater. Technol.* **2023**, 8 (2), 2201086. <https://doi.org/10.1002/admt.202201086>.

(2) Al Shboul, A.; Shih, A.; Izquierdo, R. A Flexible Indium Oxide Sensor With Anti-Humidity Property for Room Temperature Detection of Hydrogen Sulfide. *IEEE Sens. J.* **2021**, 21 (8), 9667–9674. <https://doi.org/10.1109/JSEN.2020.3010843>.

(3) Al Shboul, A. M.; Izquierdo, R. Printed Chemiresistive In 2 O 3 Nanoparticle-Based Sensors with Ppb Detection of H 2 S Gas for Food Packaging. *ACS Appl. Nano Mater.* **2021**, 4 (9), 9508–9517. <https://doi.org/10.1021/acsanm.1c01970>.

Non-destructive characterization of Ge buried structure for Porous Lift-Off

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Abstract

Single-crystal Ge membranes have recently received increasing interest for various applications, including lightweight and flexible optoelectronics and photovoltaics. Multiple methods for the fabrication of detachable single-crystal membranes have already been proposed in the literature. One of the recently reported successful methods is porous lift-off, which consists of the epitaxial growth of a Ge membrane on a bipolar electrochemically etched porous Ge layer. The thermal budget induces the formation of a separation layer containing pillars that connect the Ge membrane to the parent substrate (**Fig 1**), allowing for detachment of the epitaxial membrane and reuse of the substrate for multiple cycles. However, many challenges need to be overcome, such as the evolution of the separation layer's morphology and how to non-destructively characterize it. In this work, we report on a non-destructive characterization method by Scanning Electron Microscopy (SEM) to study the morphological transformation of the separation layer. We show that in specific conditions, it is possible to sample the pillars through an epitaxial layer by recording backscattered electrons images. Using this strategy we investigate the morphology of the buried pillars, their size and size distribution (**Fig 2.a-c**). The correlation of the SEM images before and after detachment (**Fig 2.d**) testifies to the reliability of this method and determines its limits. We discuss the advantages and the limits of this non-destructive method for characterizing the buried structure of the separation layer in the porous lift-off process.

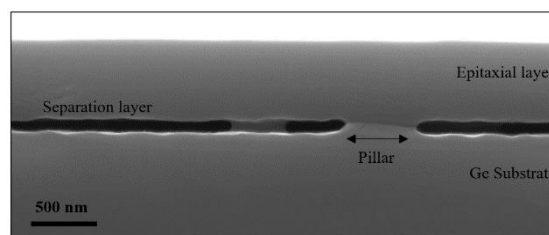


Figure 1 : Cross-section SEM images of the pillars connecting the Ge epitaxial layer to the substrate.

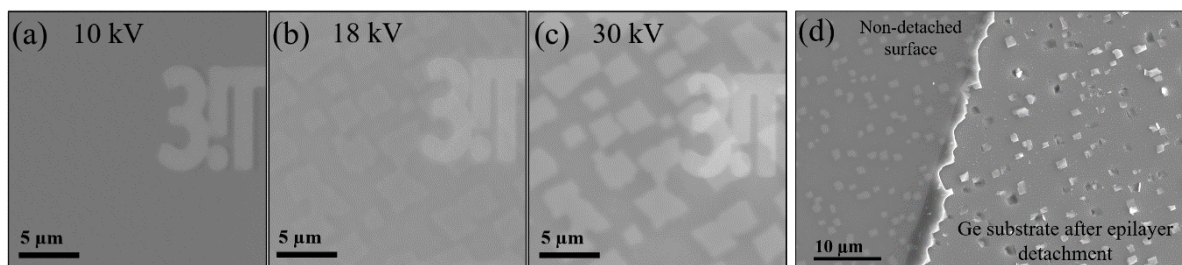


Figure 2: Top-view SEM images of pillars, a-c: non-detached epilayer with variation of beam energy, 10, 18 and 30 kV respectively. d: the interface between the detached and the non-detached surface after epilayer detachment.

LIGNIN DERIVED CATALYST FOR BIODIESEL SYNTHESIS

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Increasing dependence and overconsumption of non-renewable, pollutant-emitting fossil fuels has been declared as a primary contributor to climate change, prompting the shift to renewable energy sources. Biodiesel has emerged as a promising, more sustainable alternative energy source, primarily formed through either the transesterification of triglycerides or the esterification of free fatty acids into fatty acid methyl esters (biodiesel). However, current biodiesel production uses refined vegetable oils as feedstock which has raised concerns due to the competition with food crops and contributes a staggering 90% to the overall cost of production. Additionally, a major hurdle in the sustainability of biodiesel production is the current basic homogeneous catalysts employed react with free fatty acids in oils to produce soap, significantly contaminating the product and requiring extensive purification steps, resulting in substantial wastewater. For this reason, heterogeneous catalysts have garnered interest as more suitable alternatives. As well as being able to perform the transesterification of triglycerides, acidic catalysts also catalyse the esterification of free fatty acids present in most non-edible and waste cooking oils into biodiesel. In this study, a lignin-derived heterogeneous acid catalyst converted over 97% of oleic acid- a representative of free fatty acids- into biodiesel under optimal conditions. A basic heterogeneous catalyst was also synthesised and converted over 97% of canola oil- a representation of triglycerides- into biodiesel under optimal conditions. The combination of these catalysts can be integrated in a two-step conversion of waste-cooking oil into biodiesel. Furthermore, lignin is considered a waste by-product of the paper/pulp industry, so the upcycling of lignin into a value-added product to convert waste cooking oil offers increased sustainability as well as access to environments and economies that are limited in resources and financials.

Combinatorial Study of Systematic Aluminum Substitution into NMC Cathode Materials

Alex Hebert

Alex Hebert, Colton David, Eric McCalla

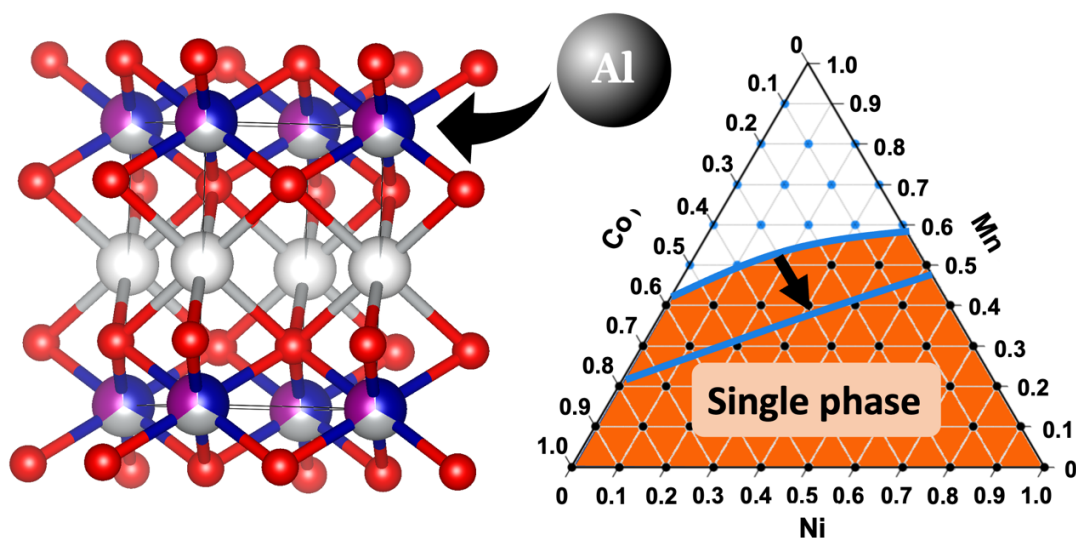
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Abstract

Li-ion batteries power our modern mobile world. They are already used in billions of devices and are powering more of our transportation every day. The cathode material of Li-ion batteries is the limiting factor in terms of battery capacity, as well as one of the culprits of battery failure. Thus, improving the cathode material is critical. The layered metal oxide $\text{LiNi}^x\text{Mn}^y\text{Co}^z\text{O}_2$ (NMC) is the current market-leader in the cathode space. Many compositions are in use with the industry pushing capacity higher with high-Ni materials. However, high-Ni compositions come at the cost of material stability, i.e., battery lifetime. To stabilize the cathode, many metals have been substituted into the material to resist material degradation. However, most studies are limited to a few key compositions of NMC. In this work, the effects of different levels of aluminum substitution are investigated by preparing and characterizing 320 different compositions using high-throughput X-ray diffraction for structural characterization and high-throughput electrochemical techniques to extract key battery metrics. This work provides insight into how accommodating different NMC compositions are to aluminum substitution and the effects of the substitutions on their electrochemistry.

FIGURE



JUST ADD SALT : RETHINKING SOLID STATE SYNTHESIS

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YOUR ABSTRACT / VOTRE RÉSUMÉ

(300 words -1page max)

The creation of rational synthetic routes to desired functional materials is a current challenge in solid state synthesis. While organic chemists have been designing and synthesizing complex molecules for over a century, a similar understanding of the synthesis of inorganic solids is still in its infancy. To create a similar understanding in inorganic solid-state chemistry, we modify the synthesis of target systems, creating a basis of rules for the design of high temperature reactions. The ideal reactions for these studies have observably different outcomes which can be attained through and tunable reaction parameters. We focus on ternary oxide systems with either energetically similar polymorphs or well understood solid solution behavior and observe differences in our final products post reaction using X-ray diffraction. To increase the tunability of our reactions, we introduce alkali and alkaline earth halide salts into the mixture, either as low concentration fluxes or as the by-products of metathesis and cometathesis reactions. These halide salts melt at relatively low temperatures and serve as a mobile phase allowing for the conduction of reactive species to complete the reaction. In addition, the presence of additional ions controls the accessible phase space of solid-state reactions, directing product selectivity. The presentation will include comprehensive work on controlling the yttrium-manganese-oxide system and introduce some of the new oxide systems which we are investigating.

Modeling Single-Atom Catalyst Sulfur Cathodes with Density Functional Theory and Machine Learning for Lithium-Sulfur Batteries

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As current batteries reach their limits, finding new battery materials is crucial. Lithium-sulfur batteries are a promising next-generation technology but face three major issues: low active material utilization, cathode pulverization, and limited polysulfide conversion leading to anode corrosion. Single-atom catalysts (SACs) deposited onto carbon-sulfur cathodes could significantly improve conductivity and cycling performance, but the large number of potential metal candidates requires computational screening using density-functional theory (DFT) modeling accelerated by machine learning (ML). ML algorithms such as random forest, support vector regression, and specialized deep learning algorithms like graph covalent neural networks are used to predict the surface-adsorption ability of metal candidates, with calculated *d*-band model features and simple material properties from open-source material databases as input data. The performance and limitations of the ML approach are then assessed against DFT results using evaluation metrics such as root mean square error and R-squared correlation. Results show that metal compounds with oxide, nitride and sulfide groups have higher adsorption values than their pure metal counterparts. Careful analysis of binding energy results, densities of states, band structures, and *d*-band characteristics of the various metal candidates provides valuable insights into the design of experimentally-viable lithium-sulfur batteries, as well as advanced interface design in the broader field of battery research.

Fabrication of high-performance MoS₂-based electric double layer transistors and study of the effect of ionic liquid anion modification on their operation

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ABSTRACT

Electrical double layer technology with ultra-high charge carrier accumulation at the semiconductor/electrolyte channel interface was creatively introduced in transistors to overcome the problem of low carrier density and high operating voltage in field-effect transistors (FETs) due to low capacitance and electrical breakdown of the gate dielectric. In the present work, electrical double-layer transistors based on molybdenum disulfide (EDLT- MoS₂) and an ionic liquid (IL) were fabricated to achieve a higher carrier density and lower operating voltage than those in the FET-MoS₂ transistor. EDLT-MoS₂ were obtained by combining a three-terminal back-gate MoS₂ FET with an ionic liquid while disabling the back-gate effect and using the ionic liquid as a top-gate dielectric. A heavily p doped silicon layer Si⁺⁺ with thermally grown 285 nm thick SiO₂ was used as substrate, while gold (Au) with chromium (adhesion layer) were used to fabricate the source and drain electrodes of the EDLT-MoS₂. Activated carbon was chosen as the gate electrode. Two different ionic liquids [EMIM][TFSI] and [EMIM][BF₄] were used as gate dielectrics in order to: obtain high performance transistors, study the IL/MoS₂ interface and identify the anion/cation pair most capable of injecting a high density of charge carriers on the surface of the molybdenum disulfide channel. The results of electrical characterizations showed that both [EMIM][TFSI] and [EMIM][BF₄] allow us to achieve a higher carrier density in the MoS₂ channel than what usually achieved by means of conventional gating with insulating oxides such as SiO₂. This allows to use our transistors at lower operating voltage. Comparing the results obtained by the two ILs, it was found that [EMIM][TFSI] achieves the highest electric double layer capacitance over [EMIM][BF₄], if one assumes that the charge carrier mobility is unchanged, as previously measured by back-gated transistors on the same device. Surprisingly, we found that the anion plays a role in the gating efficiency of our devices in spite of the fact that it is the cation that actually recalls charge carriers (electron in this case) within the FET channel. This is in agreement with theoretical predictions and modeling done by our collaborators using First-Principles Based Molecular Dynamic method (FPMD-DFT) facilitating the analysis of the obtained data and the understanding of both interfaces [EMIM][TFSI]/MoS₂ and [EMIM][BF₄]/MoS₂. Furthermore, the performances of FET gated by [EMIM][TFSI] were found to be stable over time. This work explored from a theoretical and an experimental point of view the role of the anion in an ionic liquid. This paves the way for the choice of a suitable IL for applications such as electronics or superconductivity.

UNE TRANSITION VITREUSE AU SEIN DE CHAINES UNIQUES DE POLYMERES

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Bien que connue depuis l'époque pharaonique, la transition vitreuse n'a pas encore dévoilé tous ses secrets. Elle a cette particularité de séparer deux domaines amorphes aux propriétés très différentes telles que la viscosité, le module d'Young. Le prix Nobel de physique, P.W. Anderson, décrit d'ailleurs ce phénomène comme " the deepest and most interesting unsolved problem in solid state theory "¹. Grâce à la simulation, il est à présent possible d'examiner les origines moléculaires de ce phénomène. Cependant, il est important que les systèmes simulés soient corrélés au mieux à la réalité. Une procédure spécifique est alors proposée afin d'obtenir nos systèmes d'étude à l'équilibre mécanique². Nous montrons comment l'atteinte de cet état est importante pour calculer les propriétés mécaniques et obtenir une température de transition vitreuse (T_g) reproductible. Sur la base des résultats obtenus, nous proposons que la simulation par dynamique moléculaire atomistique agisse comme une caméra ultra-rapide permettant ainsi de révéler des phénomènes qui ne peuvent être distingués autrement, et donc d'ouvrir la voie à des descriptions nouvelles de cette transition particulière et ce d'un point de vue atomistique ³. Ainsi, la transition de l'état amorphe à la phase vitreuse au sein des polymères peut être détaillée en termes de gel de degrés de liberté que sont les rotations autour des liaisons le long de la chaîne polymérique. En étudiant ces transitions conformationnelles au sein du polyéthylène, nous établissons une relation entre la dynamique locale et le diagramme classique d'énergie potentielle de l'angle dièdre autour d'une liaison carbone-carbone. Nous en déduisons un lien direct entre l'énergie d'activation et T_g ⁴. De ce fait, nous montrons le lien avec la dynamique flexible telle que décrite par de Gennes⁵. Pour présenter le lien avec la flexibilité locale, nous effectuons le lien avec le modèle RIS de Flory⁶. Cela nous permet d'appliquer ces conclusions à la chaîne unique, et d'y révéler une transition vitreuse.

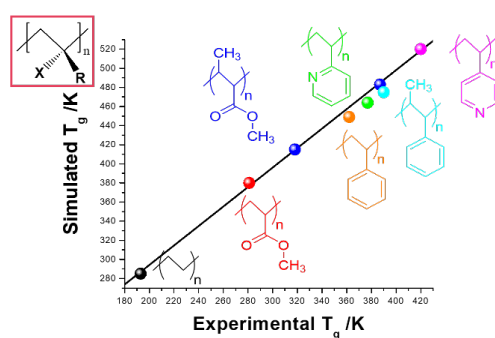


FIGURE : T_g simulées vs T_g expérimentales pour une série de polymères vinyliques

¹ P.W. Anderson, *Science* 267 (1995) 1615-1616.

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³ F Godey, A Fleury, A Ghoufi, A Soldera, *J. of Computational Chemistry* 39 (2018) 255-261.

⁴ F Godey, A Fleury, A Soldera, *Scientific Reports* 9 (2019) 1-9.

⁵ P-G. de Gennes, *Scaling Concepts in Polymer Physics*, Cornell University Press, 1979.

⁶ P Flory, *Statistical Mechanics of Chain Molecules*, Interscience Publishers, 1969.

PROCESSING/STRUCTURE RELATIONS IN INDIVIDUAL ELECTROSPUN FIBERS FOR PROPERTY OPTIMIZATION

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YOUR ABSTRACT / VOTRE RÉSUMÉ

Electrospun fibers are nanostructures formed by the solidification of an electrified jet drawn from a viscous polymer solution. They often show an exponential increase in mechanical, electrical, and optical properties at small diameters, making them promising candidates for applications in fields such as tissue engineering, selective filtration, and energy harvesting. Grasping how polymer chains orient and change conformation during electrospinning is crucial to understand the effect of processing parameters on fiber properties. Our group has developed confocal Raman microscopy methodologies to probe orientation and structure in individual fibers.

This presentation highlights the impact of three major electrospinning parameters, namely the crystallinity of the polymer, the type of collector onto which fibers are deposited, and the nature of the solvent. Raman microscopy on poly(oxymethylene) (POM) and poly(ethylene oxide) (PEO) fibers of high (~60%) and very high (~75%) crystallinity, respectively, evidenced that a higher crystallinity leads to a greater molecular orientation which is maintained over a wider range of fiber diameters (500-2800 nm).¹ PEO fibers maintained this high orientation whether they are deposited on a static collector or a collector providing additional mechanical or electric stretching. In contrast, low-crystallinity poly(ethylene terephthalate) (PET) fibers exhibited weaker orientation and, interestingly, the choice of collector strongly impacted the orientation-diameter curve and the development of the oriented mesophase.² Such variations were mainly attributed to the viscosity of the PET jet when the collector-induced stretching occurred.² Our current efforts aim to optimize this crucial strain-viscosity balance through the volatility and quality of the electrospinning solvent to reach higher orientations in low-crystallinity systems. With such studies, we hope to stimulate the larger-scale application of high-performance electrospun fibers.

1. Laramée, A. W.; Lanthier, C.; Pellerin, C. *ACS Appl. Polym. Mater.* **2020**, 2, 5025.
2. Laramée, A. W.; Lanthier, C.; Pellerin, C. *Appl. Spectrosc.* **2022**, 76, 51.

Nanostructured magnesium produced by High Pressure Torsion Extrusion for hydrogen energy storage

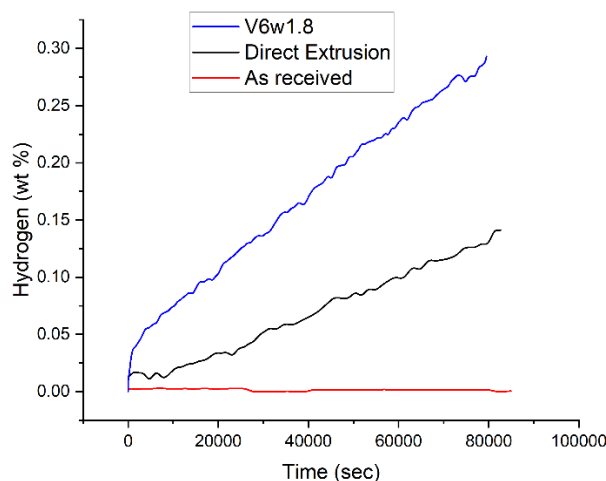
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Development of advanced materials with enhanced properties has always been a challenge for scientists to overcome the shortcoming of conventional materials for industrial applications. These efforts led to the rapid emergence of nanostructured materials with improved functional properties. Mechanical nanostructuring techniques have shown promising results in the enhancement of functional properties such as better fatigue and wear resistance, better mechanical properties, and even better performance in hydrogen energy storage for green energy applications.

This research explores the effect of a new mechanical nanostructuring technique named “High Pressure Torsion Extrusion” (HPTE) on the microstructure and hydrogen storage of magnesium. HPTE has two process parameters by which the amount of deformation can be controlled: The extrusion speed V , and the rotational speed w ; by combining these parameters, different levels of strain can be imposed on the material and therefore, different properties can be expected.

In this work, small billets of magnesium were processed by HPTE using two different process parameters: $\{v=6\text{mm/min}, w=0 \text{ (direct extrusion)}\}$, and $\{v=6\text{mm/min} \ \& \ w=1.8 \text{ rpm}\}$; then the microstructure, hardness, and kinetics of hydrogen sorption in the processed samples were studied. Results of X-ray diffraction analysis showed that the materials experienced a considerable level of microstructural refinement after HPTE. The crystallite size in magnesium reduced from the initial value of 113 nm to 85 nm in $v6w1.8$. The hardness increased after processing up to 150% of the initial values. The results of hydrogenation showed that HPTE enhanced the activation time for hydrogen absorption. The as-received material did not absorb hydrogen after one day of exposure to hydrogen gas while the synthesized specimens absorbed hydrogen up to 0.12 wt% and 0.3 wt% in the direct-extruded sample and the $v6w1.8$ sample, respectively, implying the influence of HPTE on the enhancement of hydrogen sorption in materials.



Fabrication of Monoatomic Nickel Wires Using Tribenzocyclyne Nanotubes by Self-assembly

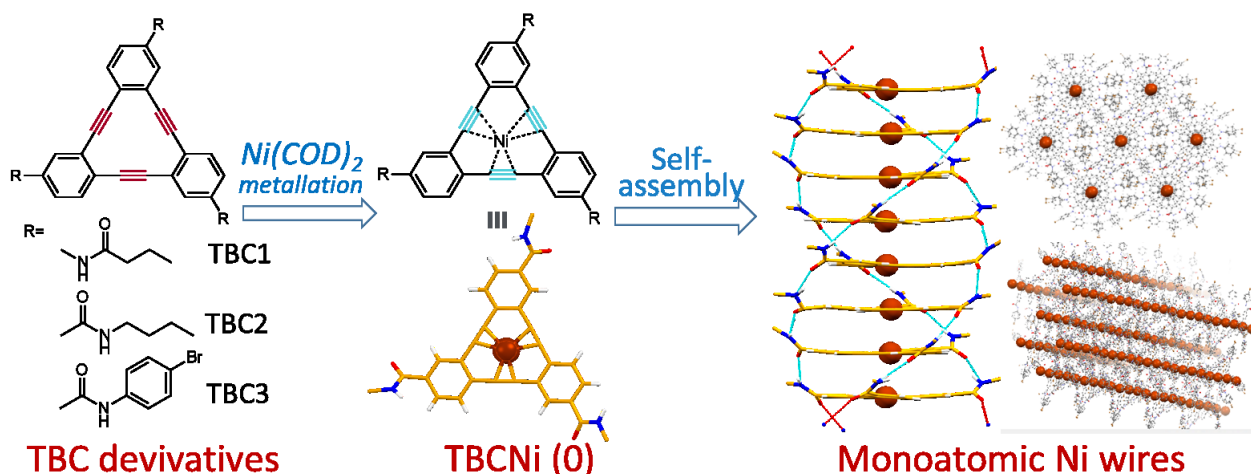
Bin Li

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Monoatomic metal wires (metal in 0 degree of oxidation) are attractive because of their promising properties such as quantum size effect. However, it is a tremendous challenge to get stable and practical amounts of these materials which hinders their studies and applications. Only a few monoatomic metal wires like Au and Pt have been constructed with inefficient expensive techniques. Here, we present a simple self-assembly method to fabricate monoatomic nickel (0) wires by using tribenzocyclyne (TBC) as template. TBC-Ni(0) complex forms a one-dimensional columnar stacking through hydrogen bonding of amide groups on the side chains of TBC, which leads to the formation of single-atom nickel wires within the nanotubes of TBC. The Ni-Ni distance are 0.33nm, 0.35nm and 0.48nm respectively which depend on the molecular distance of the columnar stacking TBC with different types of side chain. These fabricated monoatomic nickel wires will allow detailed experimental investigation of their physical properties.



Calculs des propriétés électroniques et vibrationnelles de matériaux graphène-soufre

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À l'aide de calculs utilisant la théorie de la fonctionnelle de la densité (DFT), nous avons étudié la fonctionnalisation du graphène par des atomes soufre. Nous avons tout d'abord développé différents modèles afin d'en évaluer la stabilité et nous avons déterminé les propriétés électroniques et vibrationnelles de plusieurs matériaux graphène-soufre (G-S) covalents. Les résultats de nos calculs DFT soutiennent la formation d'une liaison forte entre le soufre et le graphène. Par ailleurs, les différents modèles considérés donnent une composition chimique qui est en bon accord avec la proportion observée du rapport S/C obtenu expérimentalement suite à une réaction directe entre le graphite pyrolytique hautement orienté (HOPG) et le soufre élémentaire. De plus, des simulations de dynamique moléculaire *ab-initio* nous permettent de confirmer la stabilité des liaisons S-G à l'ambiante. Les modes vibrationnels calculés avec la DFT supportent également la signature vibrationnelle spécifique du matériau G-S observée par spectroscopie Raman.

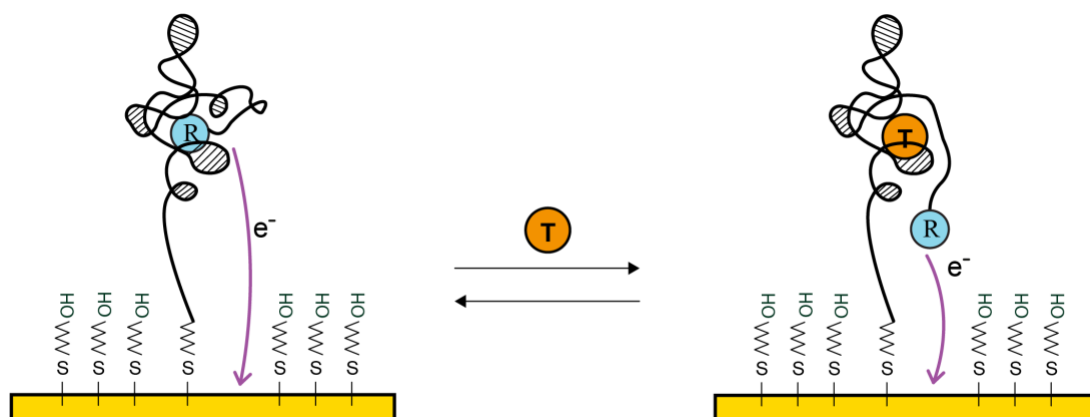
ON THE SIGNALING MECHANISM OF ELECTROCHEMICAL APTAMER BASED BIOSENSORS

Erfan Rahbarimehr

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Aptamer-based electrochemical biosensors (E-AB) have been identified as potential tools to extend the range of molecules that can be detected at the point-of-care in the context of personalized medicine. Despite the superior accuracy of electrochemical impedance spectroscopy (EIS) for interrogating E-AB sensors, the measurement of dissociation constants (K_D) using this technique for the MN4 cocaine-binding aptamer biosensor showed inconsistent results compared to solution-based isothermal titration calorimetry (ITC) upon titration with certain anti-malarial compounds. To account for these discrepancies, a novel sensing mechanism is postulated, whereby competition arises between the ligand and the redox reporter (methylene blue), which is covalently attached to the aptamer. This mechanism could be triggered by the displacement of the redox reporter from the binding site by the target molecule, or by changes in the environmental conditions that impact the redox reporter, ultimately leading to alterations in the electrochemical response of the biosensor. This proposed mechanism is anticipated to be broadly applicable to other aptamer systems, and the introduction of intercalative redox reporters with DNA binding properties could expand the dynamic range of electrochemical biosensors.



An Approach to Reduce the Environmental Footprint of Composite Electrodes for Lithium-ion Batteries with Aqueous Electrolytes

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Lithium-ion batteries are of utmost importance today due to their high energy density allowing the development of mobile applications and the storage of renewable energies. A battery is composed of a positive electrode and a negative electrode separated by an electrolyte, typically consisting of an organic solvent to transport the charge. The use of an organic electrolyte generates safety and environmental issues associated with high production costs. To overcome these problems, aqueous electrolyte lithium-ion batteries (ARLB), with a reduced environmental footprint, have been proposed in particular for stationary applications.

The electrodes, in lithium-ion batteries, are generally present in form of a composite mixture prepared using perfluorinated binders (PFAS) such as polyvinylidene difluoride (PVDF) or polytetrafluoroethylene (PTFE), also known as persistent pollutants, and toxic solvents N-methyl-2-pyrrolidone (NMP). The recent ban on the use of eternal pollutants reinforces the interest of producers to find alternative binders.

It is then necessary to turn to bio-sourced binders, renewable and ideally water-soluble binders, such as carboxymethyl cellulose (CMC), derived from wood residues. Although the preparation of electrodes with an aqueous process is less expensive, more environmentally friendly, and non-toxic, the use of CMC in ARLB poses a challenge due to its solubility in the aqueous electrolyte of the cell, which leads to a loss of mechanical cohesion and electronic percolation of the electrode.

In order to address these challenges, our research group has developed a process for preparing electrodes using a water-soluble binder in ARLB. The application of a plasma film deposition at atmospheric pressure allows for the prevention of such electrodes dissolution while allowing for the compatibility of materials at interfaces, where electrochemical reactions essential to the proper functioning of an energy storage system take place. This presentation will first detail the concept of our work. The fundamental phenomena allowing the operation of the aqueous battery will then be explained. Finally, initial tests for a large-scale application will be presented.

This work opens to new possibility of exploring better material options with good electrochemical performance and represents a first step towards a more sustainable lithium-ion battery.

HIGH THROUGHPUT STUDIES OF DOPED LLZO GARNET SOLID ELECTROLYTES

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Lithium lanthanum zirconium oxide (LLZO) is a leading candidate for solid Li-batteries due to its high lithium-ion conductivity, stability in air and against Li metal, and compatibility with high-voltage cathodes.^{1,2} Our understanding of LLZO is limited by the relatively small number of compositions which have been studied; both in the larger Li-La-Zr-O system and in the doped cubic LLZO system, which can accommodate an extremely wide range of dopants.³ To study this large number of compositions, we have applied a high-throughput methodology for synthesizing, characterizing, and testing sets of 64 LLZO electrolytes at the mg-scale. We use a citrate sol-gel synthesis whereby reagent solutions are dispensed across a well-plate to give a composition gradient. After drying and calcining the gels, the resulting powders are pelleted and sintered. We utilize high-throughput characterization techniques including powder X-ray diffraction, impedance spectroscopy, DC polarization, and electrochemical stability window testing.

Using our methodology, we have studied over 700 samples to produce a full phase stability diagram for the Li-La-Zr-O pseudoternary system.⁴ We found there is significant solubility of Li in the $\text{La}_2\text{Zr}_2\text{O}_7$ pyrochlore structure, and that both cubic and tetragonal undoped LLZO appearing throughout the system have similarly poor bulk conductivities. This previous study again emphasizes the key role dopants play in LLZO. Herein, our methodology is applied to a comprehensive doping study where 60 different dopants are evaluated under identical synthesis conditions to allow for a thorough understanding of dopant effects on structure, ionic conductivity, electronic conductivity, and electrochemical stability window. Our samples achieve high conductivities over 1 mS/cm and relative densities above 90% with our combinatorial synthesis. Since comparing dopants in the literature is often difficult due to varying synthesis methods, this systematic work is essential in rational design of these electrolytes.

¹ Q. Liu, et al., *J. Power Sources* **2018**, 389, 120-134.

² T. Thompson, et al., *ACS Energy Letters* **2017**, 2, 462-468.

³ F. Zheng, et al., *J. Power Sources* **2018**, 389, 198-213.

⁴ E. Anderson et al., *Solid State Ionics* **2022**, 388, 116087.

METHODS TO IMPROVE THE FIRST HYDROGENATION OF THE VANADIUM-RICH BCC ALLOYS

YOUR NAME / VOTRE NOM

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YOUR ABSTRACT / VOTRE RÉSUMÉ

(300 words -1page max)

Vanadium-based body centred cubic (BCC) alloys are interesting materials for hydrogen storage because of their relatively high gravimetric storage capacity (~4 wt.%) and fast hydrogenation-dehydrogenation kinetics at room temperature. However, the first hydrogenation (the so-called activation) is slow and usually necessitates high pressure/temperature. This work focuses on the effect of three different preparation methods on the first hydrogenation of the vanadium-rich BCC alloy Ti16V60Cr24: one-time cold rolling, 5 min ball milling and addition of 4 wt.% of Zr. All samples were synthesized by arc melting. Without Zr addition the alloy was single phase, but when 4 wt.% Zr was added, a secondary zirconium-rich phase was present. However, X-ray diffraction patterns only showed a single-body-centred cubic phase before hydrogenation for all samples. The crystal structure of the fully hydrogenated samples was body-centred tetragonal. The highest hydrogen capacity (3.8 wt.%) was measured for the Zr-doped alloy. The ball-milled alloy also exhibited a high storage capacity and fast kinetics. However, the maximum hydrogen storage capacity slightly decreased after cold rolling. It was found that air exposure increases incubation time for the first hydrogenation. The incubation time was shortened by cold rolling which, however, reduced the hydrogen storage capacity. The Pressure-Composition isotherms of Ti16V60Cr24 + 4 wt.% Zr at 297, 303 and 323 K were determined. The determined enthalpy and entropy of hydrides formation were -41 ± 5 kJ/mol and -134 ± 14 J/mol/K, respectively.

FIGURE

(Optional / Facultative)

TUNING CLUSTER-BASED RARE-EARTH METAL–ORGANIC FRAMEWORKS FOR WHITE LIGHT EMISSION

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Twenty-seven years after the first use of the name metal–organic framework (MOF), this class of materials is receiving more attention than ever, being considered by many as the future of materials science. These distinguished materials are composed of metal ions or clusters bonded by organic linkers, giving rise to three-dimensional network structures. Because of their very interesting characteristics, which often include extensive porosity, crystallinity, and structural tunability through controlling the metal and the organic linker building units, more than 99,000 different MOFs have so far been reported. Nevertheless, the research regarding this class of materials is still relatively young. In recent years, MOFs have been studied for a large number of applications including gas storage, drug delivery, chemical separations, catalysis, sensing, adsorption, light-harvesting and energy conversion.

Due to the special characteristics of rare-earth (RE) elements, which include scandium, yttrium, and the whole series of lanthanoids, promising new RE-based MOFs have been obtained in the past years. Among these characteristics, it is worth mentioning the high coordination numbers and distinct optical properties of RE ions, which can lead to the generation of materials with interesting photophysical and photochemical properties and unique crystalline structures.

Towards the application of photoluminescent RE-MOFs, we have been focusing on the design and synthesis of cluster-based MOFs containing multiple rare-earth metal ions, as their combination has the potential for white light emission. In this work, new bimetallic and trimetallic rare-earth cluster-based MOFs will be discussed, including the optimization of synthetic conditions, focusing on a balance between the ratio of RE-metal ions to yield the purest white light emission possible. The final materials are fully characterized by powder X-ray diffraction (PXRD), N₂ sorption, thermogravimetric analysis (TGA), scanning electron microscopy (SEM), and inductively coupled plasma mass spectrometry (ICP-MS). Finally, a complete study exploring the photoluminescent properties and photostability of these RE-MOFs is carried out.

ONE-STEP SYNTHESIS OF NiSe_2 AND NiSe_2 / RGO-PGM FOR HYDROGEN EVOLUTION REACTION

Issa Malam Mahamadou

Mohamed Siaj

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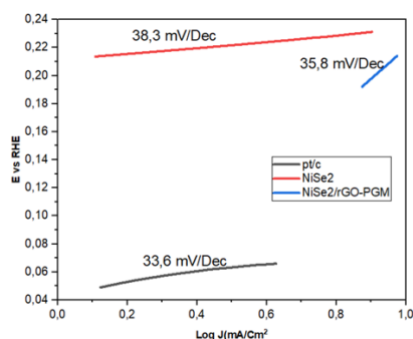
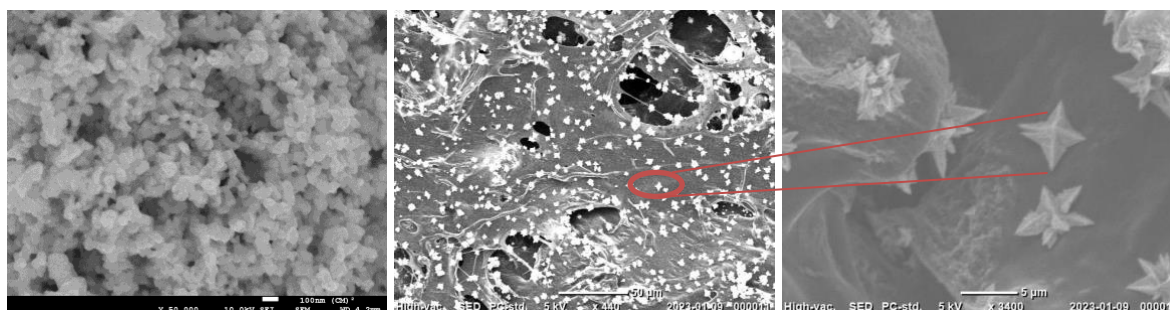
Université du Québec à Montréal, Montréal, Québec H3C 3P8, Canada

YOUR ABSTRACT / VOTRE RÉSUMÉ

The search of cheap, earth-abundant and efficient hydrogen evolution reaction (HER) catalysts is significant for sustainable hydrogen economy. Here we introduce a simple and cost-effective strategy for one-step synthesis of NiSe_2 and 3D porous NiSe_2 /RGO-PGM hybrid catalysts from our laboratory via hydrothermal method. In this talk, we will show a unique interconnected macroporous conducting carbon membrane that was prepared by cryogeletion and subsequent carbonization of the gelatin and graphene oxide cryogel. The NiSe_2 /RGO-PGM was used as electrocatalyst without binder “binder-free” for water-splitting HER. These catalysts exhibit superior catalytic performance and challenging Pt/C by a small overpotential (~ 100 mV) for NiSe_2 /RGO-PGM and (~ 230 mV) for NiSe_2 to afford $10 \text{ mA} / \text{Cm}^2$ with respectively Tafel slope $35,8 \text{ mV/Dec}$ and $38,3 \text{ mV/Dec}$ and good stability in acid, which benefits from the good electrical conductivity of NiSe_2 and NiSe_2 /RGO-PGM catalysts.

FIGURE

(Optional / Facultative)



DEFYING RATE LIMITATIONS IN LI-ION BATTERIES WITH LITHIUM INVENTORY MAPPING

Jeremy I. G. Dawkins

Martens, I. Danis, A. Beaulieu, I. Chhin, D. Mirolo, M. Drnec, J. Mauzeroll, J. Schougaard, S.

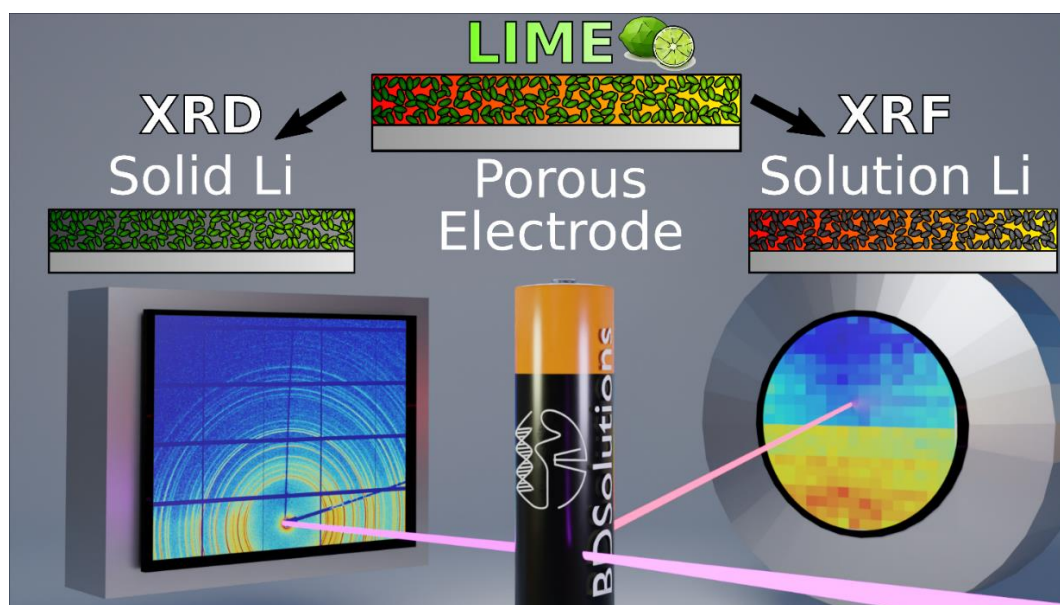
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SOLUTION PHASE CONCENTRATION GRADIENTS OF Li^+ ARE THE MOST COMMON CULPRIT FOR RATE LIMITATIONS IN COMMERCIAL LI-ION BATTERIES, AND ARE THE SOURCE OF CRIPPLING OVERPOTENTIALS, REDUCED EFFECTIVE CELL CAPACITY, ENERGY DENSITY AND POWER DENSITY. WE CAN OVERCOME THESE LIMITATIONS BY TRANSFORMING THE ELECTRODE ARCHITECTURE TO OPTIMIZE THE SOLUTION PHASE MASS TRANSPORT, BUT THIS REQUIRES INTIMATE KNOWLEDGE OF THE EFFECTIVE MASS TRANSPORT WITHIN THE POROUS ELECTRODES, INCLUDING THE CONCENTRATION PROFILE EVOLUTION WITH TIME DURING OPERATION. SIMILARLY, SOLID PHASE Li GRADIENTS OFFER COMPLEMENTARY INFORMATION ON THE STATE OF CHARGE AND CONDITION OF THE ACTIVE MATERIAL PARTICLES.

ALTHOUGH BOTH THE SOLUTION PHASE AND SOLID PHASE CONCENTRATION GRADIENTS OF Li HAVE ENORMOUS IMPACTS ON CELL PERFORMANCE, NO METHOD EXISTS TO MEASURE BOTH THESE GRADIENTS SIMULTANEOUSLY. THE SOLUTION PHASE GRADIENT HAS PROVEN ESPECIALLY ELUSIVE DUE TO THE EXPERIMENTAL CHALLENGES OF TRACKING A LIGHT ELEMENT (Li) IN A DENSE, OPAQUE AND PARAMAGNETIC MATRIX (I.E. THE COMPOSITE ELECTRODE). AS SUCH, THERE IS NO EXPERIMENTAL DATA AVAILABLE ON SOLUTION PHASE GRADIENTS THAT FORM WITHIN THE PORES OF LIB ELECTRODES. THIS GAP RESULTS IN A HINDERED EFFORT TO RATIONALLY DESIGN NEW MASS-TRANSPORT-OPTIMIZED ELECTRODE ARCHITECTURES.

IN THIS PRESENTATION, WE WILL INTRODUCE OUR WORK ON A SYNCHROTRON X-RAY METHOD THAT BRIDGES THIS GAP THROUGH TOTAL LI INVENTORY MAPPING OF ELECTRODES (LIME). LIME QUANTIFIES BOTH THE SOLID AND SOLUTION Li CONTENT OF AN ELECTRODE SIMULTANEOUSLY YET SEPARATELY, WITH EXCELLENT SPATIAL ($5\ \mu\text{m}$) AND TEMPORAL ($\approx 1-2$ MINUTES) RESOLUTION. CAPITALIZING ON LIME WILL BRING COMMERCIAL MANUFACTURERS CLOSER TO IMPLEMENTING ESSENTIAL FAST-CHARGING LIBS AT AFFORDABLE PRICES, WHILE PROVIDING LONG AWAITED DATA TO VALIDATE AND IMPROVE NUMERICAL MODELING EFFORTS. IT IS HOPED THAT THIS WORK WILL INDIRECTLY EXPEDITE ELECTRIC VEHICLE IMPLEMENTATION, AND PAVE THE WAY TO GRID-LEVEL STORAGE SOLUTIONS, THEREBY CHALLENGING THE FOSSIL-FUEL-DRIVEN STATUS-QUO AND IMPOSING CHANGE ON A STAGNANT ENERGY SECTOR.



ETUDE D'UN ELASTOMERE CRISTALLIN LIQUIDE AVEC UNE TRANSITION DE PHASE ORDRE-DESORDRE A TEMPERATURE CORPORELLE

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Rassemblant les caractéristiques de caoutchoucs et de cristaux liquides, les élastomères cristallins liquides (ECL) sont un matériau polymère prometteur pour de nombreuses technologies, telles qu'actionneur, muscle artificiel et robot souple contrôlés par des stimuli (chaleur, lumière, champ électrique ou magnétique). La base de toutes ces applications est une propriété fascinante d'ECL, à savoir qu'une transition de phase à l'échelle moléculaire, entre un état ordonné (phase CL) et un état désordonné (phase isotrope), peut induire un changement de forme important à l'échelle macroscopique. Notre recherche s'inscrit dans ce domaine émergent. Nous avons comme but de développer un ECL qui peut fonctionner comme un matériau à mémoire de forme réversible et stimuable par la température du corps ($T_{corps} \sim 37\text{ °C}$), en vue de possibles applications biomédicales. Ceci représente un défi, car les ECL rapportés dans la littérature ont généralement une température de transition ordre-désordre au-dessus de 50 °C. Notre solution est d'utiliser une nouvelle stratégie inspirée par une étude antérieure qui montre que la présence d'un macromonomère non-mésogénique (polyéthylène glycol diacrylate), comme diluant de la concentration mésogénique dans la chaîne principale, impose un effet de garder les températures de transition de phase basses. Ensuite, une propriété « autobloquante » sera apportée à l'ECL par réticulation utilisant des liens dynamiques pour améliorer sa malléabilité. Finalement, nous tenterons de renforcer la force mécanique du matériau par ajout de nanoparticules de renfort tout en conservant les températures de transition de phase.

Self-Dispersing Silica Fume Nanoparticles: A Valuable Admixture for Ultra High-Performance Concrete

Kevin Daoust

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Ultra-high-performance concrete (UHPC) is a promising material to alleviate the environmental impact of concrete which is responsible for 8% of our CO₂ emission. Compared to normal concrete, UHPC offers superior mechanical properties and durability leading to a reduction of its cross-section members and maintenance, saving material and lowering labor costs. These improved properties come from a low water-to-binder ratio and high amounts of silica nanoparticles like silica fume (SF). Proper dispersion of SF plays a crucial role for the optimisation of UHPC. At high concentrations (>10 wt%), dispersing SF is extremely challenging with conventional polycarboxylate superplasticizers and leads to challenging deployment. In this work, we evaluate the production of UHPC with SF@PEG which are SF particles with a small layer of polyethylene glycol (PEG) covalently grafted on their surface. Remarkably, UHPCs made with all SF@PEG samples show lower viscosity, longer workability and lower mixing power requirements compared to UHPC made with SF. The use of SF@PEG also allows drastic reduction of the amount of superplasticizer needed to ensure a workable dispersion. Furthermore, the UHPC prepared with SF@PEG (2.5 wt% of PEG) exhibits a 14% increase in compressive strength compared to the UHPC prepared with SF. Owing to their lower viscosity, longer workability, lower mixing energy requirements and higher compressive strengths, we envision that SF@PEG will significantly advance the manufacturing of UHPC.

IMPROVED MAGNETISM IN BORON-DOPED GRAPHENE NANORIBBONS USING NON-BENZENOID DEFECTS

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ABSTRACT

Although recent studies have reported the existence of high spin states on free-standing 7-armchair graphene nanoribbons (7-AGNR) with topological defects [1] and boron-doped nanoribbons (7-BGNR) [2], the magnetism is not robust enough to endure on a gold substrate. In contrast, previous studies on carbon-based triangulene dimers and hexamer nanostars have shown that the magnetic character of adsorbed species is not totally screened by the Au(111) substrate and magnetism persists [3-4]. With the help of first-principles DFT+U calculations, we propose to address the issue associated with weak magnetism in GNRs by incorporating non-benzenoid pentagon defects in 7-BGNRs. The presence of such defects strengthens its exchange coupling energy, for both free-standing and Au(111) adsorbed species. Our results show that the pentagonal defects in pristine 7-AGNR leads to antiferromagnetic (AFM) free-standing ground state; while on Au(111) surface, it becomes ferromagnetic (FM) with a triplet spin configuration (Fig. 1). This variation mostly originates from the p-type doping nature of the substrate. Contrarily, pentagonal defects in 7-BGNR gives relatively stable FM ground state for both free-standing and adsorbed phases on Au(111). In addition, we have found that the magnetism is strongly localized nearby the non-benzenoid defect sites of the 7-AGNR, even on the Au(111) surface. In summary, our study provides new insights into the design of magnetic graphene-based systems, and suggests a promising approach for tailoring their magnetic properties.

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FIGURE

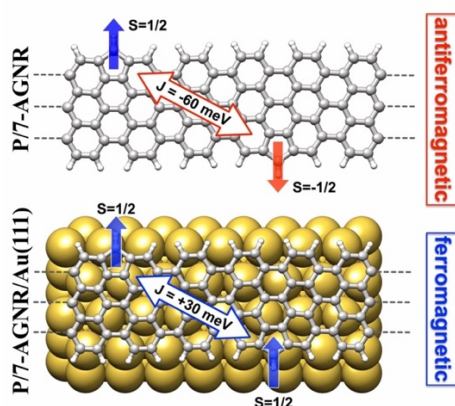


Figure 1: Non-benzenoid pentagon defects in 7-AGNR backbone introduces open-shell singlet state in free-standing phase while a FM triplet state is observed when adsorbed on Au(111) surface.

Organic nonvolatile resistive switching memory devices based on liquid crystal films

Lindiomar Borges de Avila Jr

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Memristors are two-terminal non-volatile memory devices based on resistivity switching (RS) effects. The theoretical modeling of this component was first presented in the early 1970 [1] and the experimental proof conducted in the Hewlett and Packard (HP) laboratories in 2008. Liquid crystals (LCs) are promising smart materials for application in organic electronics due to their molecular self-organizing properties. Organic resistive random access memory (ORRAM) devices can be manufactured with a layer of organic material sandwiched in a vertical structure between two conductive electrodes. Nowadays, there are many reports of materials with this application [2], but there are only few studies for LCs, making them a great research opportunity [3].

This work aims to investigate the RS effect of a columnar LC at room temperature, which combines molecular order with charge transport. The RS behavior was characterized by I-V curves (from -30 to 30V), where an unipolar behaviour was observed, with the set and reset process occurring at the same polarity. This effect was improved by doping the LC with semiconducting core/shell quantum dots of ZnO@SiO₂, which also increased the electrical stability and the ON/OFF ratio. We demonstrated the ability to write-read-erase-read, between ON and OFF states, by applying specific external voltages. A conduction mechanism responsible for the RS effect was proposed based on molecular electrochemical reduction. This work highlights the impressive ability of the columnar LC to store and read information multiple times.

Acknowledgements: This work was funded by CNPq, CAPES (#001), FAPESC, INCT-INEO, CAPES/COFECUB (#937-20 and PhC 962/20) and H2020-MSCA-RISE-2017 (OCTA, #778158).

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ELECTROCHEMICAL ETCHING STUDY OF MESOPOROUS GERMANIUM THROUGH STATISTICAL DESIGN OF EXPERIMENTS

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Owing to its mechanical and physicochemical properties, porous germanium (PGe) shows promise for a variety of novel applications, including energy storage and sensing, as well as for use as an epitaxial template for detachable lightweight and low-cost III-V based optoelectronic devices. However, the bipolar electrochemical etching (BEE) used for PGe formation is highly complex, as numerous parameters interact with each other. To optimise such a complex system, statistical methods such as Design of Experiment (DoE) are preferred. The DOE approach reduces the number of experiments needed compared to a conventional experimental design while still allowing for an assessment of the impact of each parameter.

DoE is used to shed light on two important factors: *(i)* the direct effect of parameters on the PGe characteristics, and *(ii)* the interaction between the parameters and their non-linear effects. To further reduce the number of experiments, a D-optimal design can be employed to identify the most impactful parameters affecting the PGe characteristics, allowing for the adoption of a Central Composite Design plan focusing on three key parameters. Statistical analysis can then be applied to the dataset, providing a deeper understanding of observed trends.

In this work, an optimized DoE approach is used to study the formation of PGe with tubular morphology, etched by fast BEE into a Ge substrate. The main etching parameters, such as etching/passivation current density, pulse duration, and total time, were studied to observe their direct impact on PGe structures as well as to reveal interactions and correlations between them. The PGe layers were characterized by AFM, SEM and profilometry to analyse their properties and to produce the dataset necessary for statistical analysis. Using this approach, the main trends for each parameter have been identified, allowing specific parameter intervals to be chosen when finetuning the PGe structure for a specific application.



Figure 1: Cross-section SEM view of porous germanium with tubular morphology

DECORATING METALS WITH CARBENE: OBSERVATION OF THE CARBONE-METAL BOND BY RAMAN SPECTROSCOPY

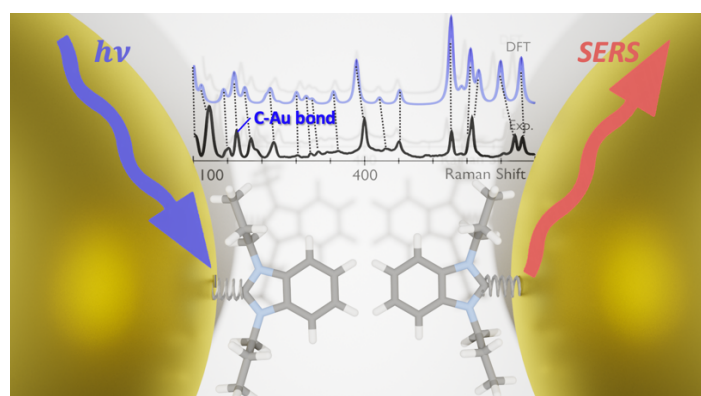
LUCILLE KUSTER

Lucille Kuster, Marilyne Bélanger-Bouliga, Ali Nazemi*, Mathieu Frenette*

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Metallic nanoparticles find many applications due to their thermal, chemical, physical and (photo)catalytic properties. Their large surface-to-volume ratio and small size make them important candidates for various drug delivery applications and non-invasive imaging applications. Metallic nanoparticles (NPs) functionalized with electron-donor molecules, such as N-Heterocyclic Carbenes (NHC), are quite stable. NHCs have a strong sigma-donor character that allows the formation of strong covalent bonds with transition metals. While many structures are proposed, unambiguous observation of the carbon-metal nanoparticle bonding has not yet been reported. In order to see this bonding between the carbene from the NHC and the metal from the nanoparticles, the C-M bond has been observed by Raman spectroscopy without destroying the sample. In Raman spectroscopy, when the plasmonic frequency of the nanoparticle is in resonance with the incident excitation laser, the intensities of the Raman peaks corresponding to the ligands on the surface of the NPs increase; this phenomenon is called Surface-Enhanced Raman Spectroscopy (SERS).

The synthesized NHCs have symmetric alkyl chains on both nitrogens—one NHC has 12 carbons on each chain and the other has 3 carbons. The metals used in this study are gold, which forms stable complexes and nanoparticles, and silver, which is less stable than gold due to its photosensitivity. Each relevant Raman peak was assigned with computational chemistry (Density-functional theory, DFT) for both the complexes and the nanoparticles bonded to the NHCs. Different levels of theory for the DFT calculations were compared to obtain optimized Raman spectra predictions. The r²SCAN-3c method was chosen as the best compromise between accuracy with the experimental SERS spectra and computation time. Each type of carbon-metal bond was observed at small Raman frequencies. This platform for studying the force of the C-M bond could provide useful insights for the development of a new generation of drug delivery assemblies.



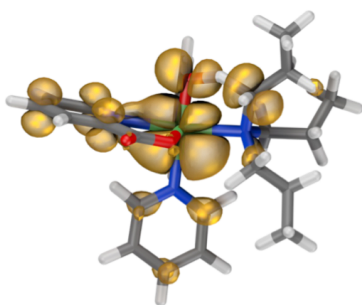
ISOLATING THE REACTIVITY OF INTERMEDIATES IN INDUSTRY-RELEVANT (PHOTO)REDOX CHEMISTRY

MATHIEU FRENETTE

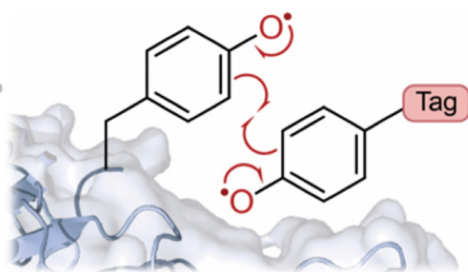
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(Photo-)Chemical reactions that involve single-electron transfers and unpaired electrons often proceed via interestingly complex mechanisms. These complex mechanisms, can in return, offer an array of useful transformations; many of these reactions occur at room temperature, without strong acids or bases, and offer reactivity that is often orthogonal to traditional nucleophile-electrophile chemistry. Pharmaceutical industry researchers have recently embraced these complex reactions and our group has helped collaborators understand the mechanisms at play.

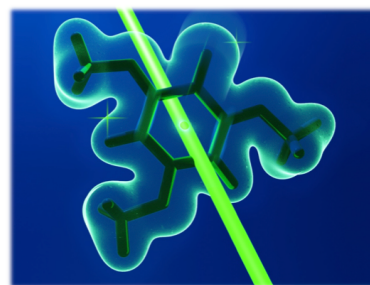
To offer mechanistic insight in redox (photo)chemistry, one strategy is the identification of key reaction intermediates. Unambiguous characterization of highly reactive species is challenging, but their discovery hints at novel reaction pathways to be explored. This talk will show increasingly strong evidence for Fe(IV)-oxo intermediates in the conversion of amines to amides,¹ for phenoxyl radicals in the photochemical tagging of protein tyrosines² and for a phenoxenium (phenol cation) in a hypervalent iodine reaction.³ The isolation and study of these intermediates using steady-state kinetics, transient absorption, and resonance Raman spectroscopy gave increasingly convincing confidence in key steps of these reaction mechanisms.



**steady-state
kinetics**



laser-flash photolysis



resonance Raman

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PHOTO-INDUCED FORCE MICROSCOPY OF CHEMICALLY MODIFIED 2D-MATERIALS SURFACES

Maziar Jafari and Mohamed Siaj

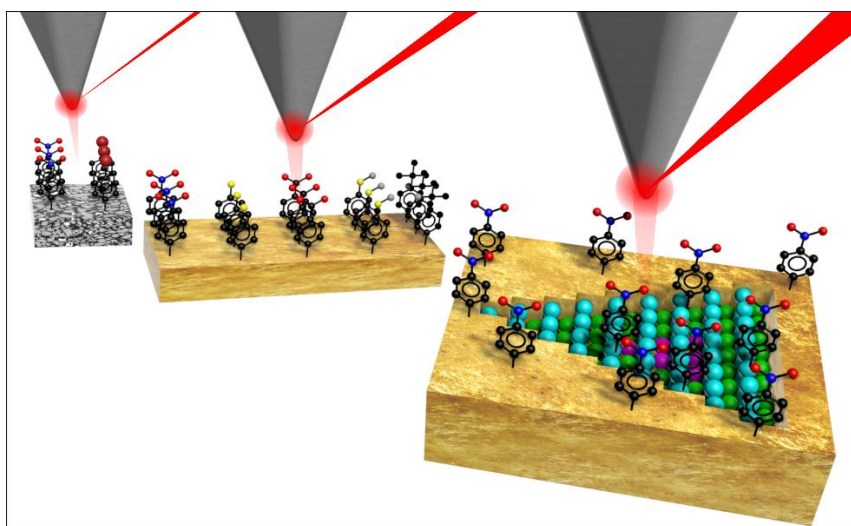
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ABSTRACT / RÉSUMÉ

Since visible light microscopy and photon-based spectroscopy are bound by the limit of diffraction of light, few-nanometer scale imaging and spectroscopy resolution is currently impossible using optical lenses found in Raman or Infrared cameras/microscopes. Scanning probe microscopy has been able to bypass this limitation using tip-enhanced near-field concentrated light. Since 2010, photo-induced force microscopy (PiFM) has evolved into a state-of-the-art local surface vibrational scanning probe microscope imaging and spectroscopy technique. Given its monolayer surface sensitivity, non-contact operational mode and <10 nm spatial resolution, rival techniques have yet to match the efficacy. 2D-materials are model substrates to examine surface chemical reactions because of their smooth and flat surfaces. Electroactive 2D-materials are of particular interest because of their dynamic electrical properties enabling electrochemical applications. Aryl diazonium salts are well-known to covalently bind to conductive surfaces by applying a reducing potential. Their binding results in a thin, uniform and well oriented organic layer covering the material surface. Aryl diazonium salts can be synthesized to present diverse chemical functional groups, suitable for observing systematic mid-IR spectroscopic varieties. In this work, we functionalized model surfaces with strongly active Infrared molecules to showcase the effectiveness of the photo-induced force microscope in identifying the grafted substituted phenyl derivatives and in chemically imaging those molecules locally. Specifically, glassy carbon electrode and template stripped gold conductive 2D-surfaces and transition metal dichalcogenide monolayers MoSe₂, WSe₂ and MoSe₂-WSe₂ in-plane heterostructure semiconductor 2D-surfaces were electrochemically grafted with several aryl diazonium salts in both protic and aprotic solvents.

FIGURE



SYNTHESIS AND STUDY OF NOVEL SIDE-CHAIN LIQUID CRYSTALLINE ELASTOMERS

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RECENTLY, OUR GROUP REPORTED A UNIQUE “AUXETIC-LIKE” REVERSIBLE SHAPE CHANGE EXHIBITED BY A LIQUID CRYSTALLINE ELASTOMER (LCE) MATERIAL. WITH A MECHANICALLY STRETCHED MONODOMAIN STRIP UNDERGOING LC-ISOTROPIC PHASE TRANSITION, BOTH THE LENGTH AND WIDTH CONTRACT IN THE ISOTROPIC PHASE, AND BOTH EXTEND IN THE LC PHASE. WE BELIEVE THAT THE STRUCTURAL PARAMETERS OF LCE, PARTICULARLY THE MESOGEN’S ASPECT RATIO AND THE FLEXIBLE SPACER LENGTH, MIGHT AFFECT THIS PHENOMENON. TO OBTAIN EXPERIMENTAL EVIDENCE, HEREIN, WE SYNTHESIZED A SERIES OF RATIONALLY DESIGNED SIDE-CHAIN LCES BASED ON THERMOPLASTIC ELASTOMER OF POLY(STYRENE-BUTADIENE-STYRENE) (SBS) TRIBLOCK COPOLYMER CONTAINING DIFFERENT MESOGENS (AZOBENZENE AND BIPHENYL) WITH VARYING LENGTHS OF THE SPACER. COMPARATIVE STUDIES WERE CARRIED OUT TO UNDERSTAND HOW THE STRUCTURAL PARAMETERS OF LCES ARE RELATED TO THE ORDER-DISORDER PHASE TRANSITION INDUCED SHAPE CHANGE. WE FOUND AN ODD-EVEN EFFECT IN THE STRETCHING-INDUCED MESOGEN ORIENTATION FOR LCES WITH DIFFERENT SPACERS. MORE IMPORTANTLY, THE RESULTS SHOW THAT IN AN LCE STRIP SUBJECTED TO LARGE STRAINS, A SUSTAINED PERPENDICULAR ALIGNMENT OF THE SIDE-GROUP MESOGENS, WITH RESPECT TO THE STRETCHING DIRECTION, IS AN INDISPENSABLE CONDITION FOR THE LCE TO EXHIBIT THE UNUSUAL THERMALLY INDUCED “AUXETIC-LIKE” REVERSIBLE DEFORMATION. LCES HAVING EITHER PARALLEL MESOGEN ORIENTATION OR RANDOMIZED MESOGEN ALIGNMENT AT LARGE STRAINS EXHIBIT NORMAL ACTUATION BEHAVIOUR; THAT IS, THE LENGTH CONTRACTS, AND THE WIDTH EXTENDS ON HEATING INTO THE ISOTROPIC PHASE, WHILE THE OPPOSITE DEFORMATIONS OCCUR ON COOLING TO THE LC PHASE.

Near-infrared lifetime mapping of rare-earth doped nanoparticles using ultrahigh-speed line-scanning microscopy

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Luminescent nanomaterials—which can be excited and emit in the near-infrared (NIR) range—have attracted great attention in a plethora of applications, including nanomedicine, biosensing, bioimaging, solar cells, and photocatalysis. Especially in biomedical applications, NIR light mitigates the drawbacks associated with ultraviolet and/or visible light (e.g. photodamage, background autofluorescence, and limited penetration depth). At the forefront of NIR-excited nanomaterials are rare-earth doped nanoparticles (RENPs) that possess exceptional optical properties, such as programmable emission, long luminescence lifetime, and high photostability. However, the NIR lifetime property of RENPs and their potential applications are rarely explored. The conventional technique in lifetime measurement, time-correlated single-photon counting, is recognized as an effective method that possesses a high signal-to-noise ratio and temporal resolution. However, slow acquisition speed still is a weak point, especially in the case of wide-field luminescence lifetime imaging that requires a longer time for two-dimensional scanning operation to form a lifetime map and in the case of a long-lived emission lifetime (from hundreds of microseconds to several milliseconds) that demands extended pixel dwell time. Here, we develop a line-scanning NIR luminescence lifetime imaging microscopy. By combining a rotating-mirror streak camera and a mechanical motor, this system offers a one-dimensional imaging speed of 140 thousand frames per second. It is applied to wide-field NIR photoluminescence lifetime imaging of several types of RENPs which are excited and emitted in the NIR region. Furthermore, the potential applications of NIR lifetimes in anticounterfeiting and nanothermometry are demonstrated.

DESIGN OF A SIMPLE AND LOW-COST CARBON-BASED CATALYST FOR CONVERTING WASTE COOKING OIL INTO BIODIESEL

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YOUR ABSTRACT / VOTRE RÉSUMÉ

Biodiesel has emerged as an ideal candidate for conventional diesel replacement. Reduction in greenhouse emissions, low toxicity and biodegradability are some of its key benefits over petroleum-based diesel. However, its production still faces significant hurdles including the inability to reuse and recover the catalysts, leading to a costly purification process. In this regard, heterogeneous catalysts have become an interesting alternative to overcome these drawbacks, as they can be easily separated, recovered, and reused. Indeed, several heterogeneous catalysts for biodiesel production have been reported, such as alkaline metal oxides, zeolites, and mesoporous supported materials. Nevertheless, these materials have some disadvantages, such as high cost and complex synthetic routes. Thus, carbon-based materials have recently come to light as a promising alternative to replace these catalysts since they offer simple and inexpensive synthesis routes, possess extremely interesting physical and chemical properties, such as high surface area to volume ratios, elevated thermal stability, and metal-free composition. Moreover, the functional groups present on their surfaces can be tuned to mimic those found in homogeneous catalysts, imparting them with outstanding catalytic activity. Here we present the use of a heterogeneous carbon-based catalyst for the (trans)esterification of waste-cooking oil to produce biodiesel. We report biodiesel conversions of 98% at 90 °C, for 3 hours, using 10 wt.% catalyst loading and a 1:36 methanol to oil molar ratio. Moreover, we investigated the catalyst tolerance towards free fatty acid (FFA) content. It showed a tolerance content of up to 10 wt.%. In order to comprehend the reaction mechanism, we further characterized its surface groups to glean an understanding of surface chemistry and the role it plays in the (trans)esterification reaction. This effective and inexpensive heterogeneous catalyst proved to be a promising substitute to the commonly used homogeneous catalysts and a novel alternative to make biodiesel production more feasible.

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

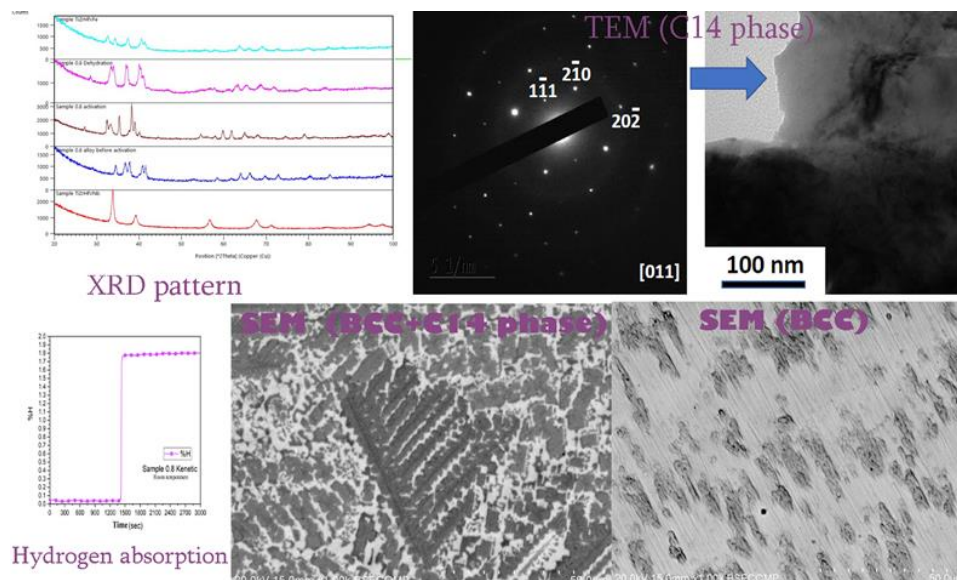
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ZrTiVHfNb high-entropy alloys have shown great potential as a hydrogen storage material due to their appreciable capacity. In this study, transition metal Fe was used to improve the hydrogen storage properties of the equimolar ZrTiVHfNb alloy by substituting Nb by Fe to form alloys of compositions $\text{ZrTiVHfNb}_{1-x}\text{Fe}_x$ ($x = 0, 0.2, 0.4, 0.6, 0.8, 1$). The microstructure evolution and hydrogen storage properties. The results show that the $\text{ZrTiVHfNb}_{1-x}\text{Fe}_x$ alloys are composed of a hexagonal C14 Laves phase and a Body centered Cubic (BCC) phase. The fraction of the C14 Laves phase increases with increasing iron content. The $\text{ZrTiVHfNb}_{1-x}\text{Fe}_x$ alloys show enhanced hydrogenation kinetics and activation in room temperature. Notably, the ZrTiVHfNb alloy can reversibly absorb 2.1 wt.% hydrogen at 350°C under 2 MPa H_2 . The increased fraction of the C14 Laves phase lead to the increase of hydrogenation rates. Moreover, the increased Fe content leads to easy activation even at room temperature and under 1.2 Mpa of hydrogen pressure.



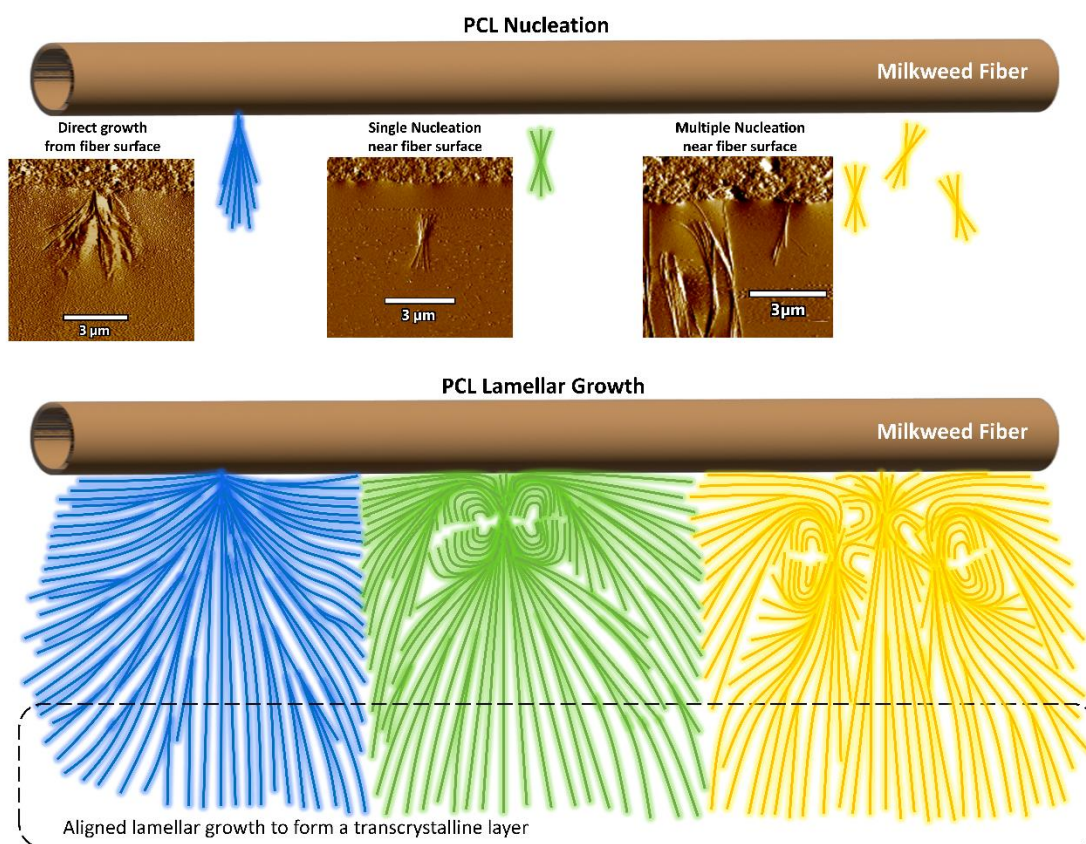
LAMELLAR GROWTH OF POLYCAPROLACTONE AT THE POLYMER/FIBER INTERFACE

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THE MORPHOLOGICAL DEVELOPMENT AND LAMELLAR STRUCTURE OF POLY(E-CAPROLACTONE) (PCL) AROUND A SINGLE MILKWEED (MW) FIBER WERE INVESTIGATED VIA VARIOUS MEANS OF MICROSCOPY. THE MW FIBER WAS TREATED WITH GRAPHENE OXIDE (GO) TO PROMOTE THE CRYSTALLIZATION OF PCL, WHICH LED TO THE FORMATION OF A PCL TRANSCRYSTALLINE (TC) LAYER ON BOTH SIDES OF THE MW FIBER. ATOMIC FORCE MICROSCOPY (AFM) WAS USED TO OBSERVE THE LAMELLAR STRUCTURE OF THE OBTAINED STRUCTURES. PAIRED WITH A HOT-STAGE, IN-SITU AFM WAS USED TO RECORD THE GROWTH OF PCL CRYSTALS FROM AND AROUND THE SURFACE OF THE NATURAL FIBER. FOR THE FIRST TIME, WE OBSERVED THE NUCLEATION AND GROWTH OF THE PCL LAMELLAE FROM THE SURFACE OF NATURAL FIBER. THE PRESENCE OF THE NATURAL FIBER INTRODUCED PHYSICAL HINDRANCE AND OPPORTUNITIES FOR THE GROWTH OF THE PCL CRYSTALS, ALBEIT THE GROWTH WAS FOLLOWING THE PRINCIPLE THEORIES AND KNOWN PHENOMENA OF POLYMER CRYSTALLIZATION. PCL TENDS TO NUCLEATE ON OR VERY CLOSE TO THE SURFACE OF THE GO-TREATED MW FIBER. IN BOTH CASES, THE PCL LAMELLAE WERE BRANCHING AND SPLAYING INTO A SHEAF-LIKE STRUCTURE WHICH THEN CONTINUED THE GROWTH TO FILL OUT THE SPACES AROUND THE MW FIBER. THE FORMED LAMELLAE THEN JOINED AND ELONGATED IN THE DIRECTION NORMAL TO THE SURFACE OF MW FIBER TO COMPLETE THE FORMATION OF THE TC LAYER UNTIL IT REACHED THE DEVELOPED SPHERULITES IN BULK.



TUNING THE INTERLAYER EXCITON IN BILAYER MoS_2 BY MEANS OF SELF-ASSEMBLED MONOLAYERS

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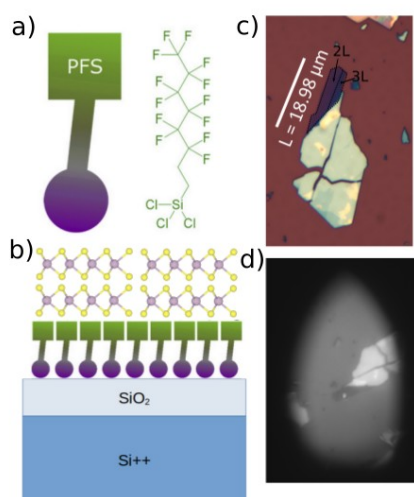
YOUR ABSTRACT / VOTRE RÉSUMÉ

The field of study surrounding Transition Metal Dichalcogenides (TMDs), a class of two dimensional materials that can be exfoliated down to a single molecular level, has recently seen large improvements and advancements. Whether in the of study of monolayer properties or in the various possibilities that stacking different materials as heterostructures open up. However, one interesting application of these materials is in their natural homobilayer form. For example, in Molybdenum Disulfide (MoS_2), there exists an interlayer exciton that emerges purely out of the interlayer interaction inside the natural homobilayer.

This exciton is unique in its ability to couple to its environment due to having both strong in-plane and out-of-plane dipole sensitivity. This project attempts to leverage this sensitivity by utilizing a method of dielectric tuning that is not commonly used for two dimensional materials, self assembled organic monolayers (SAMs). These SAMs are a group of unconjugated organic molecules that spontaneously assemble in a single molecular layer on top of a substrate. By using SAMs with a strong dipole as its functional group, it is possible to create an effective electric field across the homobilayer to couple with the interlayer exciton without external electrical or optical pumping.

In this project, we fabricate homobilayers of MoS_2 on two different SAMs, trichloro(1H,1H,2H,2H-perfluorooctyl)silane(PFS) and N-[3-(Trimethoxysilyl)propyl]ethylenediamine(AHAPS). These two molecules will form SAMs with a very strong electrostatic dipole (of opposite sign) in the vertical direction which makes them prime candidates for exerting a local electric field to the bilayer MoS_2 . We then perform optical reflectance measurements in order to directly probe the interlayer exciton and the effects of the SAM interface. This method of interfacing organic molecules to TMDs is vastly unexplored and opens a new range of possibilities for materials by using two classes of materials both known for their versatility.

FIGURE



Schematic overview of the coupled SAM and TMD system. a) Structure of PFS, one of the self assembled monolayers studied in this investigation. b) Schematic diagram of the bilayer TMD on top of the SAM. c) Optical microscope image of MoS_2 used in this investigation. d) Laser spot focused on the bilayer for exciton spectroscopy.

NANOCARBON SYNTHESIS BY INDUCTION-COUPLED PLASMA REACTOR FOR ADVANCED APPLICATIONS

Nadi Braidy

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YOUR ABSTRACT / VOTRE RÉSUMÉ

Thanks to their remarkable properties, nanocarbon, especially graphene and carbon nanotubes are ubiquitous to a wide range of applications. Advanced processing methods can produce the distinctive 1D and 2D morphological features of carbon nanotubes and graphene but typically translate into low production rates and heavy post-processing steps to remove the catalyst or support. As an alternative, carbon nanohorns (CNHs) and carbon nanoflakes (CNFs), i.e., few-layer graphene, approach the structural properties of their carbon nanotubes and graphene counterpart and can be prepared with a much higher production rate and are catalyst-free.

CNHs and CNFs are typically produced by vaporizing a carbon precursor and condensing the ensuing C-rich vapor in a controlled way [1]. The growth of different nanocarbon structures can be promoted by tuning the growth parameters such as the C-precursor partial pressure, total pressure, flow rate, and temperature. Controlled growth environments, such as those found for laser or arc-discharge reactors, are achieved at the cost of a low production rate, especially if graphite is the precursor.

We have isolated the conditions to produce CNHs (Figure a) and CNFs (Figure b,c) powders using a radio-frequency induction plasma reactor and methane as precursor [2,3]. CNFs and CNHs could be produced at a rate of 15-30 g/h using a plasma torch operated with power ranging between 15 kW and 30 kW.

We have studied the morphology of the nanopowder using aberration-corrected transmission electron microscopy (Figure 1a, inset) and Raman spectroscopy. High pressures, in the range of 80-85 kPa are essential for CNHs while lower pressures, typically 20 kPa, promote the growth of 100-200 nm-large CNFs (Figure b,c). For instance, we have explored the effect of flow rate and various gaseous promoters to isolate the optimal conditions for the growth of ~50 nm-long CNHs. Other synthesis conditions led to the growth of 50-100 nm diameter faceted carbon nanocapsules.

We report on the process map of the various carbonaceous nanomaterials that we were able to stabilize. We have coupled these observations to optical emission spectroscopy studies of the plasma torch and thermodynamic computation to shine some light on the growth mechanism of these remarkable nanostructures.

[1] Georgakilas et al. *Chemical Reviews* 2015 **115** (11), 4744. DOI: 10.1021/cr500304f

[2] Casteignau et al (2022). *Plasma Chemistry and Plasma Processing* **42** (3), 465. DOI: 10.1007/s11090-022-10240-8

[3] Aissou et al. (2022) *Tribology International* **167** 107406. DOI 10.1016/j.triboint.2021.107406

Accelerated Development of High Voltage Li-ion Cathodes

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Following the ever-growing demand for energy and the environmental concerns, efforts to electrify the transportation sector are improving rapidly; as a result, yet another large market for Li-ion technology has been opening up. The need for high energy density Li-ion batteries, in order for the development of electric vehicles, attracted scientists' attention to high-voltage cathode materials. Among which, olivine-structured, Polyanionic cathode materials (LiMPO_4) have been extensively investigated. In this category, LiCoPO_4 (LCP) and LiNiPO_4 (LNP) have received particular attention for their high redox potential of 4.8 and 5.2 V vs. Li/Li^+ , respectively, and thus high energy density. However, despite the high theoretical capacity, these materials show unsatisfactory electrochemical performance due to their low electronic conductivity and low ionic conductivity which can be attributed to their one-dimensional (1D) ion transport tunnels. Till date, there have not been experimental studies systematically done on these materials, where one can deduce the potential methods or dopant candidates with their optimum ratio, out of thousands of different samples, which might be revolutionary in the development of transport electrification era.

Here, we applied high-throughput methods to synthesize near-micron sized carbon-coated LiCoPO_4 with improved energy density and capacity retention. We systematically studied mono- and co-doping method on improving the performance of LCP. In total, 1300 materials with 46 different substituents have been synthesized and characterized. A number of substituents greatly improved capacity (e.g., 160 mAh g^{-1} for 1% In substitution vs 95 mAh g^{-1} for the pristine). However, co-doping was required to improve extended cycling. $\text{Li}_{1-3x}\text{Co}_{1-2x}\text{In}_x\text{Mo}_x\text{PO}_4$ is found to be particularly effective with dramatically improved cycling (as high as 100% after 10 cycles, vs $\approx 50\%$ in unsubstituted). While In improved the electronic conductivity of the carbon-coated materials, Mo co-doping gave larger particles and DFT calculations showed that Mo impedes the formation of Li/Co antisite defects.

USING POLYSACCHARIDE AS AN ELECTROLYTE FOR ENERGY STORAGE PURPOSES

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YOUR ABSTRACT / VOTRE RÉSUMÉ

Energy storage technologies are one of the most promising alternatives for energy transition. These technologies will also play an important role in supplying energy to light, wearable and flexible electronics. These smart and wearable electronics are one of the main components of the Internet of Things (IoT) system, defined as the connection between an electronic object and its connected interface. The value of the global flexible electronics market reached USD 31.7 billion in 2022 and its revenue forecast will reach USD 48.6 billion by 2028, due to the increasing need for IoT devices. However, serious concerns about the ecological footprint of such technologies must be addressed early in their conception and throughout the whole device's life cycle.

To meet the need for supplying these devices with energy, electronics come with batteries that must respect special requirements for their applications. Most of the time, those batteries contain polymers that can be used either as 1) electrolyte, e.g., solid polymer electrolyte or gel polymer electrolyte, to enable flexible electronics/batteries fabrication or as 2) binders in positive or negative electrodes ensuring the mechanical cohesion within the composite electrodes. Biobased polymers are one of the promising alternatives according to our environmental concerns about these devices. Their general affinity with water makes them suitable for aqueous rechargeable batteries, implying several technologies such as aqueous rechargeable lithium-ion batteries (ARLB) or zinc rechargeable batteries (ZRB).

In this study, we developed a hydrogel electrolyte made of pectin, a polysaccharide contained in the cell plants' wall, as an alternative to synthetic polymers in batteries. Hydrophobic interactions and hydrogen bonds, together with bivalent cation interactions, allow the free-standing electrolyte gelation. Electrochemical characterization has been evaluated by ionic conductivity measurements as well as its ability to be used as an electrolyte in hybrid devices, such as zinc-lithium-ion batteries.

PROBING TRENDS IN THE STABILITY OF THE RE-UIO-66 ANALOGUES THROUGH ANALYSIS BY SINGLE CRYSTAL X-RAY DIFFRACTION^A

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Long-range order — i.e., crystallinity — is a structural feature that dominates the vast majority of metal–organic frameworks (MOFs) reported as of today. Crystalline materials are advantageous to study due to their known composition and constant density, as well as the uniform distribution of functionality. When studying MOFs, crystalline structures can be used to determine the position of adsorption sites, proof of post-synthetic modification, and precise identification of pore-occupying species.

To this day, obtaining crystal structures for newly synthesised MOFs is considered a difficult task since there is not, in most cases, a significant difference between growth and nucleation rates leading to the precipitation of microcrystalline powders, rather than suitable single crystals.

In the past, our group was able to synthesise microcrystalline powders of RE-UiO-66 (RE = Y(III), Sm(III), Eu(III), Gd(III), Tb(III), Dy(III), Ho(III), Er(III), Tm(III), Yb(III), and Lu(III)) and obtain a single crystal structure for Tm-UiO-66. These materials are isorecticular to Zr-UiO-66, presenting hydroxy- or fluoro-bridged RE₆ clusters as their inorganic blocks, and terephthalic acid as their organic ones.

Herein, we report the synthesis of a series of single crystals of all the RE-UiO-66 analogues obtained through optimisation of reaction conditions. A systematic study is performed to understand the relationship between RE(III)-X (X = O, F) bond lengths holding the cluster together, and those joining the clusters to the linkers to give the network structure. Furthermore, these findings are discussed in relation to the thermal stability of the MOFs in order to form a hypothesis regarding the difficulty in synthesising lighter lanthanoid RE-UiO-66 analogues.

Effects of synthesis parameters on the anatase TiO₂ crystal growth using fluorine as capping agent

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TiO₂ serves as an important semiconductor which has many applications, especially the photocatalysis. Anatase phase TiO₂ is the most studied one due to its intrinsic reactive property as photocatalyst. According to the theoretical calculation, the (001) facet is the most reactive facet, and Fluorine is the most used capping agent to block anatase growth along [001] direction. Although there are many works about (001) facet exposing TiO₂ synthesized using HF, a systematic study about synthesis parameters needs to be done. In this work, HF concentration, Ti/F molar ratio, hydrothermal temperature, hydrothermal time, Ti source, and titanium organic complex concentration (TNBT or TTIP) were considered as the main experimental factors to synthesize TiO₂ with different facets exposing ratio, such as (101), (001) and (100). It was found that the HF weight concentration should exceed 40% to obtain (001) facet exposing TiO₂. With the increasing of HF or the decreasing of Ti/F molar ratio, the morphology changed from truncated bipyramid nanosheets with different size. The hydrothermal temperature could affect the phase purity and (001) facet exposing percentage, and ultrathin TiO₂ (3 nm) was obtained at 160 °C with diluted TNBT. It was found that the (100) facet could be maintained under 3 hours at 230 °C, however, with the increasing of hydrothermal time, (100) facet would be reduced when the time exceeded 12 hours. Also, the (001) facet would be reduced with hydrothermal time increasing, and TiO₂ NSs thickness increased. All TiO₂ samples were characterized by XRD, SEM and TEM, the crystal growth mechanism was proposed.

IN-OPERANDO PHOTO-SWITCHING OF COPPER OXIDATION STATES IN COPPER-BASED PLASMONIC HETEROGENEOUS PHOTOCATALYSIS FOR EFFICIENT H₂ EVOLUTION

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Metal nanoparticles (NP) supported on TiO₂ are known to be efficient photocatalysts for solar-to-chemical energy conversion. While TiO₂ decorated with copper NPs has the potential to become an attractive system, the poor oxidative stability of Cu severely limits its applicability. In this work, we demonstrate that when Cu NPs supported on TiO₂ nanobelts (NBs) are engaged in the photocatalytic generation of H₂ from water under light illumination, Cu is not only oxidized in CuO but also dissolved under the form of Cu⁺/Cu²⁺ ions, leading to a continuous reconstruction of nanoparticles via Ostwald ripening. By nanoencapsulating the CuO_x (Cu/CuO/Cu₂O) NPs by a few layers of carbon supported on TiO₂ (TC@C), Ostwald ripening can be suppressed. The resulting CuO_x@C NPs are photo-reduced under visible illumination to generate Cu@C NPs. This photo-switching strategy allows the preparation of a Cu plasmonic photocatalyst with enhanced activity for H₂ production. Remarkably, the photocatalyst is even active when illuminated with visible light, indicating a clear plasmonic enhancement of photocatalytic activity from the surface plasmonic resonance (SPR) effect of Cu NPs. Three-dimensional electromagnetic wave-frequency domain (3D-EWFD) simulations were conducted to confirm the SPR enhancement. This advance bodes for the development of scalable multifunctional Cu-based plasmonic photocatalysts for solar energy transfer.

PREUVE DE CONCEPT DE MATERIAUX ALCALINS ACTIVES DE RESIDUS DE BAUXITE POUR LA FABRICATION D'ADSORBANTS DE POLLUANTS

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VOTRE RÉSUMÉ

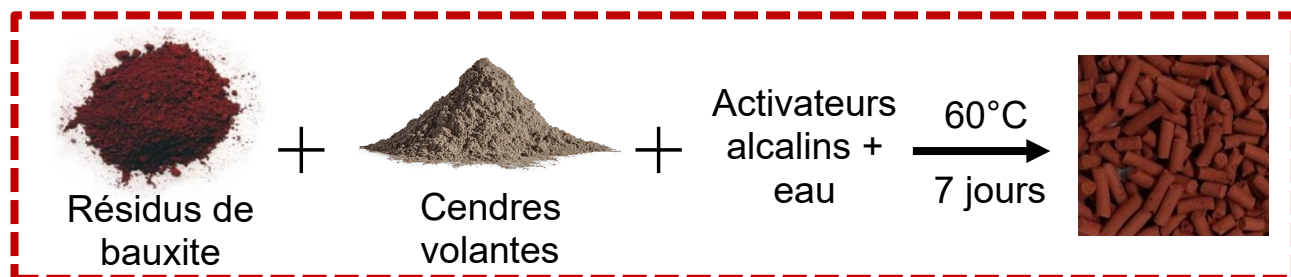
Parmi les différents types de défis liés au développement durable, la pollution de l'eau est l'un des plus surveillés au Canada, notamment pour la préservation des vastes ressources en eau potable du pays. Elle est liée à la présence de contaminants, des composés chimiques toxiques présents dans l'eau. Pour y remédier, différentes techniques existent pour les extraire, comme les adsorbants, des matériaux qui capturent et fixent les polluants à leur surface.

Les résidus de bauxite sont des déchets issus de la production d'aluminium. Leurs propriétés adsorbantes intrinsèques leur donnent l'opportunité de limiter leur empreinte environnementale. Leur utilisation permettrait de réduire l'espace de stockage nécessaire dans les bassins à ciel ouvert, tout en leur offrant une seconde vie dans le cadre d'une économie circulaire. Pour cela, il faut neutraliser leur toxicité due à leur alcalinité et aux métaux lourds présents dans leur composition, et améliorer leurs propriétés physiques.

La technologie proposée par ce projet est basée sur la géopolymérisation, une transformation physico-chimique des solides. Elle vise à activer les oxydes des matériaux et à les rendre plus réactifs avec les contaminants tout en améliorant la fixation des métaux, la résistance mécanique et la porosité. S'agissant d'une technologie récente, une étude approfondie de ses comportements et de ses améliorations doit être réalisée.

Le projet vise à former des matériaux alcalins activés en utilisant le processus de géopolymérisation pour formuler différents prototypes en utilisant une seule étape de mélange et en les coulant dans la forme désirée. Les prototypes les plus prometteurs sont testés pour vérifier leur capacité d'adsorption de contaminants tels que le phosphore, l'azote, le fluorure, le bleu de méthylène et le pentachlorophénol. Des résultats préliminaires sont présentés pour évaluer les performances d'élimination dans l'eau.

FIGURE



A Highly Stable All-Solid-State Lithium–Organic Batteries with Sulfide electrolyte in Low Temperature

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Organic electrode materials (OEMs) as one type of promising alternative for current transition metal oxides are dedicated to fabricating more sustainable lithium-ion batteries in the future. However, the high solubility of OEMs in the conventional liquid-based electrolyte severely restricted its development. As one of the several methods, using inorganic solid-state electrolyte (SSEs) fundamentally prevent the dissolution problem. Here, we demonstrated that one typical organic material 2,2'-Bis(2,3-dihydro-3-oxoindolyliden) (Indigo) showed excellent compatibility with argyrodite sulfide-based SSEs ($\text{Li}_6\text{PS}_5\text{Cl}$) in All-solid-state batteries (ASSBs). With optimized carbon additives, the Indigo-based ASSBs delivered a high capacity of 535 mAh g^{-1} , high energy density of 1123 Wh kg^{-1} , and excellent capacity retention of 91.4% after 100 cycles at room temperature, which is one of the best results for OEMs-based ASSBs. At low temperatures (-10°C), the Indigo-based ASSBs exhibited a capacity of 290 mA g^{-1} and favorable cycling stability (nearly 100% capacity retention after 100 cycles at 0.2C). Moreover, ASSBs with high active material loading (over 10 mg cm^{-2}) are also constructed and showed excellent cycling performance.

MODULATION OF RESPONSE TIME AND SYNAPTIC PLASTICITY IN ION-GATED TRANSISTORS FOR LOW-POWER NEUROMORPHIC COMPUTING

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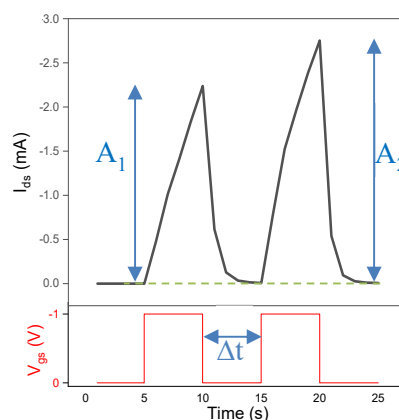
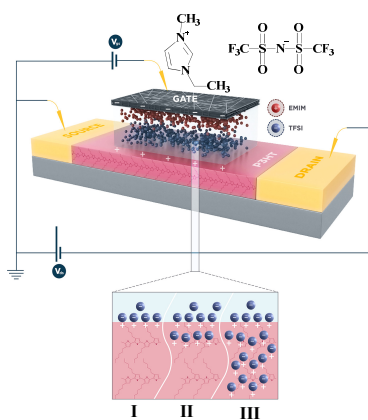
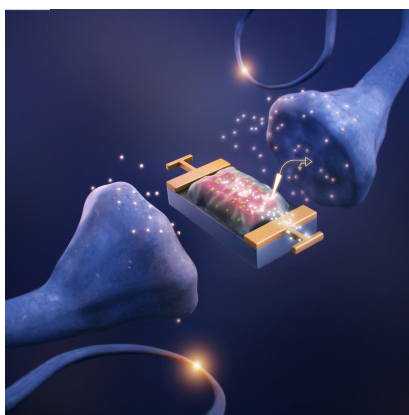
ABSTRACT:

High-performance and low-power consumption neuromorphic computing (i.e., brain-like computing) is attracting increasing attention in the materials science, device engineering, green electronics, and bioelectronic research communities. Ion-gated transistors (IGTs) as synaptic transistors, by perceiving the environment in real-time, can be studied and exploited as neuromorphic devices.

Depending on the permeability of the semiconducting channel to ions, IGTs undergo volumetric (three-dimensional) or electrostatic (field-effect, two-dimensional) doping, which leads to a wide range of response times. Long-term memory and high-speed data processing are essential for neuromorphic computing.

We propose a method to modulate the response time and synaptic plasticity of IGTs made up of poly (3-hexylthiophene, P3HT) gated by the [EMIM][TFSI] ionic liquid. We report on the effect of the frequency of the gate-source voltage (V_{gs}) pulses, the number of applied V_{gs} pulses, and the pulse duration time on IGT response time. With increasing drain-source voltage (V_{ds}) from -0.2 V to -1 V, we observed that the response time halves using a 200 ms-long square step $V_{gs} = -0.5$ V pulses. Moreover, with increasing V_{gs} from -0.5 V to -1 V the response time increases by 27% at $V_{ds} = -1$ V.

Our results shed light on the impact of various aspects of the input voltages on governing the transistor response time and synaptic functions in organic IGTs to reach low-power and fast-switching neuromorphic devices. The methodology also includes the effect of the V_{gs} sampling time on the accuracy of electric measurements of this study.



PORE CHARACTERIZATION FOR ALKALI ACTIVATED MATERIALS SYNTHESIZED USING BAUXITE RESIDUE

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Development of byproducts of materials that are produced in large volumes into usable resources is an efficient method to reduce effects of their disposal, while creating a potential revenue stream for industries. Bauxite residue (BR) is the byproduct of alumina extraction and has crossed 4 billion tons in storage. Alumina industries currently use containment facilities to store the byproduct. However, these facilities are nearly filling up, and run the risk of contaminating nearby ecosystems. An alternative for reusing BR, which is highly alkaline and is composed of numerous metal oxides, must be explored to avoid a scenario of hazardous spills. One solution is to bind BR in alkali-activated materials (AAM).

AAMs are amorphous aluminosilicate matrices that do not need temperatures higher than 100°C to be synthesized. AAMs require a precursor rich in aluminates and silicates, and an alkali activator, such as alkali hydroxide, to form. Using BR as a precursor in an AAM creates a ceramic-like material that has industrial and constructional applications. The synthesis of porous AAMs is currently being studied due to their applications. Porous AAMs that use untreated BR as principal precursor have not been sufficiently studied yet.

Porous AAMs composed of 75% BR and 14% fly ash were synthesized, using sodium metasilicate, calcium hydroxide, and sodium hydroxide as activators. The materials were mixed, and the resulting paste was molded into 2"-cubes, cured at 60°C for seven days, and analyzed. The effect of hydrogen peroxide and sucrose on the porosity of the samples was recorded. Compressive strength of the samples was measured to provide a baseline for potential application.

Resulting samples displayed up to 60% porosity, enabling applications in form of adsorbents, filters, and insulators. The procedure involves low energy usage and minimal chemical treatment, resulting in a fuel-saving and ecologically safe method to valorize BR.



Innovative zirconia-based material shaped by SLA 3D printing

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Introduction

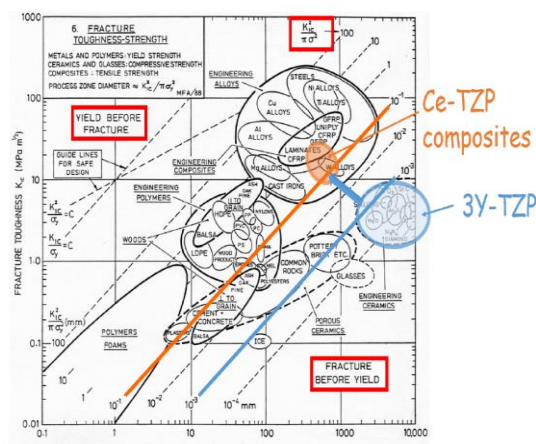
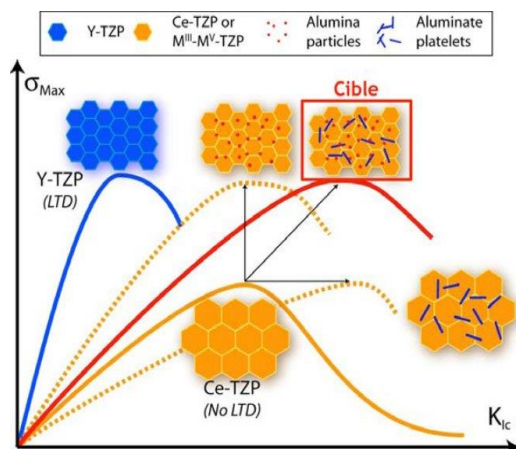
Today a strong need for high-performance ceramic materials combined with new shaping techniques appears on the market. 3D printing technology of ceramic objects is in strong development as it opens new perspectives. While ceramic materials are brittle and subject to catastrophic failure that is difficult to predict, ceria-stabilized zirconia-based composites can provide new ceramic materials with a plastic deformation domain before rupture, excellent resistance to processing flaws and a Weibull modulus approaching that of a steel. In this study, we explored the influence of SLA stereolithography shaping on this new ceria-stabilized zirconia-based material with unique mechanical behavior.

Experimental

Firstly, a slurry compatible with the CERAMAKER process was developed. Then, the specific object of the study was to evolve the influence of the shaping parameters (layer thickness, lasing power, etc.) on the green part quality. Finally, the effect of the sintering temperature on the microstructure and mechanical properties of optimized SLA-printed material was also studied.

Conclusion

Through this study, 3DCERAM has been able to prove that this new material could be shaped by 3D SLA. Different sintering parameters have been studied to optimize densification and material properties. SEM observations show original layer structures and microstructure development attributable to the shaping process.



EXPLORING THE POTENTIAL OF GEL POLYMER ELECTROLYTES FOR HIGH-EFFICIENCY LITHIUM Batteries : PRE- AND POST-TREATMENT STUDIES OF EC-BASED POLYMER BLENDS

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*As the most commonly used rechargeable energy storage device, Li batteries (LiBs) require the continuous development of electrodes and electrolyte materials in order to improve their performance. Solid polymer electrolytes (SPEs) have been presented as safer alternatives for liquid electrolytes as they tend to be non-flammable, have enough mechanical strength to resist dendrite growth, and do not leak. However, these materials tend to be less conductive than liquid electrolytes. This problem can be solved by solid-state gel polymer electrolytes (GPEs), which have lately received more attention. GPEs present a possible solution to this dilemma as they combine the ionic conductivity of liquid electrolytes with the increased safety of SPE.¹ This work presents in-situ GPE preparation from an SPE prepared via melt processing in order to take advantage of the easy processability of SPE and the higher ionic conductivity of GPE.^{2, 3} The initial SPE was prepared by combining two polymers with lithium salt via extrusion mixing. This method of GPE processing was also found to improve other aspects of the electrolyte such as thermal and electrochemical properties which were characterized using cycling voltammetry, electrochemical impedance spectroscopy, and thermal gravimetric analysis. Additionally, *t* salt-polymer interactions in the GPE were characterized using FTIR and NMR.*

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NEAR-INFRARED MULTIFUNCTIONAL NANOPLATFORM FOR DEEP-TISSUE BIMODAL IMAGING AND THERAPY

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YOUR ABSTRACT / VOTRE RÉSUMÉ

Multifunctional nanoplateforms integrating photoluminescence and magnetic resonance bimodal imaging and further, drug delivery capabilities are of significant importance in the emerging research area of theranostics. For photoluminescence technique, imaging in the second biological window in the near infrared range (NIR-II, 1000-1350 nm) has attracted more attention due to the higher resolution and deeper tissue penetration than in the conventional visible range (400-700 nm) and in the first biological window (NIR-I, 700-950 nm). Among NIR-II imaging agents, the lanthanide-doped nanoparticles (LDNPs), free of toxic lead and cadmium usually involved in NIR imaging, are emerging as new generation of promising candidates. In magnetic resonance imaging (MRI), gadolinium (Gd) is most attractive due to its strong paramagnetic properties and indeed, several Gd-based compounds have been approved by the United States Food and Drug Administration as MRI contrast agents for clinical use. In this talk, I will present our work [1] on the synthesis of “bio-safer”, NIR-emitting multifunctional nanoplateforms, and their applications in biomedicine. Specifically, we rationally designed and engineered the nanoplateforms by loading ultrasmall NaGdF₄:Nd³⁺ nanoparticles (~ 4.1 nm in diameter) into relatively large-channel mesoporous SiO₂ (mSiO₂) nanospheres for the first time. Thanks to the unique combination of paramagnetic property, and the capability of being excited by near infrared light in the NIR-I range and emitting in the NIR-II range in single-type nanoparticles of NaGdF₄:Nd³⁺, the NaGdF₄:Nd³⁺@mSiO₂ nanoplateforms realize magnetic resonance and NIR photoluminescence dual-mode tumor imaging of live mice. Moreover, the unique three-dimensional mesoporous structure of the nanoplateforms allows the efficient loading of doxorubicin molecules at a high level and demonstrates pH-responsive drug release behavior that is beneficial for cancer-targeted therapy.

Reference:

[1] Materials Today Advances 16, 100306.

A NEW EMPIRICAL CHALLENGE FOR USING ION LIQUIDS AS A DYNAMIC APPROACH TO DESIGN PDMS-BASED ICEPHOBIC COATING

SABA GOHARSHENAS MOGHADAM

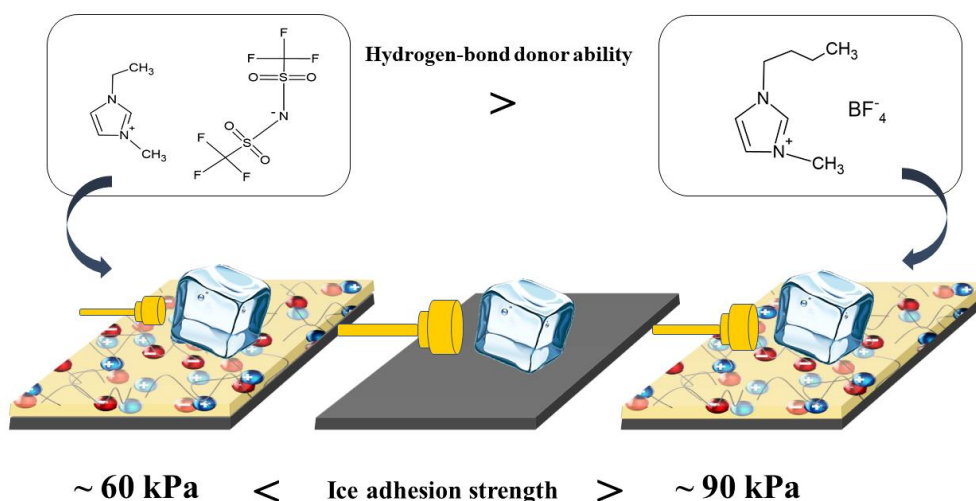
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ABSTRACT

Ionic liquids (ILs) are large organic salts with low melting points, often below 100 °C [1]. They are thought to be antifreeze agents capable of creating dynamic interface melting between ice and a substrate [2]. Ice-accretion issues have been addressed using a variety of solutions over the last few years. Designing ice protective coatings as a passive strategy such as, superhydrophobic and slippery liquid-infused porous surfaces has been ongoing for decades [3,4]. Due to fragility of current static icephobic surfaces at extremely low temperatures, there is considerable interest in finding new processing routes and materials that overcome the shortcomings associated with the current surfaces. Very low freezing temperature, low vapor pressure, wide diversity of hydrophilicity/hydrophobicity and strong hydrogen-bond donor ability based on the cation/anion choice have gained significant attention for creating thicker quasi interfacial liquid-like layer (QLL) at interface to combat icing problem [5]. Large and asymmetric chemical structure of ILs result in disrupting the ordering of crystalized ice structure, leading to creation of a lubricating layer. Their extraordinary ability to donor hydrogen-bonds to water molecules cause requiring additional energy for formation of ice nuclei from such bonded molecules. However, surfaces containing ILs are still infancy. Our contribution sets out to study a close-up of anti-icing behavior of PDMS coating containing two imidazolium-based ILs with fluorinated anions. Surface properties of coatings were investigated with respect to the relationship between wettability and ice adhesion. We were able to discriminate between the two ILs in terms of ice temperature and formation time, as well as ice adhesion strength, using differential scanning calorimetry, freezing delay time, and push-off tests. A comparison of enhanced anti-icing performance of ILs-containing coatings revealed that a minor change in chemical structure of ILs determines their potentials for anti-icing applications.



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Towards single particle electrocatalysis measurements of the oxygen reduction reaction using scanning electrochemical cell microscopy

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The oxygen reduction reaction is an important reaction at the cathode of a fuel cell as well as in metal-air batteries. Due to the slow kinetics of the oxygen reduction reaction, an efficient electrocatalyst such as platinum is currently employed in polymer electrolyte membrane fuel cells. Metallic and bimetallic nanoparticles are being explored to replace platinum with less-expensive materials such as silver and its alloys, which can enable the direct reduction of oxygen to water in alkaline conditions. However, the performance of nanoparticle electrocatalysts depends on many parameters such as the number of active sites, structure, composition, and particle size, which has motivated research in the field of single entity electrochemistry to develop new methodologies that can resolve the electrocatalytic activity of individual nanomaterials. In this work, scanning electrochemical cell microscopy, a droplet-based scanning probe method that measures local electrochemical fluxes with high spatial resolution was used to study the oxygen reduction reaction of silver electrocatalysts on carbon substrates in alkaline conditions.

The oxygen reduction reaction is a multi-step 4-electron reduction reaction following either a direct pathway where oxygen is reduced directly to water or alternatively, an indirect two-step pathway where oxygen is first reduced to hydrogen peroxide in a 2-electron reduction step, followed by a second 2-electron reduction of hydrogen peroxide to water. In alkaline solutions, the oxygen reduction reaction on a carbon substrate follows the indirect pathway generating hydrogen peroxide whereas the reduction of oxygen on silver follows the direct pathway forming water directly. The objective of this work is to enable the quantitative analysis of the electrocatalytic reduction of oxygen on individual silver nanoparticles in alkaline conditions. The working electrode area in scanning electrochemical cell microscopy is determined by the pipette diameter which is typically several hundred nanometers in size while the size of individual nanoparticles is 100 nm or less. To enable the quantitative analysis of individual nanoparticles, a low loading ratio of silver is required. As a result, a significant fraction of the working electrode area is composed of the underlying carbon substrate relative to the amount of silver electrocatalyst. This leads to a non-negligible current arising from the oxygen reduction reaction on the carbon substrate which can interfere with the current being generated by an individual silver nanoparticle. In this work, we will present our recent results that evaluate the role of silver loading and pipet diameter on the ability to resolve the electrocatalytic current generated from an individual silver nanoparticle.

Development of radiopaque PEEK filaments for 3D printing of ocular brachytherapy implants

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INTRODUCTION: Uveal melanoma is a type of eye cancer that is commonly treated with episcleral plaque brachytherapy. However, current episcleral plaques (Eps) are not personalized, resulting in poor conformity between dose patterns and tumor contours, which can lead to side effects on healthy tissues (e.g., damages to the optical nerve). Additive manufacturing (3D printing) of EPs using biocompatible polyether ether ketone (PEEK) polymer could improve the treatment precision. To enable this, PEEK filaments must be produced by extrusion, including certain additives, before being inserted into the 3D printer. This study aimed to develop 3D printable radiopaque PEEK filaments by adding tungsten (W) as an additive for the production of personalized plaques.

METHODOLOGY: Tungsten(W)-loaded PEEK filaments were extruded using a single-screw extruder. The distribution and concentration of W were measured by XRF and MPAES. Fusion temperatures was measured by DSC. The filaments printability was demonstrated using an FFF 3D printer, and the printed objects were evaluated for porosity and defects using a μ CT scanner. ImageJ software was used for CT image analysis.

RESULTS AND DISCUSSION: PEEK filaments (10 m; $\varnothing=1.75$ mm \pm 0.1 mm) with a smooth surface were successfully developed. XRF results show a uniform distribution of W in the filament. DSC analysis suggests that printing temperatures should be lowered slightly as the W concentration increases. CT images show high resolution, defect-free 3D printed objects.

CONCLUSIONS: PEEK filaments loaded with tungsten have been developed for biomedical applications, further studies could investigate modifications to enhance their properties and broaden their medical applications by incorporating other metallic additives, such as silver.

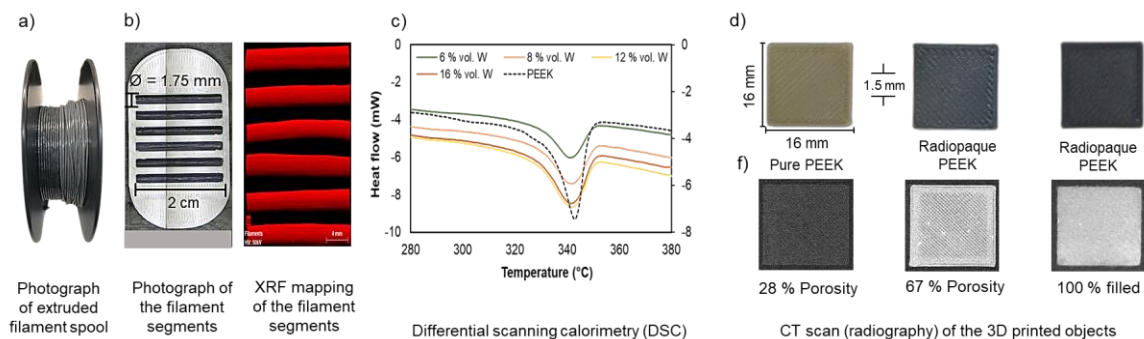


Fig: (a) Photography of the extruded tungsten-containing PEEK filament spool, (b) photography (left) and XRF mapping (right) of 6 individual segments sliced across the filament (red color refers to W), (c) differential scanning calorimetry (DSC) shows the variation of the fusion temperatures as a function of W concentration compared to pure PEEK, (d) photography (above) and CT scan images (below) of 3D printed objects in pure PEEK and radiopaque PEEK.

3D PRINTING OF NANOCELLULOSES

THEO VAN DE VEN

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ABSTRACT

This work addresses two main challenges in additive manufacturing of cellulosic hydrogels and cryogels. Those are (1) the rheological properties of suspensions of electrosterically stabilized nanocrystalline cellulose (ENCC, a member of the family of hairy nanocelluloses) are inadequate for 3D printing of hydrogels, and (2) 3D printed cellulose nanocrystal (CNC) cryogels have poor mechanical properties. The above limitations are effectively addressed by hybridization of CNC/ENCC in the presence of salt at an optimized weight ratio. Controlling the CNC/ENCC weight ratio leads to high tunability of the rheological properties of the hybrid systems, resulting in high-fidelity printing into 3D hydrogels. Similarly, high tunability in mechanical performance of the cryogels, obtained upon freeze drying of printed hydrogels, is achieved by manipulating the CNC/ENCC ratio. Compared to neat CNC cryogels, the compressive strength of the CNC/ENCC (1:1) cryogels is 78% higher. Combined, CNC bestows high printability on the cryogels, while the presence of ENCC leads to the strengthening of the corresponding super porous solid materials. Our findings open new opportunities for sustainable, biocompatible, and lightweight cellulosic structured scaffolds that can be tailored for a broad spectrum of applications.

COORDINATION POLYMERS FOR ANTIBACTERIAL APPLICATION

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ABSTRACT

Organic compounds **1-5** contain carboxylic acid (-COOH) and diaminotriazinyl (-DAT) in a single core were synthesized in high yield and used to make coordination molecules and metal-organic frameworks (MOFs). These five molecules exhibited self – complementary interaction between the -COOH and -DAT groups. The crystals of **1** and **2** grew in perchloric acid revealing that the molecules were assembled by hydrogen bonding between -COOH and -DAT groups to generate one-dimensional (1D) cationic chains which are further connected by bridging perchlorate counter ions and water to create two-dimensional (2D) network. Meanwhile, crystals **3** and **4** grew in nitric acid exhibiting a 2D extended network by hydrogen bonds between NO₃⁻ and dicationic species without self-complementary between -COOH and -DAT groups. Compound **5**, which has two -COOH groups and one -DAT group exhibited self – complementary assemble between -COOH and -DAT groups to generate a 2D network without any bridging counter ions or molecules of water. The results show high interest in self-assembly motifs and coordination motifs of organic species constructed by -COOH and -DAT in a single core. Furthermore, a binary copper (Cu) II complex, named **TD_I2E3_C01**, has been synthesized from compound **4**. The single crystal structural analysis was done, and the initial results revealed that complex **6** is constructed by a binary CuCl₂ cluster which is further chelated by two nitrogen atoms on ligand **4**. In addition, a Mn-MOF, **TD_I2E3_M01**, with the composition of Mn(**4**)₄.(DMF)₃ was synthesized. Its structural analysis showed that Mn-MOF is a 2D framework which constructed by ionic bonds by -COOH group, and coordination bonds by pyridinediaminotriazinyl (PyDAT). The antibacterial analysis revealed that the Cu II complex is a strong antibacterial agent meanwhile the Mn-MOF is not.

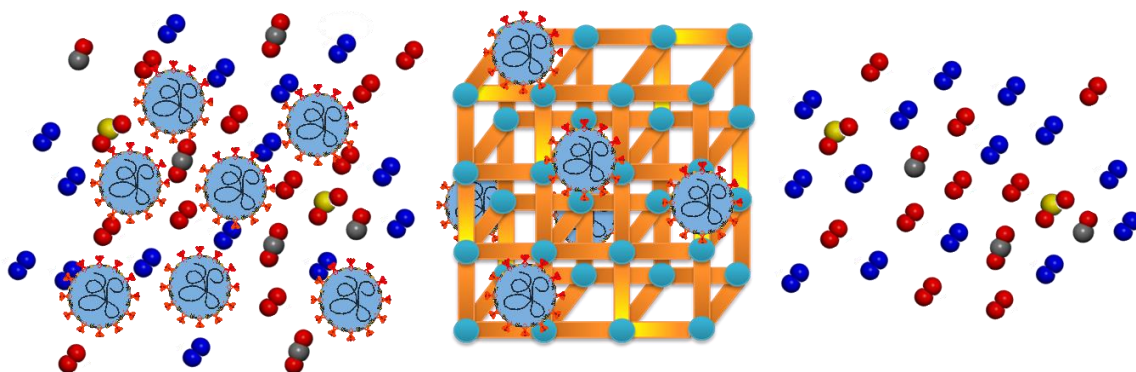


Figure 1. Adsorption of bacterial cells by coordination polymers.

Novel Plasmonic-polymer Hybrid Nanostructure for Photocatalytic H₂ Evolution Reaction

Wanting He

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Abstract

Plasmon-enhanced photocatalysis has attracted great research interest in the past decade. In principle, surface plasmon resonance (SPR) of metallic nanoparticles (NPs) can confine electromagnetic fields in subwavelength space around the NPs and contribute to photocatalysis by enhanced scattering, hot carrier transfer, near field and plasmon-heating effects. To gain benefits from the plasmonic NPs, the strong interface and short distance between the plasmonic NPs and semiconductor material are desired. Herein, we describe a design of a plasmonic-semiconductor hybrid structure, and its efficient photocatalytic activity in hydrogen (H₂) evolution reaction by water splitting. The presented novel hybrid structure is composed of a single plasmonic gold NP sitting on a self-assembled polymer sphere (Au@THPG heterodimer), like a cap with an intimate interface. The polymer sphere is made of the photon-absorbing, hyperbranched polyporphyrins g-polymer. Thanks to the plasmonic effect close to the interface, such plasmonic-polymer photocatalysts exhibited 8-fold H₂ production enhancement in the visible range as compared to plasmon-free supramolecular THPG spheres. For deeper understanding of the hybrid structure and plasmonic effect on photocatalysis in this hybrid, we further carried out a series of characterizations such as optical spectroscopy, scanning transmission electron microscope/electron energy loss spectroscopy (STEM/EELS) and photon-induced near-field electron microscopy (PINEM) technique. By doing so, we were able to reveal the strong localization of plasmonic near-fields around the Au and the Au-polymer interface. The near-fields of Au@THPG heterodimer exhibit frequency- and polarization- dependence. This work offers fundamental insights into the design and synthesis of versatile and effective plasmonic-organic based NPs for photocatalytic applications.

NOVEL BIO-SOURCED POLYOXANORBORNENE AS POTENTIAL REPLACEMENT FOR HIGH-CARBON FOOTPRINT THERMOSTABLE MATERIALS

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Polynorbornenes (PNBEs) prepared by 1,2-insertion catalytic polymerization are widely used as catalysts carrier, anion exchange membrane, photopatternable membrane and many other areas, because of their thermal stability and chemical stability. However, PNBEs hardly become ideal green materials its fossil-based materials. Impressively, Oxanorbornenes (ONBEs) is a kind of bio-sourced compounds, can be synthesized by Diels–Alder reaction between renewable furan and variable dienophiles. Here we first prepare polyoxanorbornenes (PONBEs) by 1,2-insertion catalytic polymerization, (norbornene-endo-5 σ ,2 π) Pd(II) is used as catalyst in this polymerization. Compared with other potential catalysts, (norbornene-endo-5 σ ,2 π) Pd(II) is more tolerant to products of retro Diels–Alder reaction. Although some papers already reported that only homo-PNBE is generated in NBE polymerization even rapid retro Diels–Alder and Diels–Alder reactions are occurred during polymerization, in polymerization process of ONBE(COOMe)₂, dimethyl maleate as retro Diels–Alder product rapidly inserted into PONBE polymer chain and thereby forming copolymer. Facile retro Diels–Alder reaction of ONBE is widely reported and was proved by our DFT results. DFT calculations indicate that retro Diels–Alder reaction products (thermodynamic product) are more stable than Diels–Alder reaction products. Therefore, during the polymerization, even when starting from pure monomer, retro Diels–Alder reaction products is generated and inserted into the polymer chain. PONBE(COOMe)₂ display particularly high thermostability with a 5% weight loss temperature of 397°C. Moreover, no obvious glass transition temperature (T_g) was observed in the DSC when the temperature was elevated near 350 °C. In addition, PONBE(COOMe)₂ shows strong florescence in solid state under 345 nm UV light, this polymer with AIE effect have potential to be as a thermostable fluorescent probe.

A SPRAYABLE COUMARIN-CONTAINING COMPOUND FOR PHOTOALIGNMENT OF LIQUID CRYSTALS ON CURVED SURFACE

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Abstract:

The success of the photoalignment of liquid crystals (LCs) provides displays and other optical applications with more possibilities, compared with the surface rubbing technique. Especially, it is highly demanded for applications requiring LC alignment on curved surfaces, for which surface rubbing cannot apply. Photodimerization of photoactive molecules coated on the substrate under polarized light irradiation is one of the photoalignment methods. The resulting surface alignment layer can align LC molecules deposited on the surface due to anisotropic interfacial interactions. In this work, we present a detailed study on the photoalignment behaviors of a novel coumarin-containing compound which can be spray-coated on curved surface. The photoalignment of LCs using this coumarin-containing compound is investigated by monitoring the dichroic absorption of dye-doped nematic LCs. It is found that the order parameter can reach about 0.5 by adjusting the thickness of spray layer and the polarized light intensity. In addition to LC alignment on curved surface, photo-patterned LC orientation is also conducted. The results show that the novel structure of coumarin-containing compound is promising for photoalignment of LCs.

CONTROLLABLE GRAPHENE ASSEMBLY FOR ARCHITECTURAL DESIGN

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YOUR ABSTRACT / VOTRE RÉSUMÉ

Graphene-based materials have gained great interest for broad applications and can be fabricated using graphene oxide (GO) and reduced graphene oxide (rGO) flakes as building blocks. Through controlling sheet assembly, graphene materials' architecture can be tailored to desired applications. Herein, we control the assembly of flakes at the interfaces of Pickering emulsions to develop GO and rGO materials for bone tissue engineering (BTE) and seawater electro-oxidation applications. We also demonstrate temperature-responsive rGO self-assembly by surface modification and supramolecular design.

We first obtain porous GO and rGO materials with interconnected or closed pores and tunable compositions through GO emulsions. For BTE, we create GO and rGO based scaffolds with interconnected hierarchical structures and variable compositions through emulsion-ice dual-templating.¹ Upon freezing and drying the emulsions, large and small pores can be templated by oil droplets and ice crystals, respectively. With architectures tailored for BTE, the GO scaffolds are excellent substrates for mesenchymal stem cell penetration and growth. We subsequently introduce rGO/cobalt oxide electrodes for selective seawater electro-oxidation.² We generate closed pores templated by GO emulsions enclosing catalytic Co₃O₄ particles in the oil droplets. After reduction, the rGO pore walls are permeable to water and gases while limiting the diffusion of chloride to the catalytic particles deposited on the internal pore walls. The closed rGO pores enclosing catalytic particles improve the electrode's selectivity for water oxidation application. Lastly, we achieve the graphene temperature-responsive self-assembly via an amphiphilic structure incorporating polydopamine (PDA) clusters on rGO flakes, which are not intrinsically responsive.³ The interactions between the rGO/PDA flakes and water are exploited to induce temperature-responsive self-assembly, allowing the creation of 2D nacre-like films and porous monoliths with structures tunable by temperature. Overall, our work provides insights on controllable and versatile assembly strategies for architecture design and preparation of graphene materials.

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STRATEGIES TOWARD POLYSULFIDES SHUTTLE INHIBITION FOR HIGH PERFORMANCE LI-S BATTERIES

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Lithium-sulfur (Li-S) battery is one of the most potential candidates for the next-generation energy-storage system due to their high energy density, while the application and commercial viability are severely hindered by the polysulfide shuttle and large volume change ($>80\%$) of sulfur species. A self-healing poly(urea) (PU) coating layer crossed-linked by hydrogen bonds is proposed to tackle both issues simultaneously. The dynamic hydrogen-bonding networks not only physically and chemically immobilize polysulfides but also repair the cracks and ensure the integrity of sulfur cathodes. Therefore, the Li-S batteries with PU coating layer exhibit a better cycling performance ($784.42 \text{ mAh g}^{-1}$ after 1000 cycles at 0.2C) than batteries without PU coating layer ($693.55 \text{ mAh g}^{-1}$ after 100 cycles at 0.2C). Additionally, to fundamentally address the polysulfide shuttle problem, a solid-state Li-S battery using a sulfide-based solid-state electrolyte with high ionic conductivity was designed. The specific capacity and cycle stability are further improved ($1465.38 \text{ mAh g}^{-1}$ after 100 cycles at 0.2C). The effect of the carbon materials structure as sulfur hosts on the performance was also investigated.

Controllable Synthesis and Development of One-dimensional CdS-based Photoanodes with Special Nanojunctions for Efficient PEC H₂ Production

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YOUR ABSTRACT / VOTRE RÉSUMÉ

YOUR ABSTRACT / VOTRE RÉSUMÉ

(300 words -1page max)

Photoelectrochemical (PEC) water splitting for hydrogen evolution is a highly-efficient and eco-friendly technology in solar energy conversion, but the question is still how to build an available PEC system with satisfied photoconversion efficiency. Photoactive materials as the basic component for PEC systems, have been extensively studied due to their distinct structure features. Among them, cadmium sulfide (CdS), especially one-dimension (1D) oriented CdS nanoarray has attracted considerable attention and is regarded as a promising candidate for PEC hydrogen production due to its suitable narrow bandgap (2.4 eV), excellent electrical/optical properties, larger aspect ratio and confined charge transfer path for lower carrier loss. However, bare CdS nanoarray photoanode suffers from serious surface charge recombination, photo-corrosion, and low quantum efficiency, which is greatly limiting its practical application. Here, the rational design of CdS-based nanojunctions, like Plasmon-enhanced, Z-scheme, and p-n scheme heterostructure, was employed to overcome these drawbacks for maximum solar light utilization and superior photoconversion efficiency. Specifically, a series of novel and highly-efficiently CdS-based composite photoanodes based on (i) Au NPs decorated carbon-wrapped oriented CdS nanoarray; (ii) the Z-scheme CdS/SnO₂ heterojunction with Au NPs as the electron transport medium, and (iii) 1D core-shell CdS nanorod/MoS₂ heterostructure will be discussed.

FIGURE

(Optional / Facultative)

Magnetoresistance effect in polymer field-effect transistor

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Migratory animals in nature can amazingly sense Earth's extremely weak magnetic field (~50 microtesla) and use it as a compass for the precise navigation in their long-distance migration. It has been turned out that this mysterious magnetoreception capability is closely related to the quantum spin dynamics of radical pairs from their magnetically sensitive proteins¹. Intriguingly, some lab-synthesised organic semiconductors (OSCs) can also show a similar magnetic field response but to a wider range (from sub-millitesla to tens of tesla), even at room temperature. The resistance of electrical devices made by these materials will demonstrate a noticeable variation when they are put into a magnetic field environment, which is called the organic magnetoresistance (OMAR). As OMAR is originated from the intrinsic spin dynamics which is intimately coupled with the charge transport in OSCs, it represents an ideal playground for understanding fundamental spin physics and the corresponding structure-property relationship.

Till present, most of the studies have been based on limited kinds of model OSCs with a relatively slow charge transport and a common 2-terminal diode-type device structure². Compared with a diode, the 3-terminal field-effect transistor (FET) structure provides an additional knob to tune the charge (spin) density in the semiconductor by electrostatic doping. Furthermore, the structure of additional semiconductor-dielectric interface tuned by different self-assembled monolayers would exert an important influence on charge (spin) transport. Thus, an extensional study to state-of-the-art OSCs in FET may provide more insights on the fascinating OMAR. Herein, we chose 3 typical high-performance polymers representative of p-, n-, and ambipolar-type polymeric semiconductors, respectively. Exploiting the FET structure, we studied OMAR in these polymers under both low and high magnetic fields. I will present in more detail on our systematic experimental investigation of temperature-, electric field-, interface-dependent magnetoresistance.

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DNA Chimeras as Electrochemical Biosensors for Host-Guest Measurements in Blood

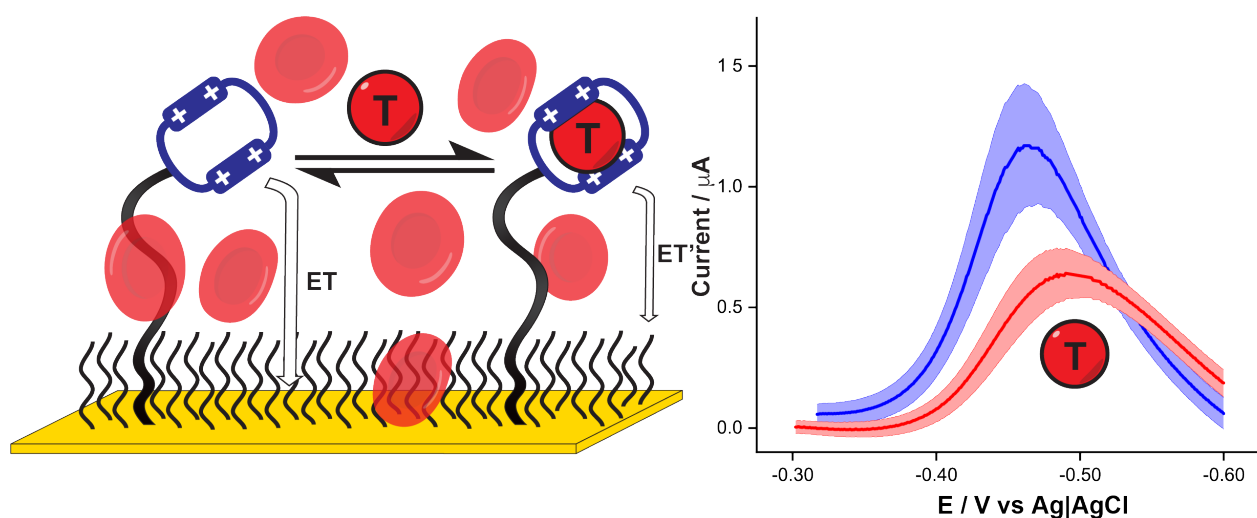
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Few sensing platforms have become ubiquitous to enable rapid and convenient diagnostics at the point-of-care. Those, however, are “one-off” technologies, meaning that they can only detect a single target and hardly adaptable to detect others. In response, we plan to develop a generalizable sensing platform that affords rapid, convenient, and continuous measurements of molecules directly in undiluted complex matrices. For this, we decided to rely on a host molecule that presents reversible interactions toward specific guest molecules to develop a new class of sensors that we coined “Electrochemical DNA-host chimeras”. As a proof-of-concept for our host-guest sensor, we decided to use cyclobis(paraquat-*p*-phenylene) (referred as “blue box”) that we attached on an electrode-bound DNA to allow measurements of biologically relevant electron-rich guest targets such as dopamine and aspirin. Doing so allows to promote host-guest complex formation that could be quantified using blue box’s electrochemistry. Because of our unique sensor architecture, we achieve, to our knowledge, the first reagentless, continuous, rapid (< 5 min) and convenient host-guest measurements directly in undiluted whole blood. We envision that given the vast library of host molecules that this represents the first steppingstone toward the development of a generalizable sensing platform for convenient and rapid measurements directly in complex matrices at the point-of-care.



Affiches / Posters

Surprising Chemistry of 6-Azidotetrazolo[5,1-a]phthalazine: What a Purported Natural Product Reveals about the Polymorphism of Explosives

AARON GABRIEL NUNEZ AVILA

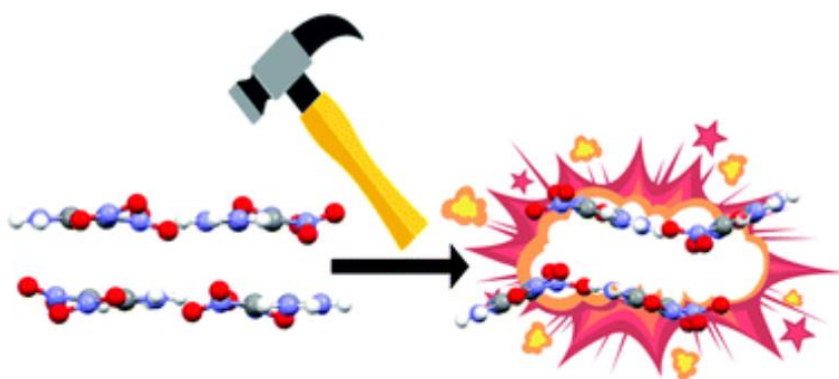
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YOUR ABSTRACT / VOTRE RÉSUMÉ

6-Azidotetrazolo[5,1-a]phthalazine (ATPH) is a nitrogen-rich compound of surprisingly broad interest. It is purported to be a natural product, yet it is closely related to substances developed as explosives and is highly polymorphic despite having a nearly planar structure with little flexibility. Seven solid forms of ATPH have been characterized by single-crystal X-ray diffraction. The structures show diverse patterns of molecular organization, including both stacked sheets and herringbone packing. In all cases, $N\cdots N$ and $C-H\cdots N$ interactions play key roles in ensuring molecular cohesion. The high polymorphism of ATPH appears to arise in part from the ability of virtually every atom of nitrogen and hydrogen in the molecule to take part in close $N\cdots N$ and $C-H\cdots N$ contacts. As a result, adjacent molecules can adopt many different relative orientations that are energetically similar, thereby generating a polymorphic landscape with an unusually high density of potential structures. This landscape has been explored in detail by the computational prediction of crystal structures. Studying ATPH has provided insights into the field of energetic materials, where access to multiple polymorphs can be used to improve performance and clarify how it depends on molecular packing. In addition, our work with ATPH shows how valuable insights into molecular crystallization, often gleaned from statistical analyses of structural databases, can also come from in-depth empirical and theoretical studies of single compounds that show distinctive behavior.



Missing Puzzle in Crystal Engineering: 2-Pyridone and [1,3,5]-Triazine-2,4-diamine, the Two Most Common Cyclic Hydrogen Bonding Sticky Sites, in a Single Core

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Keywords: diaminotriazine (DAT), pyridone, crystal engineering, structure, hydrogen bonds.

Crystal engineering is a popular subfield of materials science.¹ It deals with the design and synthesis of ordered structures by controlling the arrangement of atoms and studying their self-assembly within the crystal lattice. The term *crystal engineering* was first proposed by Schmidt² in the 1970s and defined by Desiraju in the 1990s as understanding intermolecular interactions in crystal packing to create materials with desired properties or functions³. Among the most common intermolecular interactions used as tools in crystal engineering, we find strong hydrogen bonds (e.g., O-H---O, N-H---O, O-H---N)⁴, weak hydrogen bonds (e.g., C-H---O, C-H---N...)⁵, π - π interactions, and van der Waals forces.

Herein, from a crystal engineering perspective, the intermolecular interactions in a new family of pyridone-diaminotriazine (PDO-DAT) type compounds are investigated. We have succeeded in joining these two sites in the same core molecule, highlighting their ability to self-associate by forming heteroleptic hydrogen bonds between the free hydrogen atom of the DAT group and the oxygen atom of the PDO group.

A one-pot reaction method has been successfully developed for the synthesis of eight new PDO-DAT compounds in high yield.⁶ Their identity and purity were confirmed by several characterization techniques, such as: mass spectrometry (MS), ¹H and ¹³C nuclear magnetic resonance (NMR) and infrared (FTIR) spectroscopy. Furthermore, their thermal behavior was studied using thermogravimetric analysis (TGA) and their molecular structures in the solid state were obtained by single crystal X-ray diffraction (SCXRD). In addition, to learn more about the intermolecular interactions between neighboring molecules in a crystal lattice, we used Hershfeld analysis (HS) and 2D fingerprint diagrams generated by computational chemistry software (Crystal Explorer).

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A PROMISING NEW OPTICAL NANOPROBE FOR CELLULAR IMAGING: AMINE PASSIVATED FLUORESCENT CARBON DOTS

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YOUR ABSTRACT / VOTRE RÉSUMÉ

Carbon dots (CDs) have garnered significant attention in the past decade owing to their fascinating luminescent properties and potential use in cell and tissue imaging, as well as for the study of biological processes. These quasi-spherical amorphous carbon-based nanomaterials can be tailored to emit light from the UV-NIR regions of the spectrum while offering low cytotoxicity and good biocompatibility. These properties then influence their cellular uptake, cytotoxicity, and sub-cellular localization. The physico-optical and -chemical properties of CDs are determined by the precursors, methods of preparation, and reaction conditions.

In this work, CDs synthesized from citric acid and five different amine passivating agents were characterized to reveal their properties, and determine how these properties affect their uptake and localization in cultured human cells (HFF-1; human male foreskin fibroblasts, and HeLa; human female cervical carcinoma). All CDs exhibited fluorescence with a corresponding max λ_{ex} at 350 nm and max λ_{em} at 450 nm. We found that these quasi-spherical amine passivated CDs ranged in size from 1.3 to 2.7 nm, and had similar functional groups such as carboxyl, amines and amides. There was an increase in surface charge from -21 mv to +8 mv that correlated with the increase in amine passivation. All of the CDs had low cytotoxicity in both HFF-1 and HeLa cells, with an increase in uptake that correlated with an increase in their surface charge. While all of the CDs localized to the lysosomes, suggesting entry and trafficking via the endomembrane system, there was a difference in their enrichment; some (with the most amine-passivation) most strongly co-localized with lysosomes in both cell lines. Interestingly, CDs with amphiphilic properties also localized in the cytosol likely due to passive uptake. These findings indicate that CDs could be designed to have diverse optical properties and subcellular localization, which could be explored for applications as bioimaging nanotools, and delivery agents.

DÉVELOPPEMENT D'ÉLECTROLYTES BIOSOURCÉS POUR LES PILES RÉDOX À FLUX À L'AIDE DE LA CHIMIE NUMÉRIQUE

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Un enjeu important du développement d'énergies renouvelables, mais fluctuantes, telles que l'éolien ou le solaire, est le stockage à long terme. Les piles rédox à flux permettent de pallier ce problème en utilisant des réservoirs d'électrolyte qui emmagasinent de façon stable l'énergie générée. Toutefois, l'électrolyte couramment utilisé dans ces batteries est le vanadium, une terre rare dont la quantité disponible commercialement sera insuffisante pour répondre à la demande croissante de la prochaine décennie. Une solution de remplacement est l'utilisation de molécules rédox organiques, qui ont l'avantage d'être renouvelables et d'avoir des propriétés modulables selon les groupements utilisés. Il est ainsi possible de modifier certaines propriétés d'intérêt (solubilité, potentiel rédox) en ajoutant des substituants spécifiques à une molécule de base, comme le méthyle viologène, connu pour ses réactions rédox réversibles. Les possibilités de modifications étant nombreuses, il serait utile de pouvoir prédire les propriétés des molécules sans avoir à toutes les tester. L'objectif de ce projet est de développer une méthode de calcul par chimie numérique qui puisse prédire les propriétés d'intérêt de molécules rédox, plus particulièrement le potentiel

rédox de viologènes substitués sur le cœur bipyridine. Tout d'abord, une revue de littérature et différents calculs effectués sur le méthyle viologène ont permis d'établir une méthode de calcul des potentiels théoriques par DFT en utilisant la fonctionnelle ω B97X-D, la base def2-TZVP et une représentation non explicite du solvant aqueux à l'aide du modèle C-PCM. Afin de limiter les erreurs dues aux approximations des calculs, tous les potentiels sont rapportés par rapport au potentiel du méthyle viologène non substitué, qui est utilisé comme référence. Cette méthode a été utilisée pour calculer le potentiel rédox de quatre dérivés du viologène. Ensuite, le potentiel rédox de ces mêmes molécules a été mesuré expérimentalement, et les résultats ont été corrélés aux données calculées (voir figure 1). La pente obtenue (0,89) se rapproche de l'unité, ce qui montre que la méthode de calcul utilisée permet de décrire adéquatement le potentiel rédox de ce type de composés.

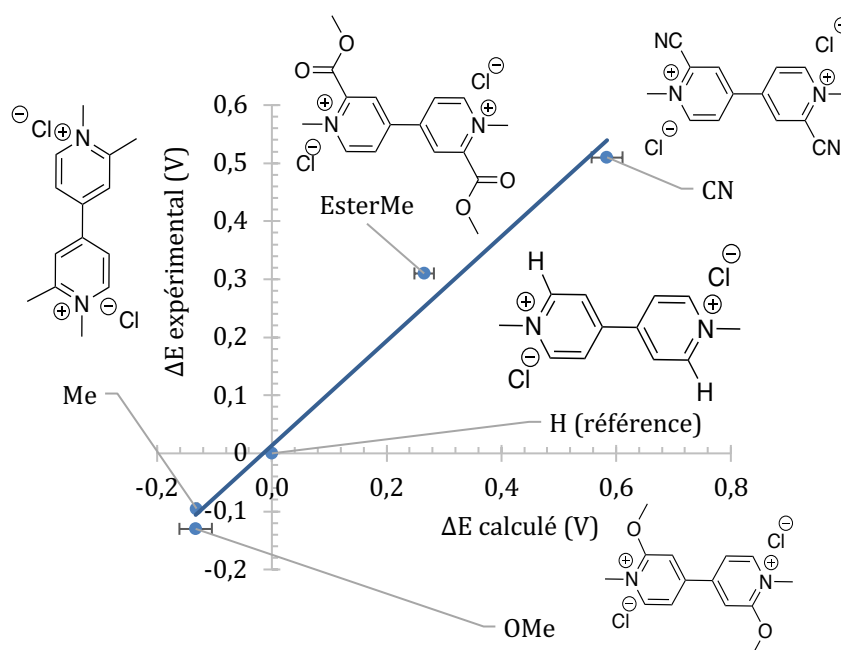


Figure 1: Corrélation entre le décalage des potentiels calculés et expérimentaux de dérivés de viologènes substitués sur le cœur bipyridine par rapport à la référence

COMPARATIVE STUDY ON THE EFFICIENCY OF NOVEL MODIFIED CHITOSAN-BASED ELECTROSPUN NANOFIBERS FOR REMOVAL OF FLUOXETINE FROM WASTEWATER TREATMENT

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YOUR ABSTRACT / VOTRE RÉSUMÉ

Pharmaceutical substances and their metabolites and conjugates are expelled from users through urine and faeces during and after medical therapy. However, drugs wind up in wastewater treatment plants, which are not built to handle this organic micropollutant. Therefore, these substances were chosen as the study's target pollutant because there is ample evidence that it has contaminated the environment. In this study, the antidepressant medication fluoxetine was removed from the solution using a new technique based on electrospun nanofibers made of N-phthalic chitosan and N-succinyl chitosan combined with polyethylene oxide (PEO) as a copolymer for electrospinnability. The electrospinning settings were tuned to achieve the best nanofiber morphology as determined by scanning electron microscopy (SEM). Adding the right chemical groups to the surface of CS through chemical modification allows for eliminating fluoxetine. The properties of modified CS were studied using Fourier-transform infrared (FTIR) spectroscopy and ¹H-NMR spectroscopy. Consequently, fluoxetine was chosen as a model pollutant to characterize adsorption using a high-performance liquid chromatography system with ultraviolet diodes array detection. The maximum removal efficiency (adsorption capacities) for N-phthalic chitosan/PEO and N-succinyl chitosan/PEO nanofibers, respectively, were 72.22% and 81.16%, which also showed that they were promising candidates for removing fluoxetine from wastewater. Finally, the application of the suggested technique was investigated, and it was confirmed that the adsorbent-modified chitosan derivatives demonstrated the capability to adsorb fluoxetine. This allowed for the efficient adsorption and removal of the pollutant. Additionally, the outcomes show that modified chitosan nanofibers that have the potential to reduce fouling in water treatment applications.

Sample preparation by filtering using SWCNTs membrane in an Electrochemical biosensor

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Electrochemical biosensors are devices that utilize the electrochemical properties of biomolecules for sensing applications. Carbon nanotubes (CNTs) have been increasingly used in microfluidic-based electrochemical biosensors due to their unique electrochemical properties, high surface area, and excellent biocompatibility. The integration of CNTs into microfluidic-based biosensors has led to improved performance in terms of sensitivity, selectivity, and response time. In this study, we introduced an electrochemical microfluidic based biosensor to filter samples before detection. To fabricate this biosensor, we have applied several approaches to have more sensitive, cheap, and more flexible biosensor. CNT membrane was fabricated by vacuum filtration and the ratio of CNT concentration was tested to obtain the best sample (more conductive, the porous membrane to filter). The ratio of CNT solution to mix with DI water should be 5:1, the pore size is 0.05 μm , and the resulting film thickness is between 0.5-0.7 μm . This membrane can be used as a filter and working electrodes. We tried several approaches, thermal printing, screen printing, Aerosol print and PDMS mold filled with ink. We need to fabricate the sample, which is cheap, easy to fabricate and also more flexible. For microfluidic based biosensor, we have tested PMMA and PDMS channels. PDMS is more flexible and easier to fabricate, but the more challenging issue regarding PDMS is bonding with other substrates. The only problem with PMMA is that this material is not flexible. We also fabricated a biosensor with thermal printing and then we injected Ferrocyanide into the channel to check CV measurements. We have compared two biosensors (one with CNT membrane filter and one with CNT working electrode without filtering the samples). The results show that when we applied a basic voltage to the electrodes, the electrolyte solution will be moved through the 3 electrodes, and we can read the signal. The one biosensor which filtered the sample with CNT filter improves the signal and the graph jumps suddenly. So, the filter improves the sensitivity of the biosensor.

TOWARDS A POINT-OF-CARE METHOD FOR THE DETECTION OF FERRITIN IN BLOOD USING A SURFACE PLASMON RESONANCE (SPR) SENSOR

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YOUR ABSTRACT / VOTRE RÉSUMÉ

The main goal of this project, in collaboration with Héma-Québec, is to develop a point-of-care method to quantify ferritin in human blood with a minimum volume of less than 200 μ L. Ferritin is a good biomarker for iron, since its main functions are to store and detoxify it. It can be found in plasma with concentrations from 90 to 150 ng/mL and 90 to 200 ng/mL in women and men respectively. In the case of anemia, a concentration under 15 ng/mL is observed and is associated with iron absorption issues, certain infections, and loss of blood. Frequent blood donors can have a decrease of iron in their blood, which motivates our goal of using surface plasmon resonance (SPR) on site at blood drives. Hemoglobin levels are measured with a fingertip puncture to determine if a donor is anemic, but not ferritin levels. The methods already suited for the quantification of ferritin are labor-intensive and not amenable to a POC approach. SPR quantifies the interactions between biomolecules. In this case, a specific polyclonal antibody to ferritin is bound on a peptide monolayer on the gold surface to capture and quantify ferritin in blood products. Multiple optimization steps will be presented to achieve the low detection limits required for ferritin: immobilization step, type of antibody, pH, secondary detection, validation in different biological matrices, surface chemistry, etc. The main challenges of this project are the size of the protein and the matrix effects. To detect the smaller concentrations, the use of nanoparticles in a secondary detection was optimized reducing background noise, the limit of detection and enhancing the signal caused by the coupling of plasmons. Lateral flow membranes were used to obtain serum directly from blood and reduce non-specific interactions caused by other components in the matrix.

NANOFIBRILLAR CONDUCTING POLYMERS FOR STRETCHABLE ELECTRODES

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ABSTRACT

In recent years, research efforts have focused on developing sustainable electronics by diverging from conventionally used metals such as ITO for conductive layers. Efforts have also been dedicated to replacing glass substrates because of their limited mechanical properties. As such, new materials with improved mechanical properties such as stretchability and bendability are of interest. ITO must also be replaced as the conductive layer in electrodes because of its brittleness. The electrospinning of conductive layers as nanofibers is an appropriate technique for producing mechanically compliant conductive layers that can potentially be used in stretchable electronics.

In this study, the potential of nanofibers that are prepared from a conductive polymer without a dispersing polymer for use in stretchable devices is explored. A self-doped conductive polymer (poly ProDOT-sulfate) was prepared, and it was electrospun into nanofibers on a stretchable and bendable substrate. Both the conductivity after spinning and mechanical properties will be evaluated towards using the stretchable electrode in flexible electrochromic device.

Adsorptive Removal of Iodate from Water using a Zr-based Metal–Organic Framework

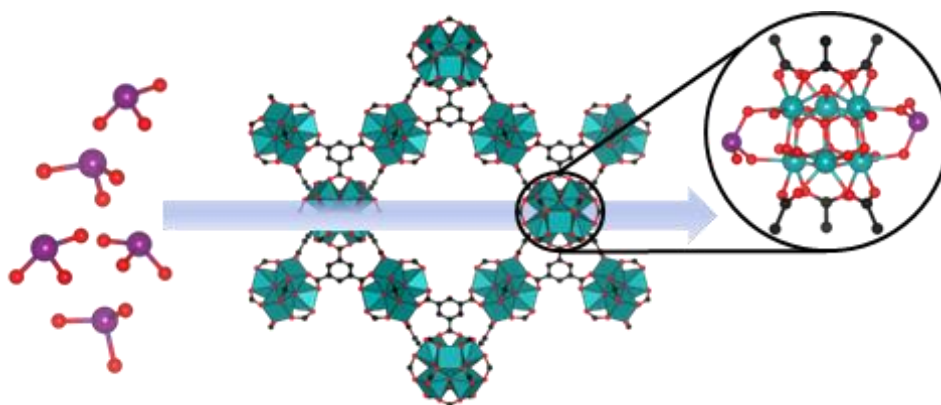
Chris Copeman

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Radioisotopes of iodine are produced as a result of nuclear fission and nuclear fuel processing, and can exist in oxic aqueous environments as its oxyanion, iodate, IO_3^- . Due to the essential nature of iodine in the human body, these radioisotopes are readily taken up, where they can accumulate in the thyroid, potentially causing hormonal problems or cancers. A Zr_6 -based metal–organic framework (MOF), MOF-808, is investigated for the adsorptive removal of IO_3^- from aqueous solutions, due to its high surface area and abundance of open metal sites. The uptake kinetics, adsorption capacity and binding mode are studied, showing a maximum uptake capacity of 233 mg/g, the highest reported by any material. The method of nodal iodate binding is studied by differential pair distribution function (dPDF) analysis of synchrotron total X-ray scattering data. Additionally, the MOF is tested for its ability for regeneration and potential for multi-cycle reuse, as well as post adsorption characterization to ensure its stability.



INFLUENCE DE LA PRÉSENCE DE MÉDICAMENTS OCULAIRES SUR LES PROPRIÉTÉS MUCOADHÉSIVES DES NANOPARTICULES D'OR

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La majorité des médicaments utilisés pour traiter les maladies de l'œil est administrée à l'aide de gouttes oculaires. Cependant, l'œil est équipé de plusieurs barrières physiologiques permettant la protection de ses tissus contre les molécules qui peuvent se présenter à sa surface. Lorsqu'une goutte médicamenteuse est administrée, moins de 0,02% des molécules actives rejoignent leur site d'action. Il est donc essentiel de développer des vecteurs de médicaments mucoadhésifs pour augmenter le temps de rétention des médicaments à la surface de l'œil et donc leur efficacité. Le laboratoire d'accueil pour ma maîtrise a démontré pour la première fois le caractère mucoadhésif des nanoparticules d'or (AuNPs). Mon projet de recherche repose donc sur l'hypothèse qu'il est possible de moduler les propriétés mucoadhésives selon les différents types de nanoparticules et les muqueuses ciblées. Mon objectif général est d'étudier l'influence de divers paramètres sur la mucoadhésion des nanoparticules d'or, afin d'optimiser leurs propriétés en tant que vecteurs de médicaments oculaires. Plus précisément, les résultats présentés ici seront liés à l'influence de la présence des médicaments sur les propriétés mucoadhésives des AuNPs. L'interaction entre les AuNPs et les mucines est caractérisée par différents protocoles de colorimétrie et de spectroscopies UV-visible et de fluorescence. Les médicaments utilisés sont le kétorolac et le flurbiprofène (qui sont des anti-inflammatoires) encapsulés à différents ratios (AuNPs : médicament) afin d'observer l'influence de ces médicaments sur la mucoadhésion. La présence de médicaments encapsulés dans les AuNPs influencent leur capacité à interagir avec les mucines, et ceci dépendamment de la nature du médicament. Aussi, les propriétés intrinsèques des médicaments altèrent notre capacité à réaliser certains protocoles par leurs interactions avec les réactifs utilisés. Les nanoparticules d'or interagissent différemment avec les mucines selon si elles contiennent des médicaments encapsulés ou non. Il est donc possible de moduler leurs propriétés mucoadhésives selon les conditions expérimentales choisies.

ACTIVE SITES STUDY AND STRATEGIES TO IMPROVE THE STABILITY OF Fe/N/C CATALYSTS IN FUEL CELLS

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As a clean energy technology, fuel cells hold great potential to significantly reduce greenhouse gas emissions while providing energy security and sustainability. The polymer electrolyte membrane fuel cells (PEMFCs) are among the most promising fuel cells because of their relatively low operating temperature and the use of H₂ and O₂ as fuels, for which the only by-products are water and heat; thus, providing clean and efficient energy. Platinum group metal (PGM) based materials are the state-of-the-art catalysts to promote the sluggish cathodic oxygen reduction reaction (ORR) in PEMFCs. However, their high cost and scarcity significantly hinder the wide commercialization of PEMFCs. The exploration of inexpensive and earth-abundant PGM-free catalysts (e.g. Fe/N/C) to replace Pt has attracted much attention. The Fe/N/C catalyst is highly active (reaching the performance of Pt) but is not sufficiently stable for practical applications. Therefore, systematic investigations into the root causes of their instability are critical and urgently needed. Fe/N/C catalysts normally consist of several different types of active sites including the single atom moiety FeN_x (mostly found as FeN₄), CN_x, Fe₃C, Fe_xN (i.e., Fe@N/C), defects, edges, etc. To obtain a better understanding of the instability causes of the Fe/N/C catalysts, we investigated the effect of the various active sites on the overall stability of the catalyst. Several chemical and physical treatments were performed on the Fe/N/C catalysts to separate the different iron-based active sites and their activities and stabilities were evaluated. We found that the typical single atom moieties (FeN_x mostly found as FeN₄) are the most performing active sites but demonstrate the least stability (especially in the first 20h of fuel cell testing). It was also demonstrated that the acid treatment on the Fe/N/C catalyst has improved its stability behavior possibly due to the formation of a thin graphitic layer on the carbide species.

DNA Chimeras as Electrochemical Biosensors for Host-Guest Measurements in Blood

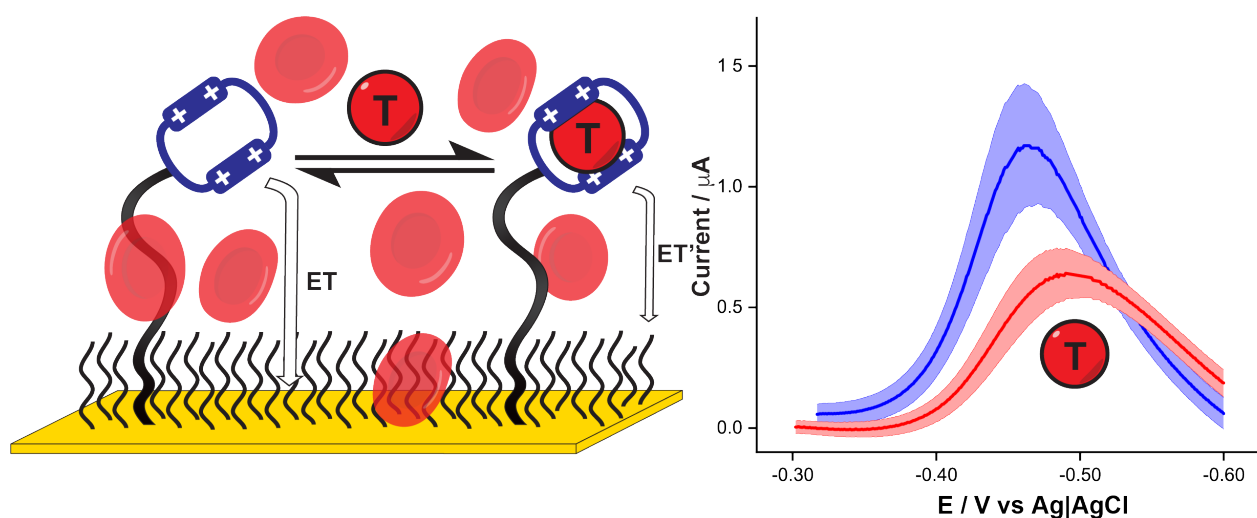
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Few sensing platforms have become ubiquitous to enable rapid and convenient diagnostics at the point-of-care. Those, however, are “one-off” technologies, meaning that they can only detect a single target and hardly adaptable to detect others. In response, we plan to develop a generalizable sensing platform that affords rapid, convenient, and continuous measurements of molecules directly in undiluted complex matrices. For this, we decided to rely on a host molecule that presents reversible interactions toward specific guest molecules to develop a new class of sensors that we coined “Electrochemical DNA-host chimeras”. As a proof-of-concept for our host-guest sensor, we decided to use cyclobis(paraquat-*p*-phenylene) (referred as “blue box”) that we attached on an electrode-bound DNA to allow measurements of biologically relevant electron-rich guest targets such as dopamine and aspirin. Doing so allows to promote host-guest complex formation that could be quantified using blue box’s electrochemistry. Because of our unique sensor architecture, we achieve, to our knowledge, the first reagentless, continuous, rapid (< 5 min) and convenient host-guest measurements directly in undiluted whole blood. We envision that given the vast library of host molecules that this represents the first steppingstone toward the development of a generalizable sensing platform for convenient and rapid measurements directly in complex matrices at the point-of-care.



PLATEFORME DE CARACTERISATION DES SYSTEMES ELECTROCHIMIQUES MAPLES

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La plateforme technologique MAPLES a été créée afin d'accélérer la recherche dans le domaine des matériaux et dispositifs fonctionnels liés à l'énergie, des batteries lithium-ion aux dispositifs électrochromiques et aux panneaux solaires. La plupart des instruments MAPLES permettent de réaliser des études sur les systèmes électrochimiques dans leur position d'utilisation prévue (*in situ*) et pendant leur fonctionnement (*in operando*) afin d'identifier pleinement les facteurs limitant les performances de ces systèmes.

Cette infrastructure est également entièrement accessible à la communauté des sciences des matériaux. En effet, nous pouvons répondre aux besoins en matière de recherche et de caractérisation des matériaux/dispositifs dans divers domaines tels que l'optimisation de dispositifs (opto)électroniques, du développement de médicaments et produits pharmaceutiques jusqu'aux analyses complexes d'échantillons environnementaux.

Notre philosophie d'opération se base sur deux piliers :

1-Partager notre expertise en électrochimie et en science des matériaux : Nous sommes prêts à aider les membres d'institutions d'enseignement ou industriels à résoudre un large éventail de questions scientifiques dans le domaine des sciences des matériaux. L'opérateur MAPLES est disponible au développement des méthodes analytiques et sert à la conduite des caractérisations sur nos instruments.

2-Développer des collaborations de recherche à long terme : Nous recherchons des collaborations avec des membres universitaires ou industriels. Ces collaborations doivent être basées sur un échange d'idées et d'informations.

MAPLES se compose de trois pôles d'instruments majeurs. Le premier pôle se compose d'instruments dédiés à la *caractérisation de structures et de microstructures*. Le second pôle est dédié aux *études de surfaces et d'interfaces*. Le troisième pôle est dédié aux *mesures électrochimiques* sur dispositifs réels.

Vous pouvez visiter notre site web au www.maples.umontreal.ca afin d'avoir une vue d'ensemble de notre infrastructure. Notre opérateur, sur place au colloque du CQMF, pourra répondre à vos questions.

First hydrogenation of gas atomized TiFe(Mn) alloy

Faranak Hosseini

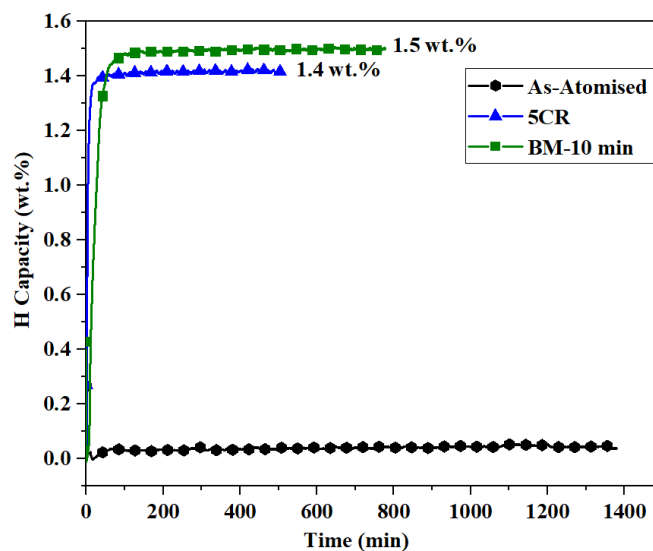
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In this study, the effect of a mechanical process, cold rolling or ball milling, on the first hydrogenation properties of TiFe(Mn) alloy was investigated. The TiFe(Mn) alloy was produced by gas atomization method by the industrial partner, GKN. Hydrogenation tests were carried out at 90° C. under a hydrogen pressure of 45 bar. The as-atomized alloy did not activate during 24 hours due to exposure to air exposure and the presence of a surface oxide layer which acts as a barrier for hydrogen gas. Five passes of cold rolling resulted to regeneration of the sample and the first hydrogenation occurred with rapid kinetics reaching full capacity of 1.4 wt% in 15 minutes. Ball milling for 10 minutes also led to activation with fast kinetics but the activation rate was slower compared to the sample subjected to cold rolling. Full saturation of 1.5% wt.% could be reached after 90 minutes. Therefore, it can be concluded that cold rolling can be a good reactivation method for TiFe alloy.

FIGURE



PREPARATION DES NANOFEUILLES D'OXYDE DE ZINC À TEMPERATURE AMBIANTE : ETUDE DES EFFETS ET DE LEURS APPLICATION DANS LES EMBALLAGES ALIMENTAIRES

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Les nanofeuilles d'oxyde de zinc à 2-D ont un fort potentiel pour la détection de gaz nocifs dans les produits alimentaires. Ce faisant, l'utilisation de cette structure pour fabriquer des capteurs pour l'industrie alimentaire aidera à améliorer la sécurité du consommateur. En effet, durant leurs cycles de vie, les aliments libèrent des gaz qui peuvent altérer leurs propriétés organoleptiques. Par conséquent, intégrer des capteurs de gaz à base de nanofeuilles d'oxyde de zinc dans les matériaux d'emballage alimentaire permettra de surveiller en temps réel les niveaux de ces gaz. Ainsi, si le niveau dépasse un certain seuil recommandé, le capteur déclenche une alarme ou un signal pour indiquer que la nourriture n'est plus sûre à la consommation. Cette technologie a un grand potentiel pour aider à réduire le gaspillage alimentaire et les déchets, un problème majeur au Canada où 2,3 millions de tonnes de denrées alimentaires comestibles sont déversées chaque année ou perdues.

Dans cette étude, nous avons procédé par la méthode de sonication à l'aide d'une sonde. Nous avons obtenu des nanofeuilles d'oxyde de Zinc à température ambiante en quelques minutes en utilisant des solutions à différents pH (e.g. pH = 7, pH = 11) sans calcination et sans avoir recours à des procédures coûteuses et longues telles que les réactions hydrothermiques¹⁻². Les nanofeuilles obtenues avec cette méthode sont très fines et leur épaisseur ne dépasse pas 10nm. Cette structure fine offre un large éventail de possibilités d'utilisation à l'échelle industrielle comme en biomédecine, dans l'industrie de l'environnement, dans les capteurs, catalyseurs et/ou des dispositifs de stockage d'énergie.

L'utilisation de cette technologie permet de réduire le temps, l'énergie consommée et par conséquent, le coût de production, tout en prévenant le gaspillage alimentaire et en réduisant les déchets, ce qui améliore l'efficacité de la chaîne d'approvisionnement alimentaire.

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THERMODYNAMICS OF RICH VANADIUM $\text{Ti}_{16}\text{V}_{60}\text{Cr}_{24-x}\text{Fe}_x$ ALLOY

FOR $x=0, 4, 8, 12, 16, 20, 24$

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ABSTRACT

The effects of the substitution of Cr by Fe on the hydrogen storage properties of the bcc alloy $\text{Ti}_{16}\text{V}_{60}\text{Cr}_{24}$ were investigated. Seven different alloys were studied: $\text{Ti}_{16}\text{V}_{60}\text{Cr}_{24-x}\text{Fe}_x$ ($x=0, 4, 8, 12, 16, 20, 24$). Micrograph of each alloy has shown two main phases such as a matrix and a bright phase. For $x=0$ and 4, the secondary phase is randomly distributed within the matrix. When $x=8$ and more, it got stick until a line of percolation is reached. Concerning the x-ray diffraction patterns, from $x=4$ to 12, the crystalline structure consists of a pure BCC while from $x=16$ to 24, C14 Laves phases appear. The lattice parameter of the BCC phase is decreasing with increasing the Fe content. This is in accordance with the Vegard's law. Moreover, the hydrogen storage maximum capacity is decreasing with increasing Fe content, this can be explained by combination the reduction of the lattice parameter of the BCC phase and the increase of the secondary phase seen in the micrographs. Pressure composition isotherm (PCI) curves were recorded at 298 K, 303 K and 323 K. Firstly, the reversible hydrogen capacity decreased with increasing the temperature and the Fe proportion. Secondly, the PCI curves permitted to deduce the Van't Hoff plot to get the enthalpy and entropy of formation of each hydride. The systematic relation between these thermodynamic parameters were then studied. We found that the enthalpy and entropy both decreased with increasing the iron content in a linear variation. That led to the conclusion of the existence of entropy-enthalpy compensation with a temperature of compensation of 240 K.

SYNTHESIS AND CHARACTERIZATION OF MUCOADHESIVE, ULTRASTABLE, AND FLUORESCENT GOLD NANOPARTICLES

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EYE DROPS REPRESENT 90% OF ALL OPHTHALMIC TREATMENTS CURRENTLY USED. THERE IS ONLY 0.02% OF EYE DROPS THERAPEUTIC MOLECULES THAT REACH THE EYE ANTERIOR CHAMBER DESPITE THEIR HIGH CONCENTRATION. THE TEAR FILM EFFICIENTLY PROTECTS THE CORNEA, REDUCING ACCESS TO THE TARGET. THEREBY, THE INCREASE OF THE DRUG BIOAVAILABILITY AND EFFICIENCY MUST COME FROM THE MUCOADHESION OPTIMIZATION OF THE DRUG DELIVERY SYSTEM. THE RESEARCH TEAM OF THE LABORATORY ALREADY DEVELOPED AND PATENTED A GOLD NANOPARTICLE SYNTHESIS THAT PRODUCES GOLD NANOPARTICLES PRESENTING ULTRASTABLE AND MUCOADHESIVE PROPERTIES. THE GOAL WAS THUS TO MODIFY THIS NANOTECHNOLOGY, WITHOUT LOSING MUCOADHESIVE AND ULTRASTABILITY PROPERTIES, ADDING A SMALL FLUORESCENT MOLECULE VIA CLICK CHEMISTRY. A FLUORESCENT PROBE WOULD ALLOW FOR NUMEROUS THERAGNOSTIC APPLICATIONS AND FACILITATE BIODISTRIBUTION/BIOACCUMULATION EXPERIMENTS. THIS FLUOROPHORE WAS COVALENTLY BONDED TO THE NANOPARTICLE AT TWO DIFFERENT RATIOS; 100% OF ALL PEGYLATED LIGANDS OF THE NANOPARTICLE BONDED THE FLUOROPHORE AND 1% OF THE LIGANDS BONDED THE FLUOROPHORE. USING DYNAMIC LIGHT SCATTERING (DLS), UV-VISIBLE SPECTROSCOPY AND TRANSMISSION ELECTRON MICROSCOPY (TEM), ULTRASTABILITY (HEATING, FREEZE-DRYING, ULTRACENTRIFUGATION, STERILIZATION BY AUTOCLAVE, RESISTANCE TO SALTS) PROPERTIES WERE SHOWCASED, ESPECIALLY FOR THE NANOPARTICLE WITH LESS FLUORESCENT MOLECULES. MUCOADHESION WAS QUANTIFIED USING THE PERIODIC ACID-SCHIFF STAIN (PAS) PROTOCOL. IMAGES OF EX VIVO CORNEAS FROM RABBITS WERE OBTAIN BY EPIFLUORESCENCE MICROSCOPY. BASED ON THESE PRELIMINARY RESULTS, GOLD NANOPARTICLES ARE A PROMISING THERAGNOSTIC SYSTEM FOR OPHTHALMIC TREATMENTS. THIS NANOTECHNOLOGY DEMONSTRATED ITS ROBUST PHYSICOCHEMICAL STABILITY, ITS INTERACTION WITH MUCINS AND ITS ABILITY TO BE TRACKED BY FLUORESCENCE EXPERIMENTS. FURTHER EXPERIMENTATIONS ARE NEEDED TO FULLY OPTIMIZE THE FLUORESCENCE WITHOUT COMPROMISING ITS STABILITY.

PREPARATION DES MATERIAUX 3D DE TYPE CHARPENTES ORGANIQUES COVALENTES (COVALENT ORGANIC FRAMEWORK, COFS) POUR LA DECONTAMINATION DE L'EAU

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RÉSUMÉ

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

Mot clés : COF, adsorption, contamination par les colorants, eau usée

CHIRALITY-INDUCED SPIN SELECTIVITY IN CONTACT ELECTRIFICATION

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CONTACT ELECTRIFICATION, ALSO KNOWN AS TRIBOELECTRIFICATION, IS A PHENOMENON BY WHICH ELECTRIC CHARGES MOVE BETWEEN DISSIMILAR MATERIALS UPON CONTACT. CONTACT ELECTRIFICATION FOR SPIN-SELECTIVE ELECTRON TRANSFER HAS ONLY RECENTLY BEEN EXPLORED IN FERRIMAGNETIC MATERIALS. ANOTHER METHOD FOR SPIN-SELECTIVE ELECTRON TRANSFER RELIES ON THE USE OF CHIRAL MOLECULES THROUGH THE CHIRALITY-INDUCED SPIN SELECTIVITY (CISS) EFFECT. HEREIN, WE HAVE DESIGNED AND BUILT A TRIBOELECTRIC NANOGENERATOR (TENG) TO INVESTIGATE THE CISS EFFECT DURING CONTACT ELECTRIFICATION. TO THIS END, WE DEMONSTRATE A CONTACT SEPARATION TENG DEVICE THAT GENERATES A STABLE ELECTRICAL OUTPUT, WHERE WE HAVE MONITORED THE VOLTAGE AND CURRENT UNDER VARIOUS SPIN FILTER CONDITIONS. SPECIFICALLY, WE HAVE PREPARED FERROMAGNETIC Ni-COATED SUBSTRATES FUNCTIONALIZED WITH CHIRAL HYBRID ORGANIC-INORGANIC PEROVSKITES (HOIPS; (R-METHYLBENZYLAMMONIUM)₂CuCl₄, (S-METHYLBENZYLAMMONIUM)₂CuCl₄, (R-1-(1-NAPHTHYL)ETHYLAMMONIUM)₂CuCl₄, AND (S-1-(1-NAPHTHYL)ETHYLAMMONIUM)₂CuCl₄).⁴ GIVEN THEIR HIGH SPIN POLARIZATION, FACILE SYNTHESSES, AND EASE OF THIN FILM PREPARATION BY SPIN COATING, WE PRESENT PRELIMINARY RESULTS OF THEIR USE IN A TENG COUPLED WITH A COPPER SURFACE TO INVESTIGATE THE CISS EFFECT UNDER THE INFLUENCE OF A PERMANENT MAGNET.

COMPUTATIONAL MOLECULAR DOCKING TO GUIDE THE DEVELOPMENT OF ELECTROCHEMICAL APTAMER-BASED BIOSENSORS.

Guy Terence Prevot

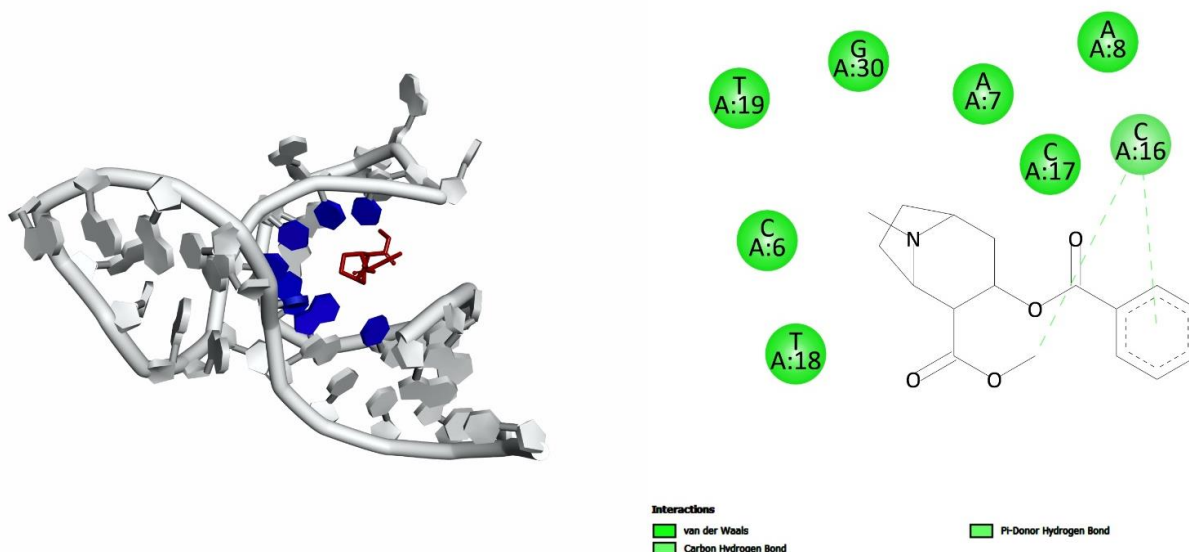
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To measure the concentration of molecules directly in complex matrices, we currently rely on analytical approaches that are laboratory-bound, cumbersome and operated by trained personnel. To transition and enable true personalized medicine requires the development of new analytical tools that provide rapid, convenient, and potentially continuous measurement of molecules directly at the point-of-care.

In this context, we are developing electrochemical aptamer-based biosensors (E-AB). E-AB sensors are comprised of a redox reporter modified aptamer (i.e., single strand of DNA or RNA selected in vitro via Systematic Evolution of Ligand by Exponential Enrichment (SELEX) to bind a specific analyte with high affinity) that are anchored on gold electrodes using thiol chemistry. Upon analyte binding, the redox reporter undergoes a binding-induced change in electron transfer, which can be measured using various electroanalytical techniques. E-AB sensors afford cheap, fast and accurate measurements of several analytes (i.e., proteins, small molecule and even cells). Due to the ease with which aptamers can be produced, E-AB sensors are deemed generalizable which could open new opportunities for personalized medicine applications.

Adapting aptamers from SELEX into E-AB sensors remains an important bottleneck hampering their widespread use. This is in part due to a lack of insights of the aptamer structures and analytes binding site. To overcome this, we have developed a computational pipeline to predict the tertiary structures of several aptamers on which we dock their analytes. With the predicted structures and identified nucleotides (see in blue and green in the figure), we reengineered aptamers to improve the analytical output of the resulting E-AB sensors. In doing so we found that all our reengineered aptamers, except ones in which we removed identified binding competent nucleotides, produced systematically larger E-AB sensors responses. We envision that using our computationally guided approach will improve E-AB sensors sensitivity and expand the library of molecules that they can monitor thus expanding what we can measure at the point-of-care.



SYNTHÈSE DE NANOLATEX PÉNÉTRANTS POUR LE DÉVELOPPEMENT DES TEINTURES DURABLES POUR LE BOIS EXPOSÉ AUX INTEMPÉRIES

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RÉSUMÉ

Le bois d'apparence utilisé à l'extérieur est sensible aux intempéries (photo-, biodégradation, humidité, etc.). D'où la nécessité de le protéger avec un revêtement durable. Toutefois, les revêtements à base de latex, très populaires, utilisés présentement ont une durée de vie limitée de 2 à 3 ans. Le mécanisme par lequel se solde la défaillance de ces revêtements est une perte d'adhésion due au :

- 1- Manque de flexibilité des résines qui les composent, lequel est corrélée à leurs hautes températures de transition vitreuses (T_g);
- 2- Manque de pénétration des résines qui les composent dans les cavités du bois, laquelle est généralement corrélée aux propriétés des résines polymériques (poids moléculaire, réticulation, groupes fonctionnels, etc.), des particules (taille, distribution, morphologie, etc.) et de la dispersion colloïdale (type et quantité d'émulsifiant, charge électrique, etc.);
- 3- Aux caractéristiques topographiques du bois après usinage (degré d'ouverture et fermeture des lumens, présence de fibrillation à la surface, etc.);

Toutefois les nanolatex sont reconnus d'avoir la capacité de mieux pénétrer le bois mais aucune étude n'en démontre la preuve. De plus, les nanolatex sont reconnus d'avoir une plus grande surface spécifique. Les nanolatex sont généralement préparés par des techniques de polymérisation en milieu hétérogène. La polymérisation en miniémulsion est la technique de choix dans le cadre de nos travaux, à cause de la faible sensibilité à l'eau des résines qu'elle génère. De plus, le planage hélicoïdal du bois s'avère une technique de surfacage, des plus intéressante, qui favoriserait la mouillabilité et l'ouverture des cavités du bois tel que les lumens tout en diminuant le niveau de fibrillation à la surface.

L'objectif principal de nos travaux consiste à synthétiser des nouvelles résines de nanolatex acryliques et/ou hybrides alkydes/acryliques afin d'évaluer leur capacité de pénétration et donc l'adhérence durable à long terme des teintures qu'elles composent.

MOLECULAR IMPRINTING ELECTROCHEMICAL SENSOR BASED ON BORON NITRIDE QUANTUM DOTS FOR FOLIC ACID DETECTION

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Folic acid (FA) also called vitamin B9, is a kind of water-soluble vitamin and considered as an essential nutrient for humans. It plays an important role in the human organism participating in metabolic reactions and biological syntheses. However, the deficiency of FA may causes many health risks such as cancer, Alzheimer's disease and some physiological disorders. Therefore, the accurate analysis of trace levels of FA is extremely important in many fields. Electrochemical sensor has attracted much attention due to its simplicity, rapidness and excellent sensitivity. In this study, a novel molecular imprinted electrochemical sensor approach based on boron nitride quantum dots (BNQDs) was presented for FA detection. BNQDs was prepared through solvothermal reaction, which then used as the glass carbon electrode modification materials to improve the sensitivity of sensing platform. Then, the o-phenylenediamine (o-PD) and β -cyclodextrin (β -CD) were selected as binary functional monomers, FA as the template molecule, which were electropolymerized onto the surface of BNQDs-CS/GCE to form the dual-monomer molecular imprinted polymer (MIP) film. Further research was conducted on the performance of the proposed sensor for detecting FA using differential pulse voltammetry (DPV) method. The results showed that the proposed sensor had excellent sensing, anti-interference, and relatively wide detection range for FA analysis. The preliminary research on the detection of FA using the electrochemical sensor based on MIP with dual-monomer can provide theoretical guidance for the detection of FA in real samples.

DEVELOPMENT OF A SHORTWAVE NEAR INFRARED SURFACE ENHANCED RAMAN SPECTROSCOPY BIOSENSOR FOR MONITORING THE RELEASE OF DOPAMINE

Hannah Williams

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ABSTRACT

Development of robust and accurate sensors has proven to be important for rapid and quantitative detection of (bio)molecules of biomedical relevance at clinically accepted detection limits. The focus of this project is to design highly sensitive nanomaterials for SERS-based optophysiology biosensors for label free detection of small organic molecules. Specifically, this sensor measures neurotransmitters (e.g., dopamine) as biomarkers of neurological disorders (e.g., Parkinson's disease) in brain tissues, and allows real-time tracking of biomarkers released by brain tissues in-vivo within real biological environments. This biosensor was built by templating a dense coating of gold nanostars (AuNS) onto tips of pulled glass fibers. Collection of data was done by rapid collection of single SERS spectra (0.25s) for label-free real-time monitoring of the release of neurotransmitters. The biosensors currently offer promising results as they detect dopamine in milli-Q water at picomolar concentrations with a $\lambda=633\text{nm}$ laser. The progression of this project is to use the biosensors with a new short-wave near-infrared (NIR) Raman system we recently built. A short-wave NIR laser ($\lambda=1064\text{nm}$) provides deeper penetration into biological materials, necessary for the detection of neurotransmitters ex vivo. Allowing for exceptional monitoring of the release of neurotransmitters through the rapid collection of SERS spectra, comparative to visible light Raman measurements. The NIR Raman system is the key to obtaining ample new data allowing for label-free monitoring of neurotransmitters in-vivo. In-vivo monitoring of dopamine neurotransmitter in brain tissue in real time will play a crucial role in understanding and tracking the health of brain tissue and the progression of neurological diseases, which is currently a global concern in the aging population.

CELLULOSIC FILTERS ENGINEERED TO CAPTURE VIRUSES

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ABSTRACT

It has recently been shown that tannic acid (TA), a naturally-occurring polyphenol, has a high affinity for extracellular, transmembrane and intracellular proteins involved in SARS-CoV-2 infectivity. Based on these promising results, TA could be used to potentially enhance the virus capture abilities of materials used in air or water filtration such as face masks and water filters. Cellulose fibers are an abundant renewable material commonly used in the fabrication of filters. It has previously been shown that cellulose can be coated with TA through an aqueous adsorption process. Our hypothesis is that the surface functionalization of cellulosic filters with TA could enhance the virus capture efficiency due to the strong interactions between TA and proteins found on the surface of the virus. The ability of filters to remove particles of different sizes is based on the porosity and effective pore size of the material. For filters made of fibers, these filtration properties can be adjusted using additives with different fiber diameters. In this work, filters made from hardwood kraft pulp fibers are developed using a highly refined cellulose fiber material possessing a large quantity of surface microfibrils as an additive. Furthermore, pectin extracted from apple pomace, an abundant and renewable resource in Quebec, can be used to coat the fibers via a transesterification reaction, serving as another additive to modulate fiber diameter and as an additional source of natural polyphenolic molecules. The effects of various filter fabrication parameters are investigated and optimized for the capture of surrogate virus nanoparticles. A cationic polymer is used to modify the nanoparticle surface charge, increasing their affinity to the cellulosic fibers. In future work, TA will be added to these filters and the filtration of nanoparticles surface modified with viral proteins will be studied.

PREPARATION OF COVALENT ORGANIC FRAMEWORK-METAL NANOPARTICLE HYBRID MATERIALS FOR CATALYTIC APPLICATIONS

Hichem Gamraoui

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Résumé:

Grâce à leur nature riche en électrons et leur capacité à former des liaisons métal-carbène exceptionnellement stables avec une gamme de métaux, les carbène N-hétérocyclique (NHC) se sont imposés comme une classe populaire et unique de ligands. Les nanoparticules (NPs) fonctionnalisées par des NHC ont démontré une stabilité thermique et chimique supérieure. En modulant la taille et la fonctionnalisation de leur surface, il est possible d'améliorer leurs propriétés et leur applicabilité. Dans ce sens une architecture hôte pour les NPs, un cadre organique covalent (COF) à base de triazine synthétisée par polycondensation sous des conditions solvothermique sera présenté. Le matériau obtenu combine plusieurs propriétés intéressantes à la fois, notamment la haute porosité qui a été utilisée pour infiltrer des complexes d'or NHC-Au dans les pores et la formation des nanoparticules après réduction. Les nanoparticules à base de COFs-Au ont été caractérisées par différentes méthodes de caractérisation comme la BET, DRX. Le COF@NHC-Au a été testé pour des applications catalytiques comme l'activité de réduction du nitrophénol.

Abstract:

Thanks to their electron-rich nature and ability to form exceptionally stable metal-carbene bonds with a range of metals, N-heterocyclic carbenes (NHCs) have emerged as a popular and unique class of ligands. Nanoparticles (NPs) functionalized with NHCs have demonstrated superior thermal and chemical stability. By modulating their size and surface functionalization, it is possible to enhance their properties and applicability. In this regard, a host architecture for NPs, a covalent organic framework (COF) based on triazine synthesized by solvothermal polycondensation, will be discussed. The resulting COF material combines several interesting properties, including high porosity, which was used to infiltrate NHC-Au complexes into pores and form the nanoparticles after reduction step. The COF-based Au nanoparticles were characterized using various characterization methods such as BET and XRD. The COF@NHC-Au was tested for catalytic applications such as activity for nitrophenol reduction.

Keywords: N-heterocyclic carbene • covalent organic framework • Gold • Nanoparticle • Catalytic application

MECHANICALLY ALLOYING OF NANOSTRUCTURED Mg_2Ni BY HIGH-PRESSURE TORSION FOR HYDROGEN STORAGE

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ABSTRACT

Mg-Ni alloys are one of the most promising candidates for solid-state hydrogen storage. However, the synthesis of Mg_2Ni is a complex procedure due to the melting point and the ebullition point of Ni and Mg respectively. As well, many unanswered questions remain about the hydriding/dehydriding mechanism of the Mg_2NiH_4 . In this study, powder mixtures of Mg-xNi (x= 5, 15, 50 wt%) were processed by severe plastic deformation (SPD) via high-pressure torsion (HPT) in order to synthesize Mg_2Ni . The phase transformation to the Mg_2Ni was confirmed by X-Ray diffraction, SEM-EDS, EBSD and TEM after the HPT process without any heat treatment. It is shown that the Mg-50Ni synthesized by HPT, can absorb hydrogen at 350° C even after air exposure, but the kinetics are still slow. The results confirm that a combination of HPT with posterior heat treatment is effective for the synthesis of Mg_2Ni by HPT. It was possible to synthesize more Mg_2Ni when Ni is increased in the mixture. Also, it was observed an increment in hydrogen uptake from 1.2 wt%, 1.5 wt% to 4,0 wt% when Ni content was increased from 5 wt%, 15 wt%, and 50 wt% respectively. Finally, results shows that the number of revolutions helps to improve the maximum hydrogen absorption during 24 hours from 3.7wt% to 5.2wt% in Mg-50Ni for 20 and 40 revolutions respectively.

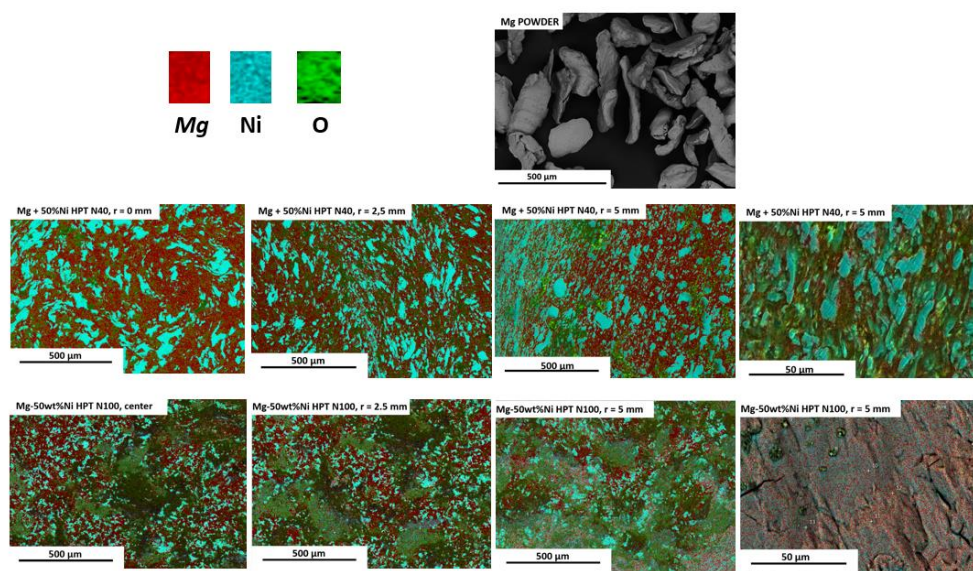


FIGURE 1. SEM-EDS ANALYSIS OF Mg_2Ni PROCESSED BY HPT AT A DIFFERENT DISTANCE FROM THE CENTER FOR 40 AND 100 TURNS.

One step synthesis of heterogeneous catalyst via plasma RF: Towards methanol production

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ABSTRACT

The valorization and capture of greenhouse gases, especially CO₂, has been studied in several works, due to their negative environmental impact as well as their interest to produce chemicals with high added value. Thus, the hydrogenation of CO₂ is the most adopted process to produce methanol, using specific operating conditions and suitable catalyst to enhance the reaction kinetics as well as promoting the selectivity of species. The purpose of this study is to develop new pathways for the development of catalysts for methanol production through physical and chemical methods. Herein, a binary catalyst containing ZnO and Al₂O₃, as well as a ternary catalyst including CuO, ZnO and Al₂O₃ were produced in a high-temperature plasma radiofrequency (RF) reactor, and then supported on mesoporous silica via an impregnation method. Plasma RF synthesis leads to 5-40 nm nanoparticles catalysts. In addition, the prepared catalysts were characterized by various techniques including XRF, XRD, TEM, TGA and BET. By using the above-mentioned techniques, the molar ratios, composition, morphology, reduction behavior and specific surface area of catalysts were studied. We investigated the impact of various operating parameters on the chemical, morphology, and crystalline nature of the NPs. Based on TEM images, most binary catalysts have a faceted structure, while ternary catalysts are irregular. These are intended for a series of test to evaluate their catalytic activity in a fixed-bed microreactor for methanol production from the direct CO₂ hydrogenation, with process optimization using response surface methodology.

Keywords: methanol synthesis, CO₂ hydrogenation, plasma RF, heterogeneous catalysts.

ONE- STEP SYNTHESIS OF NiSe_2 AND NiSe_2 / RGO-PGM FOR HYDROGEN EVOLUTION REACTION

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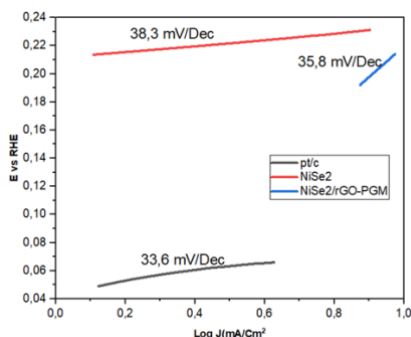
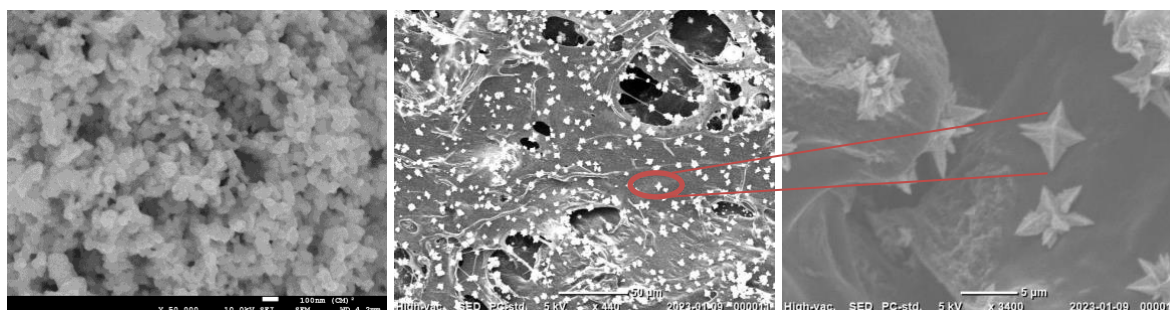
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YOUR ABSTRACT / VOTRE RÉSUMÉ

The search of cheap, earth-abundant and efficient hydrogen evolution reaction (HER) catalysts is significant for sustainable hydrogen economy. Here we introduce a simple and cost-effective strategy for one-step synthesis of NiSe_2 and 3D porous NiSe_2 /RGO-PGM hybrid catalysts from our laboratory via hydrothermal method. In this poster, we will show a unique interconnected macroporous conducting carbon membrane that was prepared by cryogeletion and subsequent carbonization of the gelatin and graphene oxide cryogel. The NiSe_2 /RGO-PGM was used as electrocatalyst without binder “binder-free” for water-splitting HER. These catalysts exhibit superior catalytic performance and challenging pt/c by a small overpotential (~ 100 mV) for NiSe_2 /RGO-PGM and (~ 230 mV) for NiSe_2 to afford $10 \text{ mA} / \text{Cm}^2$ with respectively Tafel slope $35,8 \text{ mV} / \text{Dec}$ and $38,3 \text{ mV} / \text{Dec}$ and good stability in acid, which benefits from the good electrical conductivity of NiSe_2 and NiSe_2 /RGO-PGM catalysts.

FIGURE

(Optional / Facultative)



XPS & UPS ANALYSES OF ROLL-TO-ROLL SLOT-DIE COATED PEROVSKITE SOLAR CELLS

James McGettrick

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There has been a rapid evolution of perovskite photovoltaics to a 25.8% power conversion efficiency. Coupled with the potential for low temperature deposition of solution-based layers, this allows a range of solution based manufacturing techniques to be employed for large area coatings and hence commercial scalability.

Slot-die coating is one method that shows much promise: It is a cost-effective roll-to-roll (R2R) method for coating 2-dimensional patterns, with control of film thickness and low materials wastage. However the transition from laboratory spin-coated prototypes to industrial scale slot-die coating presents a range of scientific challenges from rheological control to solution compatibility. Combining multiple slot-die coated layers is key to the development of successful devices and each layer relies on tight control and optimisation.

Here we focus on the analyses of these coatings via X-ray Photoelectron Spectroscopy (XPS) & associated surface analysis techniques. Optimisation of a layer can include a number of parameters defined either by the surface, or by very thin (<10 nm) films. XPS allows the study of the chemistry that influences wetting or adhesion in such thin layers. In addition, the extension of XPS from single point spectroscopic measurements to rastered mapping over large (cm) areas allows chemical images to be generated. Images over larger areas offer unique advantages for understanding consistency and patterning over such large areas.

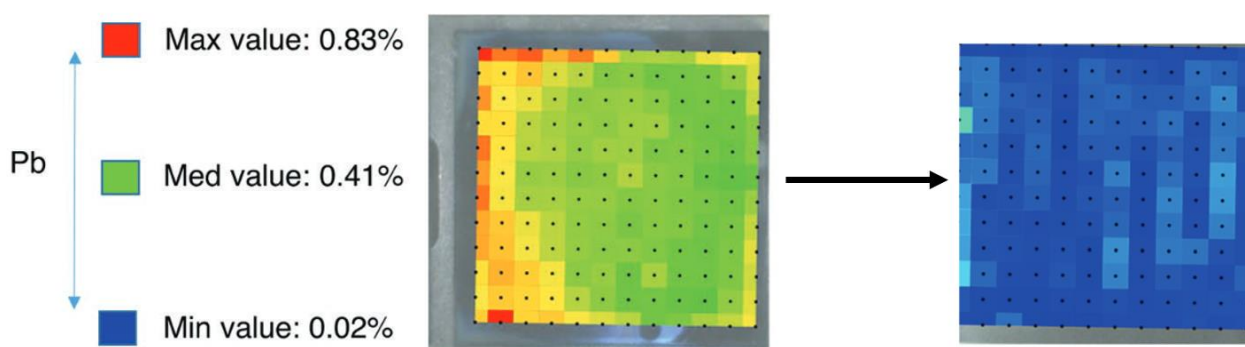


Figure. XPS elemental mapping of Pb to assess coating consistency of a PEDOT film on a methyl ammonium lead iodide perovskite. From lab spin coating to R2R slot-die coating.

ORGANIC LIGANDS / LIGANDS ORGANIQUES

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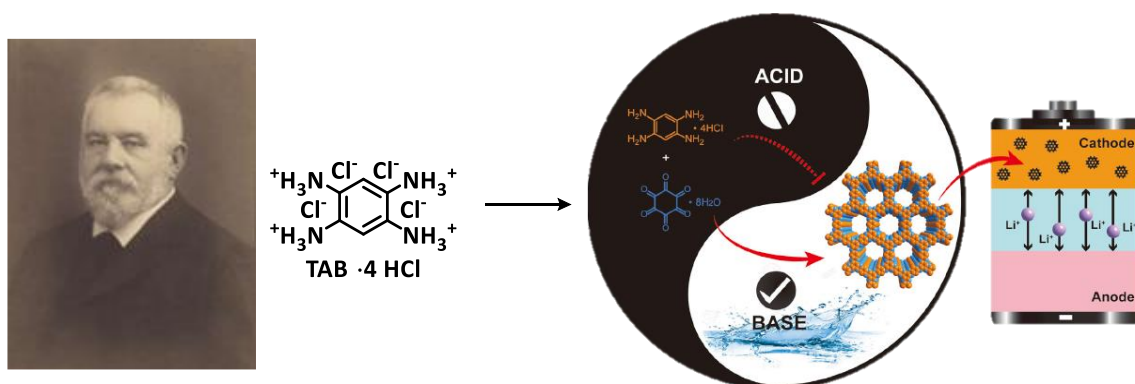
YOUR ABSTRACT / VOTRE RÉSUMÉ

(300 words - 1 page max)

LES PROTÉINES, LES ACIDES NUCLÉIQUES OU ENCORE LES LIGNANS SONT AUTANT D'EXEMPLES DE BIOMATÉRIAUX ORGANIQUES (MAJORITAIREMENT CONSTITUÉE DE H, C, O ET N) RENDANT LA VIE POSSIBLE. ILS SONT TOUS CONSTITUÉS DE MOTIFS MOLÉCULAIRES ASSOCIÉS LES UNS AUX AUTRES DE FAÇON À DICTER AU MATÉRIAU SA FORME ET SES FONCTIONS. SUR CE MODÈLE, NOUS ÉTUDIONS LA STRUCTURE ET LA RÉACTIVITÉ DE MOTIFS ORGANIQUES ABONDANTS DANS LA NATURE (ARYLAMINES ET QUINONES), FACILEMENT MODIFIABLES ET UTILISABLES POUR LA FABRICATION DE MATÉRIAUX OPTOÉLECTRONIQUES DONT LES ÉTAPES DE SYNTHÈSE ET LA CARACTÉRISATION SONT PRÉSENTÉES.

PROTEINS, NUCLEIC ACIDS, AND LIGNANS ARE ALL EXAMPLE OF ORGANIC (MOSTLY DERIVED FROM H, C, O, AND N) BIOMATERIALS SUSTAINING LIFE ON EARTH. THEY ARE ALL CONSTITUTED OF MOLECULAR MOTIFS TETHERED TO ONE ANOTHER TO DICTATE MATERIALS SHAPE AND FUNCTIONS. INSPIRED BY THIS ASCENDANT APPROACH, WE STUDY THE STRUCTURE AND REACTIVITY OF NATURALLY OCCURRING AND READILY TUNABLE ORGANIC MOTIFS (ARYLAMINES AND QUINONES) TO USE THEM FOR THE FABRICATION OF OPTOELECTRONIC MATERIALS. SYNTHETIC PROTOCOLS AND CHARACTERIZATION DATA WILL BE PRESENTED.

FIGURE



Rudolph H. Nietzsche synthesized TAB · 4 HCl in 1887

Versatile air stable molecular building bloc

TAB-derived materials

Potent optoelectronic materials

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TiO₂ Nanotubes as Semiconducting Material for Dye-Sensitized Photoelectrodes

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The use of chemical bonds to store solar energy is a promising approach to overcome the intermittency of the sun by harnessing sunlight to drive chemical transformations. One strategy to drive these processes is to use bespoke semiconductor photoelectrodes implemented in a photoelectrochemical cell to absorb light and generate charge carriers that can drive redox reactions such as the direct oxidation of adsorbed species on the photoanode. To enhance the efficiency of this process and minimize recombination of electron-hole pairs, molecular donor-chromophore-acceptor systems can be used to sensitize wide bandgap semiconductors for visible light absorption and generate high energy excited states that give rise to long-living charge separated states. Presented here are recent studies using molecularly sensitized TiO₂ nanotubes as a nanohybrid architecture for dye-sensitized photoelectrochemical cells. The highly ordered 1D-nanostructures are purpose-grown using a self-organizing electrochemical anodization approach. Nanotube mouths are found to be endowed with graphitic-like impurities and are further functionalized with a Cu(I)-based donor-chromophore-acceptor system by direct assembly at the surface. The resulting photoanode is used to generate oxidizing equivalents that can subsequently drive follow-on oxidation reactions.

INFLUENCE OF GRAPHENE OXIDE ON MECHANICAL AND MORPHOLOGICAL PROPERTIES OF NAFION® POLYMER MEMBRANES

JUAN CEBALLOS-ALVAREZ

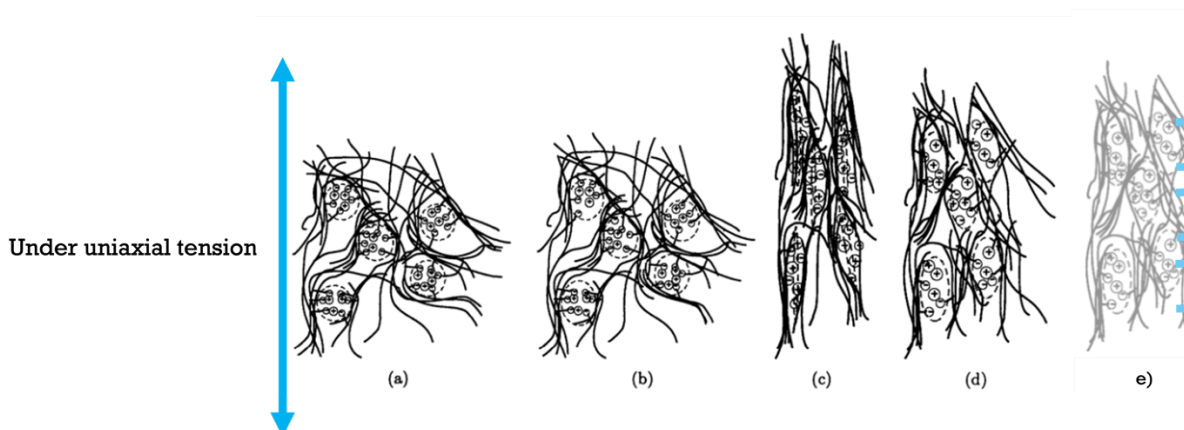
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ABSTRACT

This study explored the influence Graphene Oxide (GO) on the morphological and mechanical properties of Nafion® 115 membranes. The membrane surface was modified ultrasonically spraying a solution of GO and different annealing temperatures were tested. The nano and micro-morphology of the modified membranes were evaluated using Atomic Force Microscopy (AFM) and Scanning Electron Microscopy (SEM). Bulk and local mechanical properties were explored by tensile test and nanomechanical mapping respectively. Annealing the composite membranes resulted in an interfacial interaction between the GO and the Nafion® polymer. This method showed mechanical performance enhancement of the modified membranes (Tensile strength, elongation at brake and Young Modulus) without altering the electrical insulation of the polymer.

FIGURE



Two dimensional conceptual model of how Nafion® deforms under uniaxial tension with the backbone organized into bundles with amorphous regimes while the ionomer clusters have a circular cross section a) Prior to deformation; b) At small strain; c) At large strain; d) After load is removed; e) Hypothesis of an staple effect that GO could be having under tensile tension. Adapted with permission from Silverstein, 2008.

UN CONCEPT DE BIORAFFINERIE : DU RIZ AUX NANO OBJETS

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YOUR ABSTRACT / VOTRE RÉSUMÉ

Dans le contexte actuel de transition d'une société pétro-dépendante vers une société bio-basée, les ressources forestières représentent une alternative idéale, car elles sont une source importante de lignine et de cellulose, des biopolymères susceptibles de remplacer des produits pétro-sourcés. La culture du riz produit chaque année plus de 137 millions de tonnes de balle de riz, un résidu lignocellulosique aux faibles propriétés nutritives, mais ayant une grande concentration en silice et presque imputrescible rendant son utilisation difficile. Ces propriétés en font un candidat idéal pour la production de cellulose, d'hémicelluloses et de lignines ; des biopolymères aussi retrouvés dans le bois. Ces matériaux peuvent ensuite être transformés en matériaux à haute valeur ajoutée. L'approche adoptée dans ce projet de recherche est un concept de bioraffinerie adapté à un agro-déchet. Après analyse de sa composition, une hydrolyse acide est d'abord réalisée pour convertir le xylane de cet agro-déchet en xylose. Le résidu solide restant après l'élimination du xylane est ensuite transformé par un procédé organosolv catalytique breveté en pâte cellulosique et en lignine organosolv.

Le procédé de mise en pâte a été optimisé et les différents paramètres évalués lors processus étaient : le temps et la température d'extraction, le rapport masse de matériau/volume de solvant, la composition du solvant et la concentration en catalyseur. En utilisant une méthode électrospray, la lignine isolée a ensuite été transformée en nanoparticules de forme sphérique ayant un diamètre de 104 ± 24 nm avec un potentiel Zeta de $-31,1 \pm 2,3$ mV. Ces nanoparticules sont donc des candidates pour diverses applications comme la production de divers composites à base de polymère

Les nanoparticules de lignines produites, seules ou associées à d'autres polymères, pourront être utilisées dans des matériaux composites comme sources de molécules antioxydantes et de protection contre les rayons UV et les bactéries.

Chemical coupling approaches to synthesize VEGF protein- PEG bioconjugates.

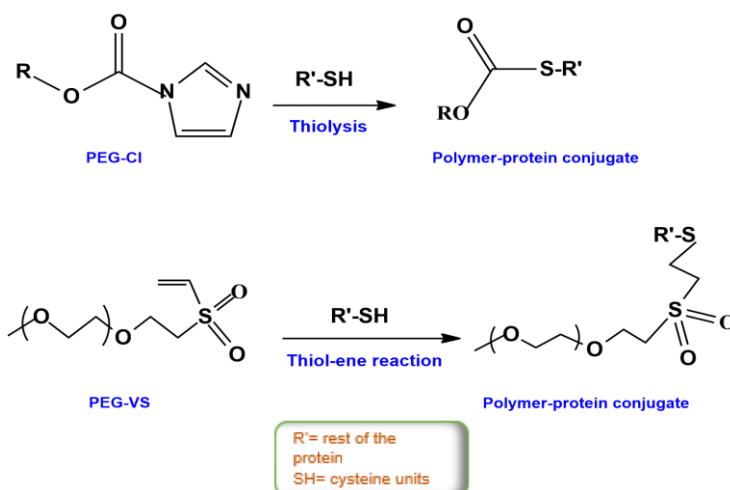
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Proteins have been extensively used in the field of biomedicine, nanotechnology, and biotechnology. In particular, vascular endothelial growth factor (VEGF) protein can promote the proliferation and differentiation of endothelial cells and thus resulting in the development of new vasculatures. Along with the therapeutic application, VEGF can also be employed to stimulate in vitro cell growth, providing novel applications. Recently, chorioallantois membrane (CAM) model developed to screen antineoplastic drugs can provide an innovative alternative to replace in vivo animal model. The addition, VEGF intends to develop a vascularized cell model which resembles an in-vivo environment. Although VEGF looks promising, its bioconjugate with bio-based polymers can improve its stability and efficiency in biological environments. The current effort aims to develop robust approaches that allow for the synthesis of angiogenic VEGF-poly (ethylene glycol) (PEG) bioconjugates. The objective is to link VEGF with activated polymer without compromising VEGF's biological activity. Our approaches explore well-known organic coupling reactions, namely carbonyl diimidazole (CDI) and divinyl sulfone (DVS) chemistries to activate hydroxyl groups of PEG. The formed activated PEG with CI and VS groups can react with reactive functional groups, particularly thiol groups in cysteine residues in VEGF protein, yielding the synthesis of VEGF-PEG bioconjugates. Gel electrophoresis has been used to qualitatively follow the coupling reaction of VEGF and activated PEG. The fabricated bioconjugates will be characterized for size and morphology in water and further evaluated for biological interactions and functions. Future direction will focus on the potential biological and tissue applications of the bioconjugates, including the fabrication of cell-encapsulated, smart (stimuli-responsive) biopolymer-based hydrogels embedded or covalently conjugated with the bioconjugates.

Submitted for poster presentation in 2023 CQMF annual meeting.



WATCHING NANOMATERIAL PHASE TRANSFORMATIONS WITH A DYNAMIC TRANSMISSION ELECTRON MICROSCOPE

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Computational initiatives like the Materials Project have amassed structure and energetic information on nearly 150,000 materials with the goal of accelerating the discovery of materials with enhanced properties. However, it remains a challenge to synthesize many of the predicted phases. Better understanding of the energy transfer mechanisms and kinetic pathways involved in phase transformations is critical for accurate prediction of the product phase and microstructure. This insight requires studying the local changes happening on the atomic and nanometer scale during this process. However, few measurements of this kind have been possible due to the extreme temporal and spatial resolution required. The Dynamic Transmission Electron Microscope (DTEM) has been recently developed to address this challenge, and is capable of imaging irreversible transformations in nanomaterials with nanosecond and nanometer resolution. In this talk, an introduction to the operating principle of this unique microscope and the challenges of snapshot imaging with electrons will be given. A current benchmark of the capabilities of the DTEM at INRS will be presented, along with planned future developments.

Phosphorus and Nitrogen Co-Doped Reduced Graphene Oxide as Superior Electrode Materials for Supercapacitors

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Abstract

In recent years, carbon-doped heteroatoms have gained considerable research interest. Doping with heteroatoms makes it possible to increase the specific capacity and improve the electrochemical performance of carbonaceous materials. Recently, N/P doping on porous carbons has been reported to have excellent performance as an electrode for supercapacitors. Supercapacitors have attracted remarkable attention as a component for energy storage and a good alternative to batteries and fuel cells. In this presentation, we will focus on phosphorus/nitrogen co-doped reduced graphene oxide (PN-rGO) material prepared by one-step pyrolysis of the functionalized GO (FGO) with hexachlorocyclotriphosphazene and *p*-phenylenediamine. Compared with the undoped rGO, the electrochemical measurements of PN-rGO exhibit enhanced capacitive properties, including high specific capacitance, remarkable rate capability, and excellent cycling stability. The outstanding performance of this resulting material as a supercapacitor electrode will be discussed in detail.

Keywords: Graphene oxide, PN co-doping reduced graphene oxide, supercapacitor, porous carbon.

MEASURING OXYGEN DIFFUSION IN CELLULAR ENCAPSULATION DEVICES MADE SIMPLE AND ACCESSIBLE

Laurier Gauvin

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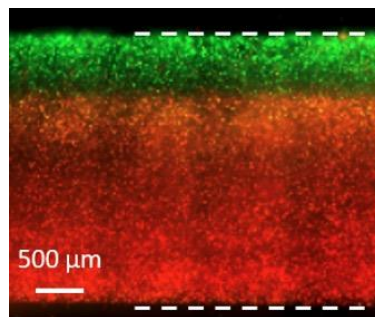
[†]These authors contributed equally to this work.

ABSTRACT

(299 words)

Transplantation of insulin-producing pancreatic islets has enabled type 1 diabetic patients to regain the ability to endogenously produce insulin leading to partial or even full exogenous insulin independence. Current therapies rely on immunosuppressants to prevent transplant rejection. The transplantation of hydrogel-encapsulated islets has been proposed as an immunosuppressant-free alternative. Whilst hydrogels allow the flow of insulin, nutrients, and oxygen, such molecules do not actively transport from the blood through the encapsulation layer, creating a diffusion-limited cell oxygen supply. As such, to bring a successful encapsulated islet transplant to fruition, diligent study must be performed to ensure that adequate oxygen is diffused into the islets. This oxygen can be quantified using various measurement techniques or can be estimated using computational fluid dynamics (CFD); however, these respectively require costly specialized equipment and the use of numerous arguable assumptions. This work presents a simple and easily reproducible system used to quantify the diffusivities of hydrogels and to analyze said diffusivities' effect on cell viability. By simply purging oxygen from a hydrogel slab using nitrogen, accurate and precise measurements of 3 types of hydrogels were produced. This setup was validated through its use on H₂O, through CFD, and through calculations of Peclet number (<0.7). Live/dead studies of MIN6 cells incorporated into the same 3 hydrogels were performed to study the effect of diffusivity on islet viability. M/G ratio was found to be a greater predictor of diffusivity than hydrogel concentration and these results were reflected in the slab viability measurements. Nevertheless, in the cell-slab experiments, at higher cells count, cell fraction was found to be the limiting factor for viability (results consistent with our Thiele modulus calculations). This work could ultimately contribute to the development of encapsulated islet devices by enabling simple and reliable benchmarking of hydrogel diffusivities and their respective cell capacity.

FIGURE



Live/dead staining of hydrogel (Protanal) to calculate oxygen supply to MIN6 cells through diffusion.

EXAMING THE ROLE OF CHIRALITY IN PEROVSKITE SOLAR CELLS

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Abstract

Silicon-based solar cells (SSC) are sustainable methods for generating electricity.¹ The incomplete absorption of the incident light by the silicon in these devices, however, limits the sun light-to-electricity efficiency. Efforts have focused on developing SSC alternatives to overcome this major limitation and for increasing the overall efficiency of solar cells. Lead-based perovskites solar cells have gained traction as alternatives to SSC. This is in part owing to their unique optoelectronic properties.² Indeed, the lower band gap of lead perovskite compared to SBS can improve the efficiency of solar cells and it also enhances the energetic compatibility of the different device layers.² Despite this advantage, the toxicity and instability of lead perovskites under ambient environmental conditions are major limitations to these perovskites in solar cells. These shortcomings could be overcome by replacing lead in the perovskite structure with other metals that have reduced deleterious effects.³ Toward this end, we examined 2D chiral tin-based perovskites as solar cell alternatives. These perovskites were prepared from ethylbenzylamine (EBA), adapted from previous reported work.⁴ They are expected to be as performant as lead perovskites courtesy of their similar optoelectronic properties. The structural and optical properties of the tin perovskites will be presented.

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ODD-EVEN EFFECT IN THE MOLECULAR ORIENTATION IN 2D AND 3D PHOSPHOLIPID ASSEMBLIES

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ABSTRACT

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

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

Titre: Vers des carburants solaires par des méthodes de photosynthèse artificielle

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RÉSUMÉ

L'hydrogène, étant considéré comme l'énergie « verte » du futur, apparaît aujourd'hui comme l'une des meilleures alternatives pour la transition énergétique mondiale d'ici 2050. Il peut être produit par électrolyse de l'eau, mais de nouvelles méthodes assez intéressantes sont en cours de développement telles que la photosynthèse artificielle (PA). Il s'agit d'une méthode qui consiste à produire l'hydrogène à partir de l'eau en utilisant l'énergie solaire captée grâce aux photosensibilisateurs (PS) (des composés capables de récolter l'énergie solaire) et en présence des catalyseurs pour accélérer la réaction.¹

On s'intéresse à l'application des complexes de coordination de cobalt(II), nickel(II) et cuivre(II) avec des ligands organiques tels que les amidine-*N*-oxides (AMOXs),² comme catalyseurs pour la production de l'hydrogène et la réduction du CO₂ dans des systèmes photocatalytiques homogènes avec des PS moléculaires (p. ex. des complexes de Ru(II), Ir(III), Re(I) ou Cu(I)).

La préparation des ligands et des complexes a été réalisée par des méthodes de synthèse organique et inorganique et leur caractérisation, a été effectuée par des techniques comme la spectrométrie de masse, l'analyse élémentaire et les spectroscopies RMN, IR et UV-Vis. Leurs propriétés redox ont été étudiées par des méthodes électrochimiques (la voltammétrie cyclique). Dans une étape suivante les tests en photocatalyse seront effectués.

¹ Segev *et al.*, *J. Phys. D Appl. Phys.*, 55(32), 323003, 2022.; ²Cibian *et al.*, *Chem. Eur. J.*, 2015, 21, 9474.

Optimization of the dosimetric hydrogel formulation for low-dose rate brachytherapy

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Introduction: Brachytherapy is a cancer treatment method that uses radioactive sources near or into a tumor to kill cancer cells. An accurate dosimetry tool is needed to validate the dose profile deployed by personalized brachytherapy implants before using them on real tumors. Gel dosimeters are potential tools for this purpose. The changes induced in the gel upon radiation is by MRI acquisition to record 3D dose distribution. Current gel dosimeters are not adapted to these implants. They are mainly used for high-energy radiation dosimetry. Thus, an accurate gel dosimeter is essential for low-dose-rate brachytherapy. Methacrylic acid (MAA)-based gels (MAGIC) show a stable dose distribution and can be prepared easily. Low melting point and self-polymerization of MAA are problematics of MAGIC gels. Chemical modifications on MAGIC gel would address mentioned problems. This study aims at developing a gel suitable for personalized brachytherapy implants.

Methodology: To optimize MAGIC gel formulation, gelatin and paraformaldehyde solutions (0.5, 0.75, 1 and 1.25 %w/w) were separately prepared, and mixed at 45°C. Copper (II) sulfate pentahydrate and L-Ascorbic acid solutions, and MAA were added at 37°C. The gel solution was poured into glass tubes sealed and gelified at 4°C. To compare the gel sensitivity before and after 30 Gy irradiation (137Cs), the relaxometry measurements were done. T2-weighted MRI scanning was done (TR/TE/FOV/Matrix= 3000/120ms/60mm/96×96) and the signal intensity was integrated.

Results: MAGIC gel with 0.5% paraformaldehyde melted above 25 °C. Preparation of MAGIC gel with higher concentrations (1.25%) was difficult due to high viscosity. Gel with 0.75%w/w paraformaldehyde was foggier than 1% w/w resulting in a darker MRI image. The signal fall was 771, while it was 390 with 1% w/w paraformaldehyde.

Conclusion: The addition of 0.75% w/w paraformaldehyde increased the melting point of MAGIC gel, decreased the MAA self-polymerization and increased the gel sensitivity.

STUDY OF TRANSPORT PHENOMENA IN NEXT GENERATION LITHIUM BATTERIES ASSISTED BY 3D PRINTING

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Lithium-ion batteries (LIB) have a major role in the global energy future as they currently offer the best alternative for energy storage. The increase in energy demand is driving the development and optimization of high-performance batteries. With the specific objective of improving energy densities, studying the limiting phenomena such as the transport of species through the batteries' components is essential. In this regard, using a new emerging technology such as 3D printing to process some of the batteries' components could answer some issues. Thanks to its design flexibility compared to conventional manufacturing methods, this technique offers the possibility of creating customizable and complex architectures that could help unravel limiting phenomenon.

More specifically, 3D printing is an interesting way to design solid electrolytes. This study aims at showing how the structure, the composition and the configuration of the solid electrolyte composites will affect the systems properties and thus its electrochemical performances. A first part of the study consists in evaluating the feasibility of 3D printing a solid composite electrolyte with a complex architecture. Thus, 3D printing techniques will be discussed as well as the formulation of a ceramic formulation. Other aspects will be addressed such as the ink printability studies via rheology, the processing of different structures via print fidelity studies and the conductivity of the 3D printed architectures.

Optimization and Development of Aptamer-Based Biosensors for Point-of-Care Methotrexate Detection and Chemotherapeutic Drug Monitoring

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ABSTRACT

Methotrexate (MTX) is a commonly used chemotherapeutic agent that requires therapeutic monitoring to reduce the risk of toxicity in patients. In this study, two different biosensors were developed to detect MTX. The first biosensor is a label-free electrochemical aptasensor, which was developed using aptamers selected via the Systematic Evolution of Ligands by Exponential Enrichment (SELEX). The MTX₆ aptamer was selected based on its highest affinity and was used to develop the aptasensor, which exhibited excellent sensitivity and selectivity towards MTX, with a limit of detection (LOD) of 0.11 pg/ml. The aptasensor was also highly selective for MTX over analog compounds and demonstrated good recovery when tested with human serum spiked with MTX, indicating its potential use in point-of-care testing for therapeutic drug monitoring (TDM) of MTX.

The second biosensor is a fluorescence apta-assay using truncated aptamers in a competitive displacement assay. The assay uses a fluorophore-quencher pair that separates when MTX is present, resulting in an increase in fluorescence intensity. The truncated aptamer-based competitive displacement fluorescence assay offers a highly specific, rapid, and cost-effective method for detecting MTX, making it a promising tool for clinical diagnostics and treatment monitoring in point-of-care settings. The truncated aptamer displayed a superior binding ability to MTX (K_d 0.18 nM) in contrast to the full-length aptamer's (K_d 85.5 nM). The assay has a low detection limit of 17 pM and can detect MTX in the presence of various chemotherapeutic drugs and antibiotics. Overall, both biosensors show significant potential for clinical diagnostics and TDM of MTX concentrations, ultimately improving the therapeutic outcomes of patients undergoing MTX treatment.

Keywords: Methotrexate, TDM, Aptamers, SELEX, Electrochemical label-free aptasensor, Competitive displacement assay, Truncated aptamer, Aptasensor, Fluorescence assay.

PERFORMANCE OF TITNIUM OXYNITRIDE NANOPARTICLES WITH CONTROLLED COMPOSITION ON HYDROGEN GENERATION

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Abstract

Hydrogen gas produced by photocatalytic water splitting is a promising candidate for replacing fossil fuels, if an appropriate photocatalyst can be found. We consider titanium oxynitride for this application. While titanium oxide has a high band gap and high recombination rate, and titanium nitride is unstable in water, the oxynitride has the potential to combine the strong points of each of its parent materials while diminishing each materials downside. Photocatalytic water splitting requires the effective adsorption of reactant molecules/ions at the surface for electron transfer, which is intrinsically determined by the surface atomic arrangement. This arrangement can be tuned by controlling the relative amounts of oxygen and nitrogen in TiO_xN_y . However, characterizing the relative amount of each anion has historically been an analytical challenge. In this report, TiO_xN_y is synthesized by nitridation of titanium oxide under ammonia gas with varying N/O ratios. N and Ti composition is calculated by colorimetric and gravimetric methods respectively, and the complimentary techniques allow for the overall composition to be accurately determined. Through understanding and controlling the composition of the heteroanionic species, we will determine the structure property relationship with respect to photocatalytic activity in the titanium oxynitride system.

High-throughput synthesis and characterization of layered oxide cathode materials for sodium-ion batteries

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Sodium-ion batteries are seen as a promising alternative to lithium-ion batteries due to the abundance and low-cost of sodium. This may make grid-scale energy storage accessible. In recent years, manganese-based sodium layered oxide cathodes ($\text{Na}_x\text{Mn}_y\text{M}_z\text{O}_2$, where M is a dopant), have gained significant attention.[1] In this study, we used our high throughput (HTP) methods to systematically study the effect of different transition metal doping on these cathode materials and assess their crystal structure, electrochemical performance, and air/moisture stability.[2] In detail, HTP sol-gel method was used to prepare different doped samples. After sintering, HTP-XRD was performed to identify phases and determine the structural changes caused by doping. Then, HTP-cyclic voltammetry (CV) was performed to obtain the charge/discharge voltages and specific capacities. Finally, an accelerated ageing process was carried out at various humidity levels over several weeks to understand the relationship between compositions and air stability. We found 20 different transition metals that can be integrated into the layered Na-Mn-O structures, including several previously unstudied dopants such as Ga and Rb. Several pure P2, P3 and O3 sodium layered oxides structures are identified. For the undoped sample, a P2/P'2 biphasic material is obtained through slow cooling. However, with the presence of dopants such as Ni and Fe, pure structures are obtained with smooth CV curves, suggesting fewer phase transitions via doping. A series of novel cathodes yields excellent battery performance, including high specific capacities above 200 mAh g^{-1} and good capacity retention after ten cycles. Moreover, air/moisture stability analysis is conducted for co-doped samples, and it is found that as little as 5% Li in co-doped samples can stabilize the layered structure dramatically. Therefore, these findings about the effect of transition metal substitution via high throughput screening can serve as a new and rapid approach for the rational design of battery materials.

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Évaluation de l'impression 3D de matériaux polymères *via* des techniques de caractérisation avancées

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La fabrication additive, également connue sous le nom d'impression 3D, consiste à déposer de manière robotique un matériau ou un mélange de matériaux de manière additive en suivant des mouvements cartésiens (X, Y, Z), conformément à une architecture préalablement programmée à partir d'une conception assistée par ordinateur (CAO). La nouvelle méthode de fabrication additive par extrusion pneumatique en fondu ouvre une nouvelle voie pour étudier les relations entre la structure – mise en forme – propriétés des matériaux. Pour établir de telles relations, plusieurs techniques de caractérisation avancée sont utilisées, telles que la rhéologie (thixotropie, rhéofluidification), la profilométrie (uniformité, rondeur) et la calorimétrie différentielle à balayage (DSC). Ces techniques permettent de rationaliser le comportement du polymère à différentes étapes du processus d'impression, telles que la vitesse de déposition le changement de phases cristallines, la solidification de l'architecture et son uniformité par rapport au fichier CAO. Plusieurs projets interdisciplinaires ont découlé de ces caractérisations. L'un de ces projets vise à intégrer l'intelligence artificielle (IA) afin d'optimiser l'impression et de moduler les propriétés de n'importe quel polymère rapidement, et de prédire la possibilité d'imprimer un nouveau polymère avec des propriétés cristallines spécifiques. Pour mieux comprendre les phénomènes survenant pendant le processus d'impression, plusieurs simulations computationnelles dynamiques de fluides (CFD) seront effectuées. Ces simulations permettront de visualiser et de comprendre au niveau local les forces et les contraintes associées à l'extrusion pendant l'impression 3D. L'ensemble de ces résultats permettront d'accélérer les relations entre les procédés de mise en forme d'échantillons et leurs propriétés.

DIRECT INK WRITING OF POLYMERS FOR ANTIMICROBIAL PURPOSES

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Direct ink writing (DIW) is an additive manufacturing (AM) technique that allows ease of use, high processing speed, tunable printing parameters and precision at a microscopic scale for the design of self-standing three-dimensional structures rivaling classical manufacturing methods such as molding and coating. The wide range of applicable materials, versatility of possible printing substrates and intricacy of structure design make it possible to tailor specific architectures or properties for the manufacturing of functional materials. More specifically, functional polymer materials are of particular interest, as the monitoring and alteration of process parameters in DIW allows for the adaptation of the printing process to a very broad selection of polymer materials. In this work, DIW printing processes were optimized for a variety of passive and functional polymer materials comprised of amorphous and semi-crystalline thermoplastic polymers. Physicochemical characterization of printed structures and incorporation of antimicrobial additives such as silver and assorted photosensitizers were explored, along with print fidelity are herein presented for a variety of printing conditions and starting materials. The influence of polymer morphology was studied in detail, as well as presence of additives and other factors likely to impact the printing process and resulting architectures' properties. The functionalization of these polymer materials through a polymer matrix/additive solute system helps further our understanding of how the printing process influences the properties of functional materials and how passage from passive to functional polymer materials can be achieved in conjunction with modern manufacturing techniques such as DIW. Pending further rheological characterization and biological assays, functional antimicrobial polymer materials manufactured by DIW such as the ones presented in this work could incite progress in fields like water disinfection and reaction catalysis.

A prospect beyond biodetection: Optical sensors via interparticle energy transfer between rare earth doped nanoparticles

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Interparticle energy transfer (IPET) refers to the distance-dependent energy transfer between an absorbing ion and emitting ion placed in different nanocrystals. This forms the basis of many optical sensors as IPET occurs only in the presence (or absence, depending on sensor design) of the target molecule, causing changes in the emission spectra.

Rare earth doped nanoparticles (RENPs) are a group of nanoparticles that can be excited in the near-infrared (NIR) range, and can convert low-energy excitation photons into high-energy photons (ultraviolet (UV), visible (Vis)) through a multiphoton process called upconversion. Simultaneously, they can emit in the NIR range at lower energies than the excitation wavelength, a single photon luminescence process called downshifting.

Many RENP-based optical sensors have designs that restrict their function to detection, as emitted wavelengths have limited biomedical application. Here, we exploit the unique optical properties of RENPs and study IPET-based optical sensors constructed of two types of RENPs, upconverting RENPs (uc-RENPs) and downshifting RENPs (ds-RENPs). In the presence of the target analyte, emission from uc-RENP may excite ds-RENP via IPET, causing emission of higher energy photons that can be used to trigger specific reactions as well as NIR photons that can be harnessed, all using a single excitation wavelength.

In this study we aim to prove the occurrence of IPET between Tm-doped RENPs (the uc-RENPs) and Nd-doped RENPs (the ds-RENPs). We hypothesize that upon NIR excitation, emission from Tm-doped uc-RENPs is absorbed by Nd-doped ds-RENPs if they are in close proximity. We synthesized core-shell RENPs and functionalized them with complementary DNA strands. Hybridization of DNA strands reduced interparticle distance and allowed IPET to occur, as shown by a decrease in UV/Vis emission intensity from uc-RENPs observed only in the presence of DNA-functionalized ds-RENPs. These results lay the foundation for utilizing RENP-based IPET systems for further biomedical applications.

ELECTROCHEMICAL APTAMER-BASED BIOSENSORS FOR METHOTREXATE MEASUREMENTS IN INTERSTITIAL FLUID

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High Dose-Methotrexate (HD-MTX) therapy is commonly used in the treatment of certain malignancies (i.e., leptomeningeal metastases, acute lymphoblastic leukemia, and osteosarcoma). However, MTX pharmacokinetic variability is highly significant between patients. As a result, MTX therapeutic drug monitoring (TDM) is essential to ensure therapy effectiveness and avoid potentially fatal side effects induced by delayed MTX elimination.

Typically, once MTX is administered, its concentrations in blood are measured with timed intervals until below 0.1 μM . Routine MTX monitoring is conducted mainly by liquid chromatography and immunoassays. Chromatographic methods are time-consuming and require expensive instruments operated by well-qualified personnel. Immuno-assays are, in contrast, performed using high-throughput and relatively fast automated analyzers with minimal sample handling. Nevertheless, immunoassays cannot be conducted in every clinic since large analyzers and reagent kits are costly. Although blood samples are typically used in TDM, for certain patients (i.e., those with fragile veins, neonates, and infants) frequent blood draws could prove difficult or impossible. Given that the MTX pharmacokinetic profiles in blood and interstitial fluid (ISF) are similar, MTX dosing in ISF could be an alternative to clinical practice.

In this context, we have developed electrochemical aptamer-based (E-AB) biosensors, a platform technology supporting high-frequency, direct, and real-time molecular measurements in undiluted complex matrices (i.e., blood, serum, saliva, urine). To obtain such performance, E-AB sensors are composed of a redox-reporter-modified aptamer (i.e., single-stranded oligonucleotides identified *in vitro* via Systematic Evolution of Ligand by EXponential Enrichment to bind a specific target of interest with high affinity) which is attached to a gold electrode via a self-assembled monolayer. Upon target binding, aptamer undergoes a conformational change, producing measurable readouts easily monitored using electrochemical techniques (i.e., square-wave voltammetry, and chronoamperometry). In this study, we demonstrate real-time and direct MTX measurements in undiluted interstitial fluid with a fast response time (~ 60 s). We envision that the developed method could be used to personalize HD-MXT therapy at point-of-care.

THE EFFECT OF CHEMICAL STRUCTURE OF PEG/PDMS COPOLYMERS ON ICE NUCLEATION TEMPERATURE OF POLYURETHANE-BASED HYBRID COATINGS

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ABSTRACT

The possibility of ice accumulation on surfaces has been recognized as a potential disruptor in various industries, including transportation, energy production, and telecommunications. The resulting issue can lead to catastrophic event and substantial economic losses[1, 2]. Different approaches have been developed to reduce ice accumulation on surfaces, including active and passive anti-icing strategies. Passive methods use engineered materials to protect surfaces, while active methods rely on external energy sources. Passive methods have lower operational costs as they do not require additional power sources. Nonetheless, the most important challenge of passive methods is their durability [3]. Polyurethane (PU) coatings are a prevalent choice due to their highly desirable properties. Their remarkable durability, adhesion, and ability to resist environmental factors, make polyurethane (PU) coatings a compelling choice to design the icephobic coatings[4]. In this study, the surface and ice nucleation temperature of PU-based coatings modified with PEG-PDMS copolymers of varying molecular weights were studied. Fourier-transform infrared spectroscopy (FTIR) was used to evaluate the curing of PU/PEG-PDMS coatings. The roles of molecular weights and chemical structure of PEG-PDMS copolymers as well as formation of hydrogen bonding between water molecules and hydroxyl and other linkage on wettability and ice nucleation temperature has been deeply investigated by DSC and Kruss machine equipped with a cold chamber. It was observed that the addition of PEG-PDMS copolymers to PU generally lowered the ice nucleation temperature more than 25%. This is due to the promotion of hydrogen bonds between the surface and water molecules by the hydrophilic groups in the coatings[5]. The presence of these groups forms a quasi-liquid-like layer at the ice-surface interface, which delays ice nucleation. The formation of hydrogen bonds between water molecules and hydrophilic groups increases the viscosity at the interface, reducing the mobility of water molecules. As a result, the quasi-liquid-like layer (QLL) formed at the interface has a higher viscosity at lower temperatures, slowing down the transition of water molecules from liquid to solid phase [6]. The results indicated that the ice nucleation temperature is affected by the terminal groups (methoxy or hydroxyl), molecular weights, and siloxane content concentrations.

Keywords: Icephobic Coating, Polyurethane, PEG/PDMS, Ice Nucleation Temperature,

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RATIONALLY DESIGNING FLUOROPHORES WITH ELECTROACTIVITY FOR ELECTROCHROMIC DEVICES

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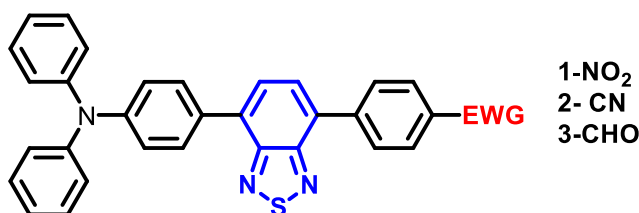
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Abstract

Donor-Acceptor-Acceptor (D-A-A) fluorophores were prepared and evaluated for both their intrinsic emission and electroactivity. Triphenylamine (TPA) was selected as the donor owing to its electroactivity, notably its reversible oxidation. TPA was covalently connected to a benzothiadiazole acceptor which was connected to various electron withdrawing groups (EWG) to complete the D-A-A fluorophore. The effect of varying the EWG of the D-A-A fluorophore on the spectroelectrochemical and fluorochemical properties were investigated. The electronic push-pull fluorophores were found to be solvatochromic and had a broad emission spanning the visible to NIR regions. The reversible redox behavior of TPA enabled an electrochemically mediated visible color change. The radical cation formed by electrochemical oxidation strongly absorbed in the near infrared region and it was contingent on the EWG. The electrochemical reversibility concomitant with the visible color changes makes the D-A-A fluorophores viable materials for use in electrochromic applications. Their intrinsic emission intensity could also be reversibly modulated with an applied potential. The fluorescence on/off behavior can also be exploited for us in functioning devices. Overall, electrochemically mediated color switching and reversible on/off emission behavior of the fluorophores make them ideal as dual-role materials in chromic devices. An acrylate chain to the D-A-A fluorophore was incorporated and successfully copolymerized on ITO device. Further investigation with the performance of the device is under progress.



Combination of Spectrofluidic Devices and Attenuated Total Reflection Infrared Spectroscopy for Plastic Biodegradation Study

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Synthetic polymers have become more prevalent in the environment due to their widespread use and inadequate disposal practices. The stubbornly resistant nature of plastics to degradation leads to their accumulation and saturation in the environment, which is a significant concern. Although physicochemical methods have been used to break down synthetic polymers, their effectiveness is limited, and they can release harmful byproducts into the environment. Microorganisms found in landfills and dumpsites have been observed to utilize plastics as their primary source of carbon, energy, and biomass, indicating their potential as a means of plastic degradation. The use of microfluidic devices, also known as Lab on a Chip (LOC), to study microorganisms is a developing field, with the miniaturization of the system providing new opportunities. The combination of FTIR with precise spatiotemporal using microfluidics is targeted for a LOC system that can provide an accurate view of biologically catalyzed plastic degradation which can inform kinetics and mechanistic studies. In this work, we integrated an ATR crystal in a LOC device and cultured plastic-eating bacteria in a channel. With the help of our lab-made ATR spectroscopy microfluidic assay accessory, we were able to obtain 1D FTIR images of bacteria distribution in a wide channel or conduct parallel experiments to test effect of conditions on bacteria growth simultaneously. Moreover, we embedded an ATR crystal covered with plastic film and cultured bacteria for long-time experiment. The use of ATR spectroscopy with plastic-eating bacteria in a long-term experiment can provide insight into the efficiency and effectiveness of these bacteria in breaking down plastic. This approach has potential applications in bioremediation and waste management.

STUDYING ELECTRODE DISTRIBUTION IN ROTARY FREESTANDING TRIBOELECTRIC NANOGENERATORS

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ABSTRACT

Triboelectric nanogenerators (TENGs) were first reported in 2012 by Wang et al. and are based on the triboelectrification concept, which corresponds to the movement of charges between two materials through contact or friction.¹ Four configurations have been developed to take advantage of TENG output, by using the charges induced in the electrodes to develop applications such as sensors, energy storage or power sources.^{2,3,4} Among them are rotary TENGs, which have demonstrated high performance according to their design and operating parameters.⁵ However, for those new to the field of TENGs, determining the appropriate electrode configuration is often a challenge. Herein, we describe three rotary TENGs by using: (1) a conventional stir plate, (2) ball bearings and (3) a salad spinner, to evaluate the relationship between electrode distribution and TENG output. It was determined that the distance, rotary mechanism, and the number of electrode portions can influence TENG voltage output and signal.

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INFLUENCE OF POLYMER CRYSTALLINITY AND MOLECULAR WEIGHT ON THE ORIENTATION OF ELECTROSPUN NANOFIBERS

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ABSTRACT

Electrospun nanofibers are unique polymer materials that often present an exponential increase in mechanical, thermal, optical, and electrical properties at reduced diameters. This behavior is largely correlated to the degree of molecular orientation within individual fibers.¹ Understanding how various electrospinning parameters affect orientation is thus a key requisite for structure and property optimization. In this work, we used polarized confocal Raman spectroscopy to shed light on the influence of two polymer characteristics, their crystallinity and molecular weight, over the relationship between fiber diameter and molecular orientation. Results show that nanofibers made from a highly crystalline polymer, poly(ethylene oxide) (PEO), exhibit an exceptionally high orientation that is maintained over a broad range of diameters,² whereas amorphous polystyrene (PS) fibers show the more commonly reported exponential increase in orientation. In PS fibers, higher molecular weight correlates with an increase in both the orientation values and the proportion of oriented fibers at any given diameter range. Together, these results suggest that increasing the number of effective crosslinking points between polymer chains, which slows down relaxation processes, is key to obtaining higher orientation. The presence of crystals in PEO fibers and, to a smaller extent, the increased number of entanglements per chain in PS fibers with high molecular weight both act as such crosslinks. This work contributes to a better comprehension of molecular orientation in electrospun fibers and guides the preparation of fibers with improved orientation-dependent properties.

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Surface plasmon resonance: a tool to facilitate translation of aptamers into electrochemical aptamer-based biosensors

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Electrochemical aptamer-based (E-AB) biosensors have demonstrated unprecedented capabilities for the continuous monitoring of molecules in undiluted complex matrices and directly in the body. E-AB sensors are comprised of a gold electrode functionalized with a redox reporter-modified aptamer and an alkanethiol self-assembled monolayer. Binding-induced conformational change of the aptamer displaces the redox reporter relative to the electrode surface resulting in changes of its electron transfer properties which are monotonically correlated to target concentration. While this class of sensors possess many attributes over current gold standard analytical techniques, translating aptamers towards a fully deployed sensor still represents a major bottleneck. This is in part because aptamer sequences are selected in solution and their behavior on an electrode is reported to change, ultimately causing discrepancies in binding affinities and loss of sensitivities. Moreover, testing several sequences remains costly and time consuming.

In response, we are developing a combined electrochemical-surface plasmon resonance (eSPR) approach to facilitate the translation of aptamers into E-AB sensors. As a proof-of-concept for our approach, we functionalized a gold prism with several methylene blue-modified DNA of different lengths before challenging the sensor with its complementary DNA. Doing so allowed us to concomitantly monitor the relative signal changes, affinity, and binding kinetics in both plasmonic and electrochemical response approaches for direct comparison. Although both techniques produced similar sigmoidal profiles, the relative signal change observed in SPR was one order of magnitude higher than the electrochemical response. Combining SPR with electrochemistry, however, allows to take into account the contributions of the applied potential on the gold film. We envision that our eSPR approach could be used as a benchmark to vet and help engineer aptamers without the need for costly redox reporter modifications so that they could translate more efficiently into the E-AB biosensors sensing platform to in turn accelerate their ability to deploy at the point-of-care.

SEPARATION MEMBRANES FUNCTIONALIZED WITH CARBOXYLIC ACID-CONTAINING CO₂-RESPONSIVE POLYMERS

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ABSTRACT

Stimuli responsive polymers often exhibit structural and conformational variations in response to mild environmental alterations. They have gained much interest due to their potential in a wide range of applications. Among the various stimuli, carbon dioxide (CO₂) has emerged as a trigger in recent years due to its safety, low cost, biocompatibility, low toxicity, and abundance. One noteworthy application of CO₂-responsive polymers is to make separation membranes, whose pores, permeability, and filtration selectivity can be adjusted or controlled by bubbling CO₂ through the solution. CO₂-responsive polymers are especially appealing due to their ability to undergo solubility switch in water through simple addition or removal of the gas, without chemical contamination. CO₂-responsive membranes known to date use tertiary amine-based polymers. Upon CO₂ aeration, the tertiary amine groups form charged ammonium bicarbonate, and the soluble polymer presents an extended chain conformation in water, which in turn converts the membrane to the pore-closure state, and the pore surface charge switches from neutral to positive. In the present study, we aim to make membranes with opposite gas switching behavior by designing, synthesizing, and investigating a novel carboxylic acid-based CO₂-responsive polymer grafted onto cellulose nanocrystal membrane. In this case, upon CO₂ bubbling the polymer switches from negatively charged to neutral state and becomes less soluble, which results in polymer chains collapse and pore opening. Upon removal of CO₂, the polymer returns to a more soluble state and the pores revert to a closed state. This type of membrane will broaden the accessible functions and applications.

Seeking Rules Governing Mixed Molecular Crystallization

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MIXED CRYSTALS RESULT WHEN COMPONENTS OF THE STRUCTURE ARE RANDOMLY REPLACED BY ANALOGUES IN RATIOS THAT CAN BE VARIED CONTINUOUSLY OVER CERTAIN RANGES. MIXED CRYSTALS ARE USEFUL BECAUSE THEIR PROPERTIES CAN BE ADJUSTED BY INCREMENTS, SIMPLY BY ALTERING THE RATIO OF COMPONENTS. UNFORTUNATELY, NO CLEAR RULES EXIST TO PREDICT WHEN TWO COMPOUNDS ARE SIMILAR ENOUGH TO FORM MIXED CRYSTALS CONTAINING SUBSTANTIAL AMOUNTS OF BOTH. TO GAIN FURTHER UNDERSTANDING, WE HAVE USED SINGLE-CRYSTAL X-RAY DIFFRACTION, COMPUTATIONAL METHODS, AND OTHER TOOLS TO STUDY MIXED CRYSTALLIZATIONS WITHIN A SELECTED SET OF STRUCTURALLY RELATED COMPOUNDS. THIS WORK HAS ALLOWED US TO BEGIN TO CLARIFY THE RULES GOVERNING THE PHENOMENON BY SHOWING THAT MIXED CRYSTALS CAN HAVE COMPOSITIONS AND PROPERTIES THAT VARY CONTINUOUSLY OVER WIDE RANGES, EVEN WHEN THE INDIVIDUAL COMPONENTS DO NOT NORMALLY CRYSTALLIZE IN THE SAME WAY. MOREOVER, CLOSE AGREEMENT OF THE RESULTS OF OUR EXPERIMENTS AND COMPUTATIONAL MODELING DEMONSTRATES THAT RELIABLE PREDICTIONS ABOUT MIXED CRYSTALLIZATION CAN BE MADE, DESPITE THE COMPLEXITY OF THE PHENOMENON.

DÉVELOPPEMENT DE MATÉRIAUX HAUTEMENT RÉFLÉCHISSANTS PRÉSENTANT UN FORT CONTRASTE DE POLARISATION

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Les nanofibres électrofilées sont des nanomatériaux unidimensionnels préparés en appliquant un champ électrique élevé à une solution de polymère. Ces fibres suscitent un intérêt considérable en raison de leur facilité de traitement et de leurs propriétés mécaniques et optiques, qui sont souvent bien supérieures à celles de matériaux préparés de manière conventionnelle, dû à une orientation moléculaire très élevée. Des travaux récents ont également montré qu'un nombre limité de polymères présentent, dans certaines conditions, des réponses optiques particulièrement intenses causées par des quasi-particules appelées polaritons. De nombreuses applications pourraient bénéficier de la combinaison des qualités optiques associées aux nanofibres et aux polaritons.

Dans ce contexte, nous avons développé, caractérisé et optimisé des tapis de nanofibres électrofilées hautement orientés présentant une réponse polaritonique. Les fibres ont été préparées à partir de polyoxyméthylène (POM), un polymère robuste connu pour sa capacité à générer des polaritons. La réponse optique des tapis a été suivie par spectroscopie infrarouge (IR) à réflexion spéculaire polarisée et optimisée par divers post-traitements des fibres. De cette manière, il a été possible d'augmenter leur réflectance de 3 à 60 % tout en présentant un excellent contraste de polarisation.

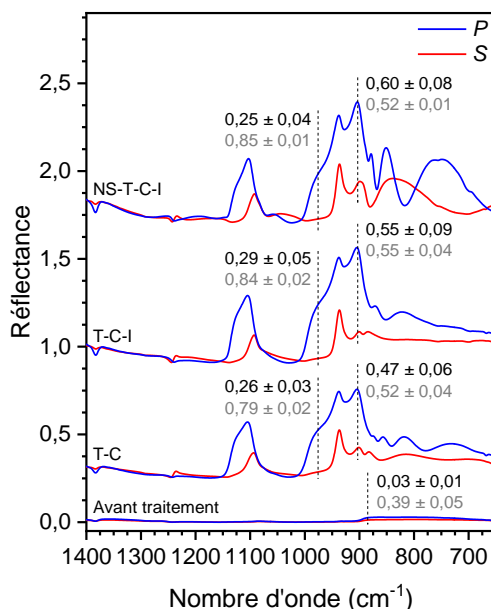


Figure 1. Spectres de réflexion spéculaire polarisée des tapis de POM soumis aux combinaisons des traitements optimisées en comparaison à un tapis non-traité.

SYNTHESIS OF RADICAL-BASED FLUOROPHORES FOR STIMULI RESPONSIVE DEVICES: A PROOF OF CONCEPT

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Abstract

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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Interface Engineering of Nickel-based Electrocatalysts for Enhancement of Water-splitting Performance

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ABSTRACT

Exploring highly active and stable bifunctional water-splitting electrocatalysts at ultra-high current densities is remarkably desirable. Interface engineering is a remarkably efficient route to boost both HER and OER intrinsic activities through coupling different active components for constructing heterostructures as bifunctional electrocatalysts. Herein, three-dimensional (3D) heterostructured transition metal-based electrocatalysts were prepared via the interface engineering, including 3D core-shell $\text{Ni}_x\text{S}_y@\text{MnO}_x\text{H}_y$ heterostructure nanorods grown on nickel foam ($\text{Ni}_x\text{S}_y@\text{MnO}_x\text{H}_y/\text{NF}$), 3D nickel-iron phosphides nanosheets modified by MnO_x nanoparticles grown on nickel foam ($\text{MnO}_x/\text{NiFeP}/\text{NF}$), and 3D Mn-doped $\text{Ni}_2\text{P}/\text{Fe}_2\text{P}$ heterointerface nanoflowers grown on Ni foam (Mn-doped $\text{Ni}_2\text{P}/\text{Fe}_2\text{P}$). The above electrocatalysts exhibit excellent bifunctional activities and stability for water splitting, especially at high current densities. These works shed a light on exploring highly active and stable bifunctional electrocatalysts by the interface engineering strategy.

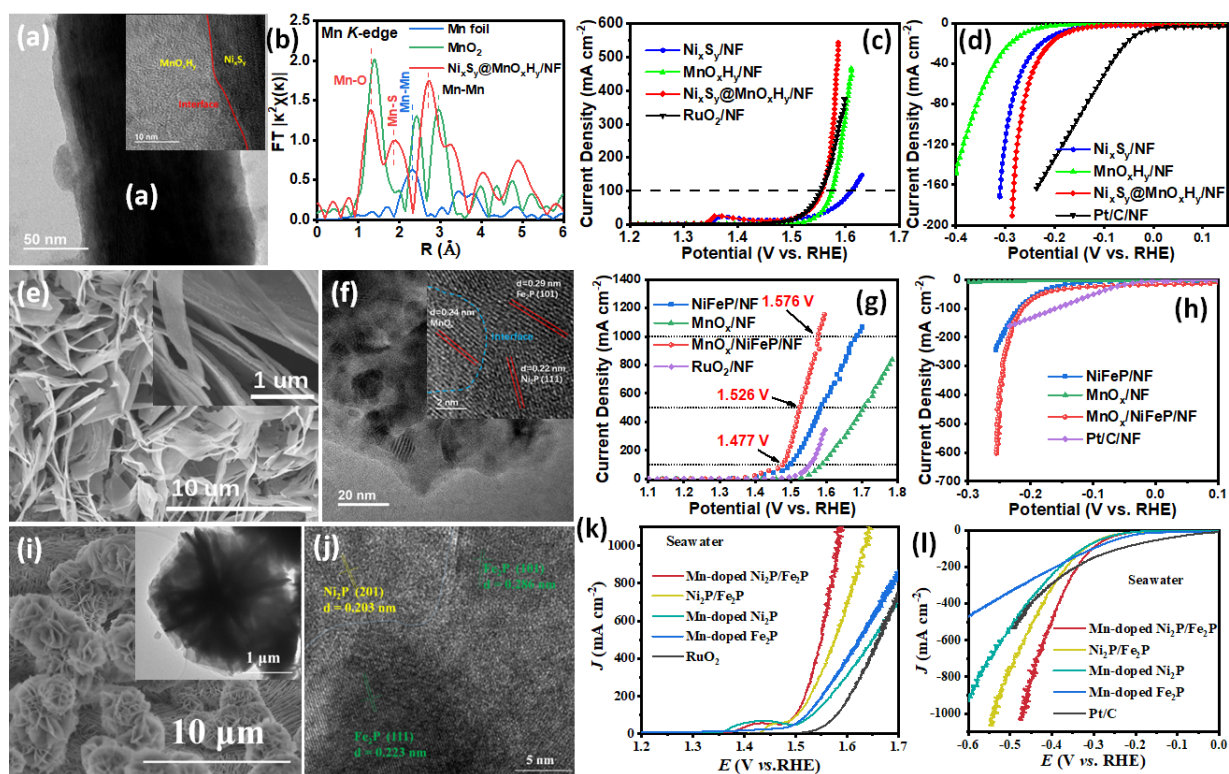


Fig. 1 (a) TEM image, (b) Mn K-edge FT-EXAFS oscillation functions $k^2\chi(k)$, (c) OER and (d) HER curves in 1.0 M KOH freshwater of $\text{Ni}_x\text{S}_y@\text{MnO}_x\text{H}_y/\text{NF}$; (e, f) SEM and TEM images, (g) OER and (h) HER curves in 1.0 M KOH freshwater of $\text{MnO}_x/\text{NiFeP}/\text{NF}$; (i, j) SEM and TEM images, (k) OER and (l) HER curves in 1.0 M KOH seawater of Mn-doped $\text{Ni}_2\text{P}/\text{Fe}_2\text{P}$.

LA MICROSCOPIE A SONDE BALAYANTE (SPM) AU LABORATOIRE DE CARACTERISATION DES MATERIAUX (LCM)

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Depuis janvier 2001, le Laboratoire de caractérisation des matériaux (LCM) offre à la communauté de recherche du Québec l'accès à une variété de techniques de caractérisation de pointe. Des professionnels de recherche y assurent la formation ainsi que le soutien technique. Nous décrirons brièvement les diverses techniques en microscopie à sonde à balayage (SPM) disponibles au LCM. Au-delà de la topographie, la SPM exploite la détection d'un éventail de propriétés physiques pour cartographier, avec une résolution latérale nanométrique, les propriétés nano mécaniques, électriques, électrochimiques, magnétiques et même l'absorbance IR d'une surface. En tant que technique, la SPM ne se limite pas à certaines conditions environnementales spécifiques, elle peut être réalisée sous vide, dans l'air ou en milieu liquide et à des températures variées. L'instrumentation de pointe et l'expertise qu'on y retrouve, font du LCM une des infrastructures spécialisées du Québec pour l'imagerie de matériaux nanostructurés et des couches minces à l'échelle du nanomètre et du micron. Notre installation SPM est utilisée par plus d'une centaine de scientifiques chaque année. Nos installations sont ouvertes à tous les chercheurs provenant des milieux universitaires et industriels, à des tarifs abordables.



EFFETS DE CONFINEMENT SUR LE MÉCANISME ET LES VITESSES D'INTERCONVERSION DES ISOMÈRES DE SPINS NUCLÉAIRES DE H₂O.

PATRICK AYOTTE

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Dans les conditions qui caractérisent le milieu interstellaire, les temps d'interconversion entre les isomères de spins nucléaires (ISN) de la molécule d'eau isolée, o-H₂O \leftrightarrow p-H₂O, ont été estimés à plusieurs milliards d'années. Cependant, des études spectroscopiques ont révélé que le processus d'interconversion se produit spontanément, à des températures aussi basses que 4K, lorsque la molécule d'H₂O est confinée dans des matrices de gaz inertes (Ne, Ar, Kr, Xe, p-H₂) ou encore, lorsqu'elle est piégée au sein du C₆₀, c'est-à-dire sous la forme d'endofullerènes, H₂O@C₆₀.

Les dépendances des coefficients de vitesse d'interconversion et de la constante d'équilibre avec la température (T = 4K - 30K), pour divers isotopologues de la molécule d'H₂O (H₂^AO, A = 16, 17, and 18) dans différents milieux de confinement (gaz rares, C₆₀) seront rapportées [1]. Le modèle du rotateur asymétrique quantique, confiné dans un puit de potentiel harmonique isotrope en trois dimensions, procure une description satisfaisante des spectres rotationnels et rovibrationnels de la molécule d'H₂O confinée révélant, dans la foulée, la topologie du potentiel de confinement. De plus, ce modèle renseigne sur l'origine des couplages entre les degrés de liberté rotationnels et translationnels et sur les mélanges des états ro-translationnels qui en découlent [2]. Nous proposons de nouvelles voies d'interconversion des ISN de H₂O et expliquons comment le confinement pourrait assouplir les règles de sélection très strictes des couplages hyperfins dans la molécule isolée. L'amélioration de notre compréhension des effets de confinement sur les mécanismes, et sur les taux d'interconversion des ISN de H₂O pourrait nous guider vers l'élaboration de meilleures stratégies de stockage [3] pour des échantillons hautement enrichis [4] en o-H₂O ouvrant de nouvelles perspectives pour l'application de la RMN pour l'étude des dynamiques interfaciales, de la catalyse hétérogène, de la corrosion et des mécanismes d'interconversion hétérogène des ISN.

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NANOFURNACES FOR CATALYSIS POWERED BY INDUCTION HEATING

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Most of the chemical industry uses building-size reactors that require a large amount of energy to provide the necessary heat to the reaction mostly produced by the combustion of combustible gas. With cheap sources of electricity available, changing to an induction heating process could be an excellent way for the industry to improve the spatiotemporal control of their processes and save on energy.

We have developed a novel microreactor for catalytic reactions that can be energized by induction heating. It uses the high potential of the nanofurnace principle to provide the necessary heat source for the reaction. The ferromagnetic particles interact with the magnetic field and convert electromagnetic energy into heat directly on the reaction site. With this method, heat transfer is much more efficient than traditional resistive heating.

The microreactor is manufactured in Teflon and can withstand the high temperatures achieved by the reactor. The reaction chamber is heated by a planar inductive coil. An IR camera bolometer probes the reaction chamber through a ZnSe lens closing the catalytic chamber which allows the measurement and control of the temperature of the system.

The catalytic particles used are bifunctional, they behave as a nanofurnace and as a catalyst. The bed's thermal gradient is generated by the heat of the reaction and by the thermal exchange with the optical glass and reactor core.

We show the possibility of heating catalytic microreactor by induction heating coupled with magnetic NPS. Then we aim to demonstrate the efficiency of this system, compare it with conventional heated reactors and open new shape opportunities for future development of induction heating in catalytic process.

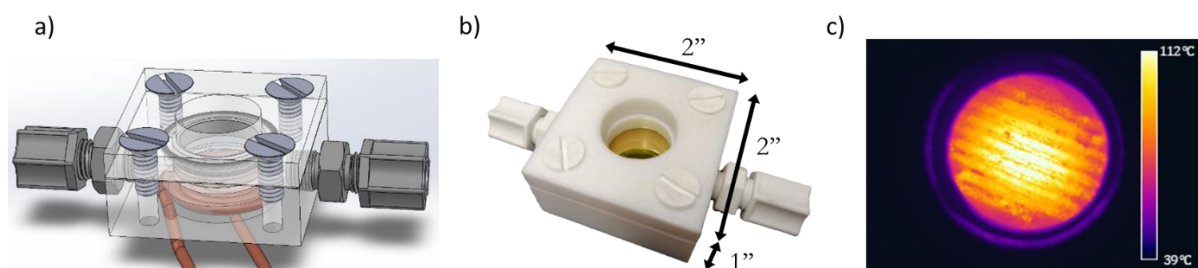


Figure 1 : a) CAD of planar microreactor for induction heating, b) manufactured planar microreactor, c) thermal imaging of catalytic chamber captured by FLIR M25 bolometer with microreactor energized with induction heating (250 A, 300 kHz).

Controlling stacking of benzene-1,3,5-tricarboxamide analogs in the crystal state through adjustment of their intermolecular hydrogen bonds, π - π stacking and substitutions at positions 2,4,6.

Pierre-Philippe Roy

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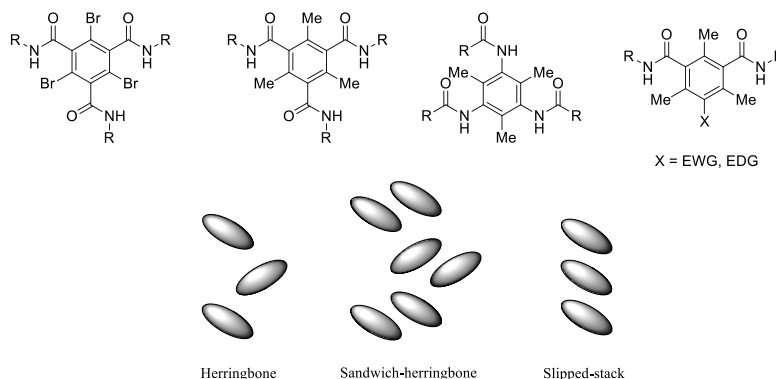
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The self-assembly properties of benzene-1,3,5-tricarboxamides (BTAs) cemented its place as an important building block in the field of supramolecular chemistry. Through intermolecular hydrogens bonds between the amides and π - π stacking, BTAs can, under the right condition, self-assemble into supramolecular polymer that find application in both the material and biomedical fields. One of the most interesting features for this class of compound is the face-to-face stacking arrangement between consecutive aryl rings stabilised by three hydrogen bonds, giving rise to helicoidal columns.

While extensive studies are done on the effect of amides substitutions on the self-assembly properties of BTAs, the effects of substitutions at the positions 2,4,6 on the aromatic core remains largely an unexplored area of research. In this context, we report the synthesis and crystallographic analysis of new C and N-centered BTA derivatives, crowded at the positions 2,4,6 with methyl or bromide substitutions. By comparing crystal structures, it is possible to observe that while hydrogen bonds play a significant role for the stabilisation of the columnar assembly of our molecules, the stacking pattern is strongly influenced by pi interactions. Increasing the electron density of the main aromatic ring through substitution with weak electron donating groups such as methyl stabilise a herringbone and sandwich-herringbone pattern. Analogs substituted with weak electron-withdrawing groups, such as the 2,4,6-tribromide, stack in a slip-stack column. Steric interaction from the amide's substitution can further influence the stacking pattern by destabilising the herringbone stacking pattern, making the slip-stack column the preferred arrangement.

Further modulation of the electronic properties of the aromatic ring is possible by replacing one of the three amides by electrons withdrawing or donating groups. 2,4,6-trimethyl-1,3-dicarboxamide stack in slip-stack column when functionalised with electron pulling groups. Otherwise, electron donating groups make the herringbone or sandwich-herringbone pattern the more stable columnar arrangement for the dicarboxamide analogues.



GROWTH OF CALCIUM PHOSPHATE LIESEGANG RINGS IN AGAR GEL

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Calcium phosphate (CaP) is an important inorganic compound with a wide range of applications, from biomedical^{1,2} to environmental applications³. Herein, we observe the emergence of Liesegang rings of CaP and investigate the phase transformation of CaP along agar gel *via* a reaction-diffusion process. In this work, three different forms of CaP were obtained: (i) dicalcium phosphate dihydrate ($\text{CaHPO}_4 \cdot 2\text{H}_2\text{O}$; DCPD), (ii) octacalcium phosphate ($\text{Ca}_8\text{H}_2(\text{PO}_4)_6 \cdot 5\text{H}_2\text{O}$; OCP), and (iii) hydroxyapatite ($\text{Ca}_{10}(\text{PO}_4)_6(\text{OH})_2$; HAp). The reaction-diffusion system plays a key role in this phase transformation, as the Ca^{2+} diffuses through the agar gel containing HPO_4^{2-} and reacts to form Liesegang rings of CaP. Growth of different forms of CaP within the same tube were observed by varying the initial concentrations of the reactants. X-ray diffraction (XRD) analyses confirmed the presence of different forms of CaP under varied experimental conditions. Different forms of CaP can coexist due to their kinetic formation and thermodynamic stability differences. Overall, these experiments highlight the diversity of CaP under reaction-diffusion conditions.

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$\text{Ti}_x\text{Hf}_{1-x}\text{VZrNb}$ as a negative electrode material for Ni-MH batteries

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YOUR ABSTRACT / VOTRE RÉSUMÉ

(300 words -1page max)

High entropy alloys (HEAs) attracted much attention as a promising material for hydrogen storage due to their unique properties. In this study, $\text{Ti}_x\text{Hf}_{1-x}\text{VZrNb}$ is investigated as a negative electrode material for Nickel-metal hydride batteries. Alloy is synthesized by arc melting and characterized by electrochemical charging/discharging for hydrogen absorption/desorption. X-ray diffraction (XRD) analysis revealed that the single body-centered cubic (BCC) phase disappears with increasing Hf concentration and decreasing Ti concentration in $\text{Ti}_x\text{Hf}_{1-x}\text{VZrNb}$ ($x = 0$ to 1). Alloys forming BCC exhibit higher discharge capacity than those having mixture of BCC and C15 Laves phase. The discharge capacity is significantly improved in Hf substituted alloys.

FIGURE

(Optional / Facultative)

L'impression 3D pour la compréhension de la production d'oxygène singulet dans des matrices polymères

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La fonctionnalisation de la surface d'un objet 3D permet l'accès à différentes propriétés intéressantes tel que l'inactivation photodynamique (*Photodynamic Inactivation* ; PDI). La PDI est une méthode qui permet l'élimination de bactéries et de virus en utilisant l'oxygène singulet comme élément cytotoxique produit à l'aide d'un photosensibilisateur. Notre projet repose sur l'hypothèse d'inclure ce photosensibilisateur dans l'objet 3D (i.e. dans la formulation utilisée pour l'impression) au lieu de fonctionnaliser la surface de l'objet déjà imprimé. En utilisant l'impression par écriture directe de formulation (*Direct-Ink Writing* ; DIW), ce projet explore la corrélation entre la structure, la forme et les propriétés d'un matériau en termes de production d'oxygène singulet, et ce, en imprimant un polymère contenant un photosensibilisateur. Une méthode a été développée pour mesurer la vitesse apparente de production d'oxygène singulet de manière indirecte afin d'évaluer l'effet de différents ratios surface sur volume pour les architectures imprimées. Les résultats montrent que la surface et le volume exercent une influence sur la production d'oxygène singulet. De plus, la rhéologie et la profilométrie ont permis de caractériser l'imprimabilité et la fidélité d'impression de la formulation.

INFLUENCE DE LA PRÉPARATION SUR LA STABILITÉ CINÉTIQUE DES VERRES MOLÉCULAIRES

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Résumé

Les verres moléculaires sont des matériaux ayant la possibilité de former un état vitreux et sont communément utilisés dans les médicaments et les systèmes optoélectroniques. L'étude de verres à base triazine a démontré que cette habileté provient en partie de leur capacité à faire des ponts hydrogènes.¹ Une recherche antérieure a mis en évidence l'influence de la température du substrat lors de la déposition de films de verre sous phase vapeur (PVD) sur leur stabilité cinétique et leur orientation moléculaire.² Ceci suggère que les conditions de préparation ont un impact sur certaines propriétés des verres. Nous avons ainsi évalué l'impact du solvant (DCM, benzène) et de la technique de préparation telles que la déposition par goutte (*drop casting*), le dépôt à la tournette (*spin coating*) et l'électronébulisation (*electrospraying*) sur la formation de pont hydrogènes du G94, un composé qui possède trois groupements amines donneurs de ponts hydrogène et deux groupements auxiliaire méthyle ce qui lui confère une grande facilité à former une phase vitreuse (fig.1). Puisque la formation de ponts hydrogène tend à faciliter la vitrification, la fraction de groupement amine faisant des ponts hydrogènes a été évaluée par spectroscopie infrarouge en transmission et par des analyses de décomposition spectrale SMMA (*Self-Modelling Mixutre Analysis*). Un supplément de ponts H de 9,4% pour le DCM et de 10,4% pour le benzène a été trouvé entre les conditions de préparation et l'état de référence. Ainsi, cette recherche contribue à d'optimiser notre contrôle sur la cristallisation des verres moléculaires afin de d'augmenter leur durabilité sous une forme vitreuse.

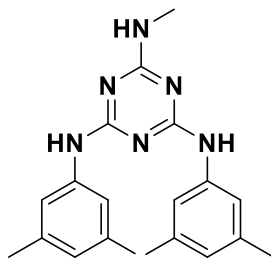


Figure 1. Structure G94.

1. *Phys. Chem. Chem. Phys.* **2016**, *18*,1681.
2. *J. Phys. Chem. B* **2017**, *121*, 2350.

INNOVATIVE ZIRCONIA BASED MATERIAL SHAPED BY SLA 3D PRINTING

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INTRODUCTION

Today a strong need for high-performance ceramic materials combined with new shaping techniques appears on the market. 3d printing technology of ceramic objects is in strong development as it opens new perspectives.

PURPOSE

based composites can provide new ceramic materials with a plastic deformation domain before rupture, excellent resistance to processing flaws and a Weibull modulus approaching that of a steel.

MATERIALS & METHODS

In this study, we explored the influence of SLA stereolithography shaping on this new ceria-stabilized zirconia-based material with unique mechanical behavior. Firstly, a slurry compatible with the CERAMAKER process was developed. Then, the object of the study was to evolve the influence of the shaping parameters (layer thickness, laser power, etc.) on the green part quality. Finally, the effect of the sintering temperature on the microstructure and mechanical properties of optimized SLA-printed material was also studied.

RESULTS

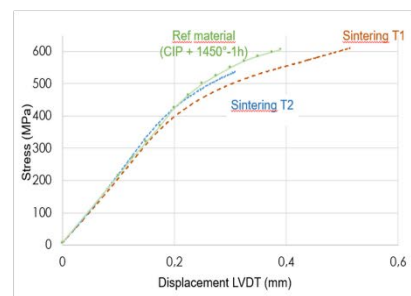
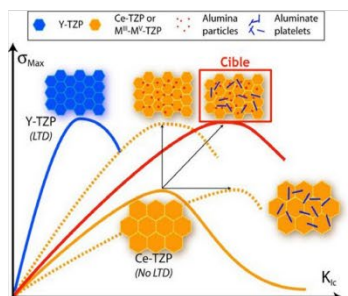
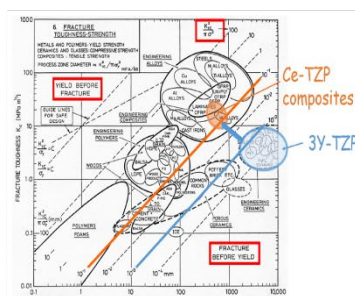
The new zirconia based material that has been developed shows mechanical properties with plastic behavior before rupture and a Weibull modulus of 40. ceria-stabilized zirconia can therefore admit a critical defect much more important than traditionally used Zr3Y (100 μ m instead of 1 μ m).

DISCUSSION

Through this study, 3DCERAM has been able to prove that this new material could be shaped by 3D SLA. Different sintering parameters have been studied to optimize densification and material properties. SEM observations show original layer structures and microstructure development attributable to the shaping process.

CONCLUSION

New zirconia-based ceramic composite material with high fracture toughness to make less invasive, strong and stable implants was developed by SLA printing. We have obtained excellent properties (Weibull modulus, fracture toughness and stress resistance) much better than those of traditional 3Y zirconia.



MICROMACHINING COMPRESSION MOLDING FOR FABRICATION OF HYDROPHOBIC AND ICEPHOBIC MICROPILLARED SILICONE RUBBER SURFACES

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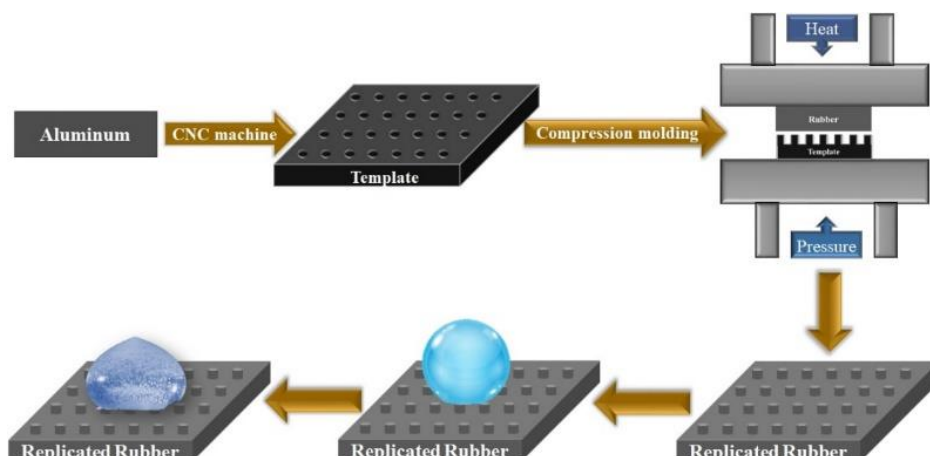
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Superhydrophobic materials could be a promising anti-icing technology that various techniques, such as self-assembly, plasma treatments, and lithography, can be used to produce micro- and nanostructured superhydrophobic surfaces. However, the practical application of these methods can be challenging due to complex engineering procedures, high fabrication costs, limited material suitability, environmental concerns, and low robustness. To address these issues, a simpler approach that involves micromachining to create micro holes and compression molding to generate replicas with micro- or nanostructures can be used. This method can significantly reduce fabrication time and costs, be applied to a wider range of materials, and provide highly reproducible results.

This study examines the effects of micro cylindrical pillar geometry on wettability and ice nucleation time. As a cost-effective, non-toxic, and efficient method of fabricating micropillars on silicone rubber surfaces, micromachining and direct replication were used to design and fabricate a set of micropillars. It is investigated experimentally whether wetting properties (contact angle and contact angle hysteresis) and anti-icing properties (ice nucleation time) are enhanced by patterned silicone rubber surfaces with cylindrical pillars of varying sizes and pitch distances.

Based on our experimental results with a limited range of pillar diameters and spacings between pillars, it appears that Cassie wetting occurs when the microcylindrical pillar diameter decreases and the space increases, while Wenzel wetting occurs when the pillar diameter increases and the space decreases. As a result of changing the surface geometry, the ice-substrate contact areas were different, resulting in a different freezing delay time. A change in micropillar geometry could make it easier to control surface wetting and anti-icing properties in superhydrophobic and anti-icing surfaces.

Keywords: Micromachining, Compression molding, Pillar array, Hydrophobicity, Ice nucleation time



ALGINATE MICROBEADS CONTAINING MAGNETIC NANOPARTICLE FOR MRI TRACKING OF ENCAPSULATED ISLETS

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ABSTRACT

Introduction: Encapsulation of pancreatic islets within hydrogels is being investigated to protect the cells from the immune system for type-1 diabetes therapy. However, when the cells are implanted *in vivo*, it is essential to develop strategies to monitor them. MRI is an attractive imaging modality to visualize soft tissues at anatomical resolution, but it is necessary to incorporate a contrast agent. Recently, ultrasmall superparamagnetic iron oxide nanoparticles (USPION) constitute an excellent alternative to gadolinium-based compounds as “positive” contrast agent for enhancing the signal in T_1 -weighted MRI.

Objective: This study aims to develop and demonstrate the retention of PEG-stabilized USPION within alginate microbeads for *in vivo* MRI follow-up of encapsulated pancreatic β -cells.

Materials&Methods: The synthesis of PEG-stabilized USPION was carried out through the thermal decomposition of iron-oleate complex followed by phosphate-PEG(5K)-COOH ligand exchange. The physicochemical and magnetic characterization was done by using DLS, TEM, FTIR, TGA and NMR relaxometer. Nanoparticle-containing alginate microbeads were obtained by an emulsification (water-mineral oil) and internal gelation process (triggered by acetic acid). The nanoparticle's retention was assessed by relaxivity measurements and T_1 -weighted MRI scans.

Results: USPION-PEG were successfully synthesized with a size less than 5 nm required to be an effective positive contrast (TEM: 4.8 ± 0.6 nm, DLS: 35 ± 4 nm); which was confirmed by the relaxivity ratio ($r_2/r_1=3.4$). The presence of PEG ligand at the surface of the iron oxide core after the ligand exchange was confirmed by FTIR and TGA. Nanoparticles were retained within the alginate microbeads for 3 months and the microbeads were visible in T_1 -weighted images with a good contrast.

Conclusion: The synthesized PEG-coated USPION demonstrated to provide a positive contrast to alginate microbeads for T_1 -weighted MRI. Overall, this study demonstrated preliminarily that the obtained MRI contrast-enhanced alginate microbeads could help monitor the outcomes of pancreatic islets transplantation in type 1 diabetes therapy.

POLYETHYLENE TEREPHTHALATE DEGRADATION BY NOVOZYM AND NAOH: A QUANTITATIVE ATR-FTIR SPECTROSCOPY STUDY

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Polyethylene terephthalate (PET) is a popular polymer due to its excellent physical properties, but its non-biodegradable nature has become an environmental concern as it can persist for hundreds of years. The characterization of PET enzymatic degradation can be challenging due to the slow rate of the process. Attenuated-total-reflection (ATR) Fourier-transform-infrared (FTIR) spectroscopy is a surface sensitive technique that is commonly employed to monitor PET degradation due to its sensitivity to detect the several functional groups simultaneously and can report on quantitative changes to components present in the spectra during degradation reactions. After reviewing articles on FTIR spectroscopy in PET degradation, we found reports that misinterpreted spectral findings, including the intensification of carbonyl and ester peaks, and the amorphous peak as indicating a crystalline peak. In this study, we determined the PET degradation, after recording several hundred ATR-FTIR spectra and performing integration analysis at different days of incubation with cutinase and NaOH solution. Integrations results revealed that hydrolysis occurred in both PET film and beads, as evidenced by the continuous decrease in three ester bands with each advancing incubation period. The 2nd derivative spectra were utilized to deconvolute the complex bands particularly esters peaks and enabling the identification of precise band locations for integration. Furthermore, we observed an increase in several peaks associated with trans conformations, indicating an increase in crystallinity, and gauche conformation peaks were decreased due to a reduction in the amorphous region. A new peak corresponding to ethylene glycol, which is one of the precursors of PET, was also observed. Our results demonstrate the potential of ATR-FTIR spectroscopy as a rapid, non-destructive, and sensitive analytical tool for the assessment of PET degradation. The integration of large spectral datasets at different incubation periods allowed the identification of amorphous and crystalline bands precisely, with continuously decreasing and increasing intensities, respectively.

SYNTHESIS OF CARBON NANOSPHERES BY CATALYTIC CHEMICAL VAPOR DEPOSITION (CCVD)

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The mechanical properties of carbon nanostructures make them promising for use as reinforcing fillers in the matrices of various composites. In this work, we are interested in synthesizing carbon nanospheres (CNSs) since their morphology allows good dispersion and distribution in a polymer matrix. In the next generation of multifunctional materials, CNSs are expected to be used as polymer reinforcements to improve some mechanical properties, including Young's modulus, mechanical impact strength, abrasion, and wear resistance. The chemical vapor deposition (CVD) method was used to synthesize CNSs since it provides a powder of high purity and makes it possible to control the size of the nanoparticles. The principle of this method (CVD) is based on the catalytic decomposition of acetylene under a nitrogen atmosphere and at high temperatures [900 – 1000°C] to obtain CNSs. This study aims to optimize the process parameters to produce CNSs with an average diameter of less than 100 nm, minimal accretion level, and a high production rate. In this work, we obtained CNSs with an average diameter of 96 nm for a ratio of $N_2:C_2H_2 = 40$ at 1000°C for one hour of reaction time. But we managed to have just a 2 g/h production rate. For this reason, we have built another large-scale reactor to have at least 20 g/h of CNSs. The dependence of CNSs size on temperature and $N_2:C_2H_2$ ratio can be understood in terms of nanoparticle residence time and catalyst activation.

Keywords: Carbon nanospheres, Chemical vapor deposition (CVD), Catalytic decomposition, acetylene.

HAIRY NANOCELLULOSES FOR THE SYNTHESIS OF NOBLE METAL NANOPARTICLES

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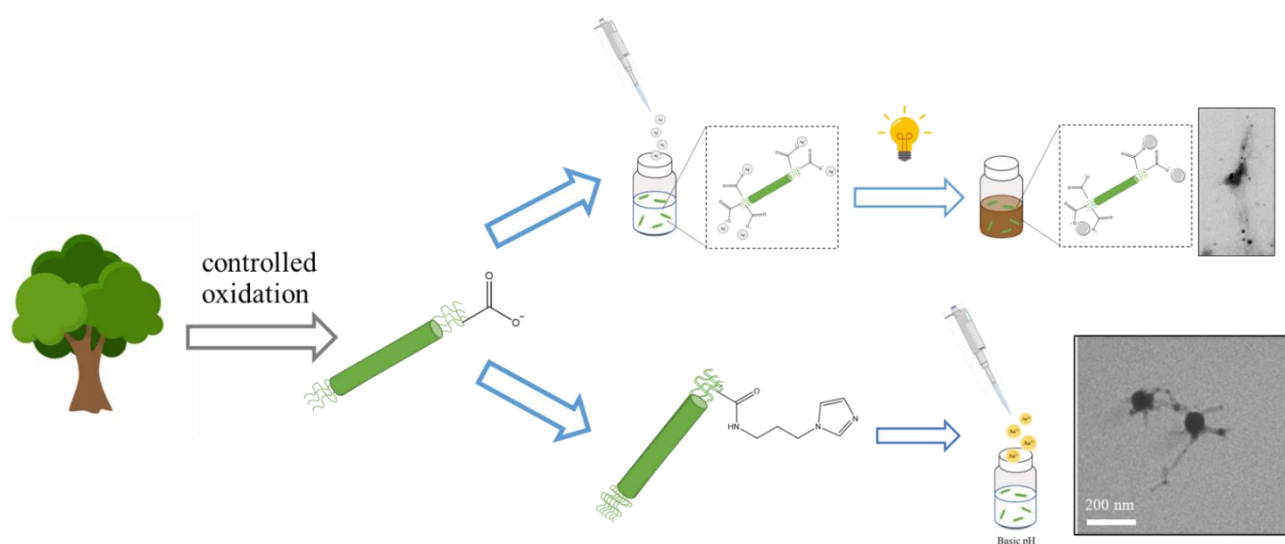
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Nanocelluloses are an emerging class of materials that have innovative applications in many fields. Cellulose is the world's most abundant biopolymer and is a renewable, biodegradable, and biocompatible material with easily modified surface chemistry. Through a two-step oxidation process a novel type of nanocellulose consisting of both crystalline and amorphous regions can be obtained. This nanocellulose has been termed hairy nanocellulose, due to its unique morphology of a crystalline rod with amorphous polymer hairs extending from each rod end. It can be prepared with a large number of carboxyl groups that offers opportunities for further functionalization.

The unique properties of hairy nanocellulose make it an excellent green alternative to conventional stabilizing agents for metal nanoparticles. This study describes the decoration of hairy nanocellulose with small and monodisperse silver nanoparticles in a green in-situ synthesis. We also detail the preparation and characterization of hairy nanocellulose derivatives designed to act as stabilizers for gold nanoparticles. Furthermore, we describe the in-situ synthesis of gold nanoparticles using the hairy nanocellulose derivatives as both the reducing and stabilizing agent. Unique structures of gold nanoparticles and hairy nanocellulose are reported. The morphology of hairy nanocellulose is utilized to prepare novel star-like and web-like composite structures with gold nanoparticles. We highlight how the morphology and versatile surface chemistry of hairy nanocelluloses makes them excellent candidates for the preparation of metal nanoparticles.

Keywords: hairy nanocellulose, natural biopolymers, metal nanoparticles



SYNTHESIS AND CHARACTERIZATION OF GRAPHENE EPISULFIDE

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RÉSUMÉ

Les batteries Li-S font face à de multiples obstacles comme la faible stabilité chimique de la cathode due à la navette des polysulfures, des pertes irréversibles de capacité et de durée de vie les empêchant d'être commercialisées. Les nanostructures de carbone ont été étudiées afin de résoudre ces problèmes en stabilisant la cathode par deux méthodes, l'adsorption chimique et le confinement physique, avec des résultats variables de piégeage de soufre et de performance de batterie. La formation de liaison covalente entre le carbone et le soufre est une troisième approche rarement appliquée au graphène [1].

Cette présentation résume la synthèse et la caractérisation de nouveaux composés appelés épisulfures de graphène (GS). Ces composés GS sont synthétisés par une réaction en phase gazeuse avec des conditions de pression et de température modérées, sans solvants ni catalyseurs. Les produits sont caractérisés par spectroscopie Raman, XPS et appuyés par des calculs DFT. Ces résultats suggèrent que la signature vibrationnelle de GS est conforme avec des groupes épisulfures à la surface du graphène.

[1] Fang, R.; Xu, J.; Wang, D.-W. Covalent Fixing of Sulfur in Metal–Sulfur Batteries. *Energy Environ. Sci.* 2020, 13 (2), 432–471. <https://doi.org/10.1039/C9EE03408K>.

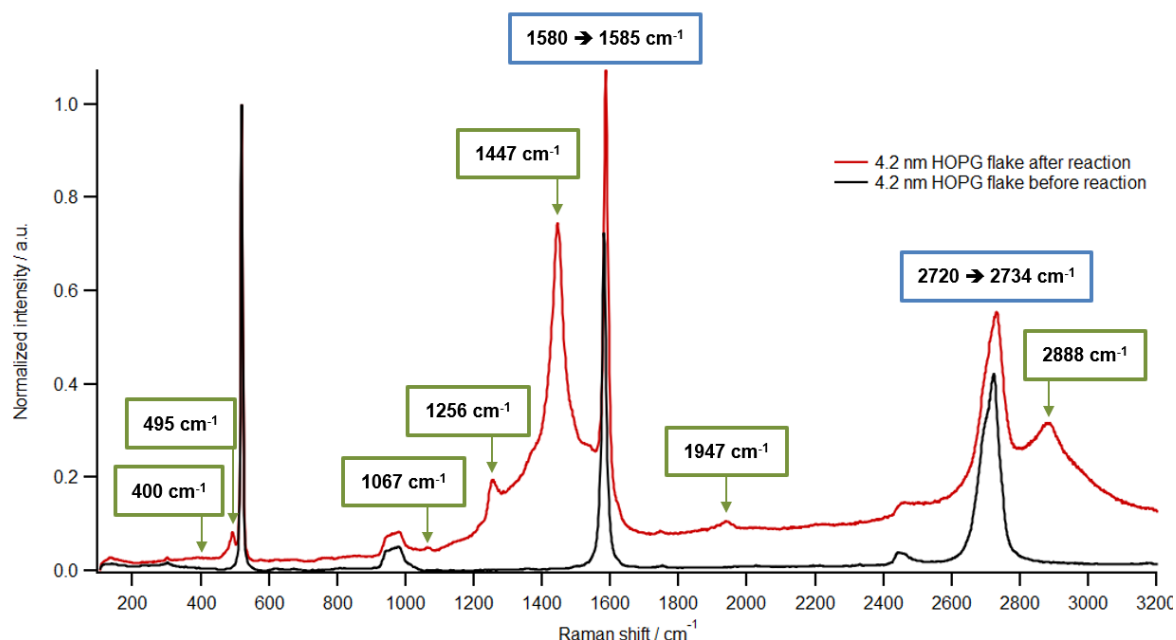


Figure: Raman spectra before and after reaction on HOPG flakes.

Atomically Dispersed N-coordinated Cobalt Atoms as Highly Active and Durable ORR Catalyst for Zn-Air Batteries

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The development of inexpensive, highly active and stable non-noble-metal catalysts for the oxygen reduction reaction (ORR) is critical for the practical applications of electrochemical energy conversion devices, while grand challenges remain. Herein, we report a facile ammonium salt etching strategy to construct an electrocatalyst with atomically dispersed Co sites embedded on N-doped porous carbon (CoNC), which demonstrates excellent ORR performance in alkaline electrolyte. The NH_4Cl -treated catalyst exhibits equivalent or even better ORR performance than those of commercial Pt/C catalyst, for example, with an onset potential of 1.06 (vs 1.01 V for Pt/C) and half-wave potential of 0.893 V (vs 0.873 V for Pt/C). Additionally, methanol tolerance tests show that the CoNC catalyst is immune to methanol poisoning in actual operation, which is much better than the Pt/C catalyst. Moreover, this NH_4Cl -treated CoAC catalyst is stable in a long-term operation up to 110 h, which is superior to most Co-based catalysts. This work provides a promising strategy for the synthesis of next-generation highly active and durable Pt-free ORR catalysts for Zn-air batteries and beyond.

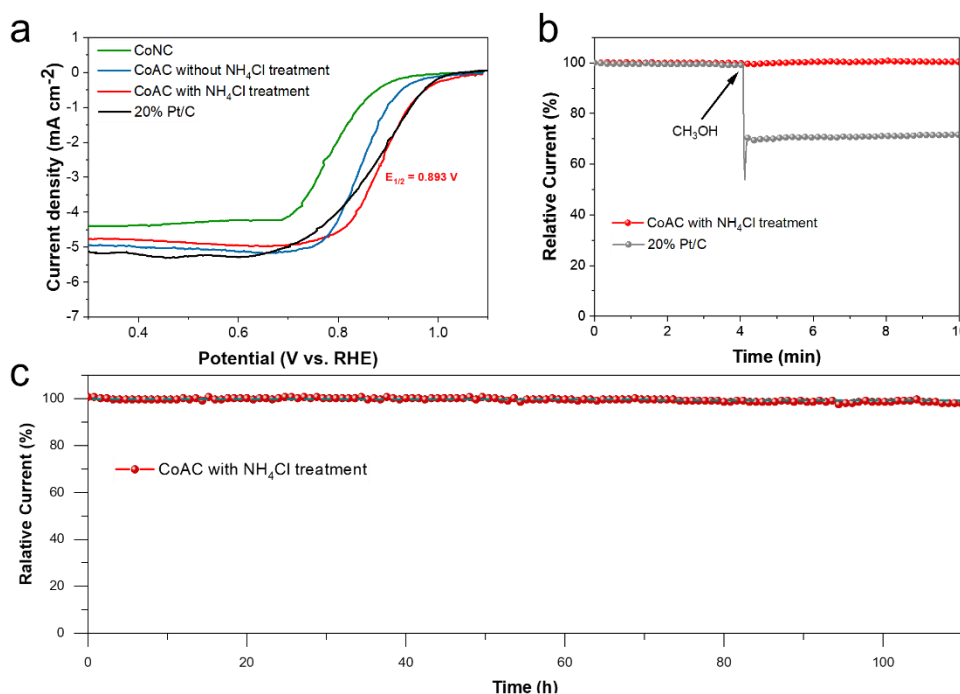


Figure 1. (a) ORR polarization curves of CoNC, CoAC without NH_4Cl treatment, CoAC with NH_4Cl treatment, and commercial Pt/C (20%) catalyst in 0.1 M O_2 -saturated KOH solution, scanning rate of 5 mV s^{-1} at 1600 rpm. (b) Methanol tolerance test of CoAC with NH_4Cl treatment catalyst and commercial Pt/C (20%) catalyst at 0.5 V with a rotation rate of 1600 rpm. 20 μL methanol is injected into the 0.1 M O_2 -saturated KOH electrolyte (200 mL) at 4 min. (c) The current-time chronoamperometric response in O_2 -saturated 0.1 M KOH solution at 0.8 V with a rotation rate of 200 rpm.

Development of a Novel Copper-Graphene Composite Coating with Enhanced Antibacterial Properties Using Inductively-Coupled Plasma Torch Spraying

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Abstract

Copper (Cu) has been used as an antibacterial agent for a long time. Recent research has found that incorporating graphene into copper coatings can enhance their antibacterial properties. However, the implementation of copper-graphene composite coatings is limited due to the high cost and scarcity of copper and the challenge of achieving a uniform distribution of graphene in the copper matrix. To address these issues, a new process for coating a metal substrate with a homogeneous composite made from copper nanopowder and graphene nanoflakes (GNFs) was developed in this study. An inductively coupled radio frequency plasma torch was used to spray a suspension of Cu powder and GNFs, creating a 15-25 μm -thick coating with good dispersion of GNFs within the Cu matrix. The quality and microstructure of the Cu-GNF coatings were evaluated using several techniques, including transmission electron microscopy, scanning electron microscopy, Raman spectroscopy, and X-ray diffraction. The results showed that the Cu-GNF coatings had exceptional antibacterial activity, with a 99% reduction of *Escherichia coli* within an hour.

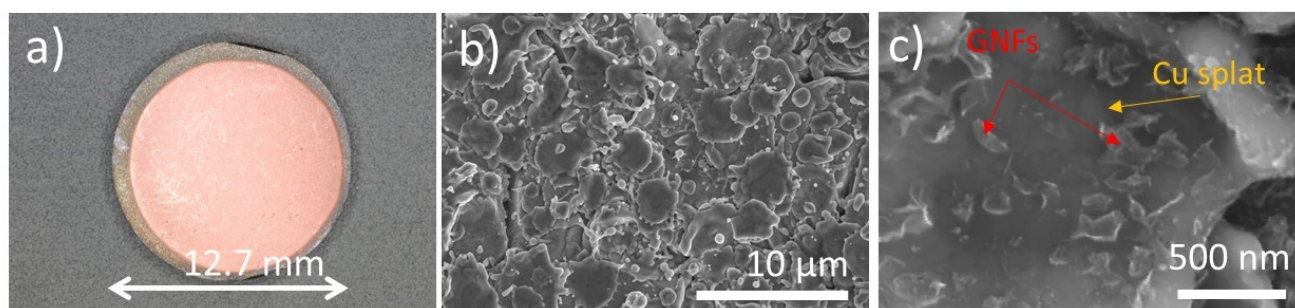


Figure 1. (a) optical image of Cu-1wt.%GNFs composite coating deposited using IC plasma. (b) SEM image of the top surface of the Cu-1wt.%GNFs coating. (c.) High-magnification SEM images of the different morphologies within the Cu-1wt.%GNFs coating.

UNDERSTANDING THE BIOLOGICAL INTERACTIONS OF METAL ORGANIC FRAMEWORKS TO INFORM WATER TREATMENT NANOTECHNOLOGY

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Abstract : Metal organic framework (MOF) nanomaterials possess desirable properties, such as high surface area, high porosity, and tunability of properties for the removal of contaminants in water. MOFs have been studied significantly for organic contaminant removal; however, minimal research has been aimed at understanding or utilizing the interactions of MOFs with biological systems, especially for the aim of water treatment for biological contamination. This project aims to develop design guidelines that correlate the physicochemical properties of various MOF nanomaterials with functional properties of interest for environmental applications. This was performed by testing four MOFs of various size, morphology, and composition and characterizing their antibacterial efficacy and how they impact the cellular integrity of microorganisms. Four zinc-based MOFs : ZIF-8, ZIF-90, Zn-MOF-74, and MOF-5 were chosen especially due to previous studies exhibiting zinc's bactericidal capabilities. The toxicity of the different MOF nanomaterials was analyzed after performing three hour exposures on bacterial cells while using concentrations varying from 100 to 500 µg/mL of each material. *Escherichia coli* was used as the model organism for these exposure experiments. From this data, one is determining toxicity endpoints: No Observable Effect Concentrations (NOEC), Lowest Observable Effect Concentration (LOEC), and Effective Concentration inducing 50% inhibition (EC₅₀). These toxicity endpoints will be correlated with the different material properties to identify the most important determinant for the toxicity of these MOF nanomaterials. Simultaneously, another project is being performed to correlate these MOFs antibacterial efficacy with their aqueous stability for potential application in water treatment.

VIOLOGEN DERIVATIVES TO IMPROVE PERFORMANCE OF AQUEOUS ORGANIC REDOX FLOW BATTERY.

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Renewable energy sources like wind and solar power are great alternative for a clean way to produce electricity but have the inconvenience to fluctuate. To address this issue and promote the implementation of renewables sources, scientists are developing new ways to store energy while the production is at a maximum for a subsequent release when there is demand. Redox flow batteries (RFBs) are the most appropriate solution and are increasingly gaining attention for stationary, large scale electrochemical energy storage. One variation of RFBs are aqueous organic redox flow batteries (AORFBs), where water-soluble organic molecules are use as the redox couple. Viologen type molecules are particularly well-suited as a negative potential species to develop cheaper and better AORFBs with great scalability, reversibility and long-term stability. In this study, viologen derivatives were synthesised with various N-functional groups to explore the impact of the substituent on their solubility, viscosity and redox potential. We showed that the use of short chains of poly(ethylene glycol) improved the solubility of the viologens derivatives which could lead to batteries with higher capacity. The asymmetric viologen (with two different substituents) provided a higher solubility and the reduction potential was unaffected by the chemical nature of the substituents. We demonstrated that the 1-(3-sulfonatopropyl)-1'-(bisethylene glycol)-4,4'-bipyridium (SPr-V-PEG2) showed a much-improved solubility (2.7 M in 1M KCl) and low viscosity (3.4 mPa*s at 1M) compared the symmetrical sulfonatopropyl derivative. As such, the most promising derivative, SPr-V-PEG2, was selected for further evaluation in a labs-scale RFB prototype cell. The compound was studied at various concentrations to assess the maximum energy density that can be reached and the effect of concentration on cycling life by achieving a comparison to the symmetrical 1,1'-bis(3-sulfonatopropyl)-4,4'-bipyridium (SPr-V-SPr).

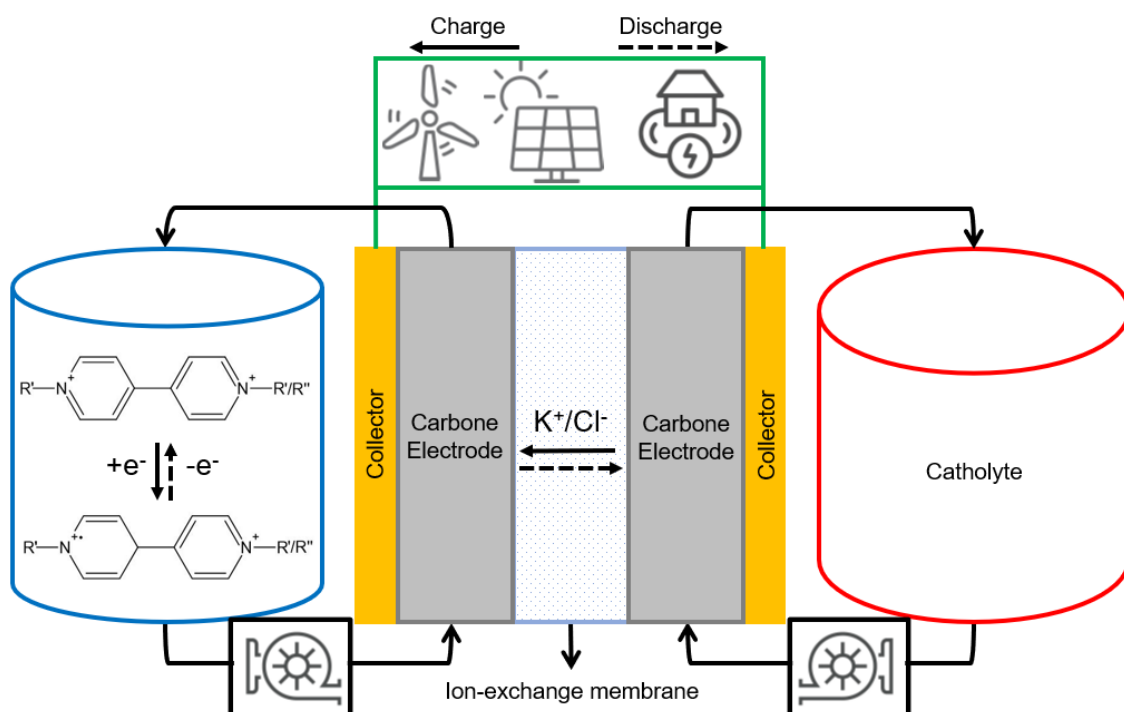


Figure 1 : Redox flow battery scheme with viologen redox couple reaction as the anolyte.

Cyanobacterial material classification with machine learning

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Our research project focuses on using microspectroscopic tools and machine learning algorithms to classify different species of cyanobacteria, a type of biological material that is extensively found in natural environments and plays a critical role in local ecology, especially in the Arctic and semi-Arctic regions.

Cyanobacteria are not only essential for the local ecosystem but also widely applied in food and fuel industries. However, classifying different species of bacteria living together is a challenging task for almost all fields of study focusing on biological material.

To address this issue, we applied non-invasive microspectroscopic techniques, including fluorescence spectroscopy using a confocal laser scanning microscope and Fourier-transform infrared spectroscopy conducted in the Canadian Light Source synchrotron facility. These techniques enable me to characterize the physiological state of cyanobacteria and identify differences between different species.

To classify the different species of cyanobacteria, multiple machine learning models were applied, including random forest, support vector machine, and neural network, to optimize the classification methodology.

The results of this study have significant implications for the fields of material science, ecology, and biotechnology, as it provides a powerful tool for the identification and classification of biological materials, including cyanobacteria. This research also contributes to our understanding of the ecological roles of cyanobacteria in natural environments and their potential applications in food and fuel industries.

PHOTO-CHARGING A LI-ION BATTERY INTEGRATING AN ELECTRONICALLY CONDUCTIVE AND LIGHT ACTIVE POLYMER

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ABSTRACT

The binder in an operating battery plays an important role of consolidating the active materials in the device. It further ensures the materials adhere to the electrode and it prevents their delamination during battery operation. While the role of the binder is to mechanically reinforce the electrode, it is electrochemically inert and it does not enable the operation of the device. It would be beneficial to take advantage of the dead mass of the binder for it to actively contribute to the electrochemical functioning of the battery. Key properties to integrate into the binder are electroactivity, electronic conductivity, and light harvesting. The latter would make the battery rechargeable with light. An important step towards storing sun light for use during dark periods and intermittent sunlight.

Leveraging the light harvesting and photoreduction capacities of a perylene diimide dye, we developed a polymer that could play multiple functions in a lithium-ion battery. The polymer was designed to be electronically conductive, harvest sunlight, and convert sunlight to electricity while also playing the conventional cohesive role of a binder. This was motivated by solution and solid-state studies that showed the dye could promote redox reactions with the active material in a lithium-ion battery: lithium iron phosphate (LFP).¹ It will be shown that the polymer binder in an operating device can harvest light and generate a charge.

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STUDY OF PH-RESPONSIVE POLYMER MEMBRANE

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Membrane technologies occupy an important position in research and development in industry due to the numerous applications. Since stimuli-responsive polymers can change their physical, chemical properties or morphology depending on the environment conditions (pH, temperature...), their integration in membranes may enable control in the separation or filtration process, thus enhancing the capacity of membranes to extract a specific target from the sample. In the present study, we prepare a pH-responsive polymer membrane by using poly(4-vinyl pyridine) (P4VP) as additive in polyvinylidene fluoride (PVDF), one of the commercial membranes. The adopted approach is to use non-solvent induced phase separation to fabricate the porous membrane and, at the same time, investigate the effect of various parameters in making the membrane (pH, temperature of coagulating bath), with the purpose of developing an ability to control the assembly of the stimuli-responsive polymer additive on the surface of the membrane. Preliminary results will be presented. Developing a general method for creating stimuli-responsive membranes from commercial ones will open the door to new applications.

STUDY OF A NEW ELECTRICALLY RESPONSIVE LIQUID CRYSTAL ELASTOMER

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Liquid crystal elastomers (LCEs) combine the features of both liquid crystals (ordered structure, anisotropic properties) and rubbers (entropic elasticity). These materials have been widely investigated as soft actuators because of their reversible, stimuli-controlled deformations with quick response. If LCEs are also endowed with electrical conductivity, they can be used for not only actuation but also sensing applications. However, the challenge is how to render LCEs electrically responsive while retaining the actuation capability. In the present work, we adopt a new approach by synthesizing a semi-interpenetrating polymer network (semi-IPN) comprised of a non-crosslinked poly(ionic liquid) (PIL) and a crosslinked LCE. Our preliminary results show that some degree of controlled phase separation between the two polymer components, which is crucial for ionic conductivity and order-disorder phase transition induced reversible shape change, could be obtained by varying the preparation conditions. Moreover, the actuation behavior and sensing through change in electrical resistance of this new LCE are investigated.

Engineering effective charge separation and hole transfer on nanopyramid-shaped BiVO₄-based nanoarray photoanodes towards photoelectrochemical water splitting

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YOUR ABSTRACT / VOTRE RÉSUMÉ

(300 words -1page max)

Directly converting solar energy through photoelectrochemical (PEC) technology is an advanced strategy to realize clean energy production. Semiconductor photoanodes as critical components play an important role in the overall photoconversion efficiency. Therefore, plenty of PEC research studies focus on the development of highly-efficient photoanodes with simultaneously satisfied optimal optical absorption, wonderful quantum efficiency, and long-term photostability, but are still challenging. In this regard, bismuth vanadate (BiVO₄) exhibits great potential because of its high theoretical photocurrent density of 7.5 mA cm⁻² (based on the band gap of 2.4 eV), high photovoltage of ~1 V, and superior photochemical stability in a near-neutral aqueous medium. However, the practical PEC performance of single BiVO₄ photoelectrodes is still limited by their rapid body carrier recombination rate and short hole diffusion length. In this presentation, we will show how one-dimensional (1D) oriented BiVO₄ nanoarchitecture (nanopyramid arrays) could be applied to define the charge transfer pathway with less carrier loss and facilitate ion diffusion with reduced bulk charge recombination. In which a collaborative strategy of electrochemical treatment and MoS₂ as a heterojunction was employed to further enhance the overall photoconversion efficiency by enriching oxygen vacancies and making unidirectional charge transfer channels. The obtained data for E-BiVO₄/MoS₂ photoanode to effectively convert the solar energy into chemical energy for significantly promoted water splitting will be presented.

FIGURE

(Optional / Facultative)

ACETYLATED CARBOXYLATED CELLULOSE FILMS

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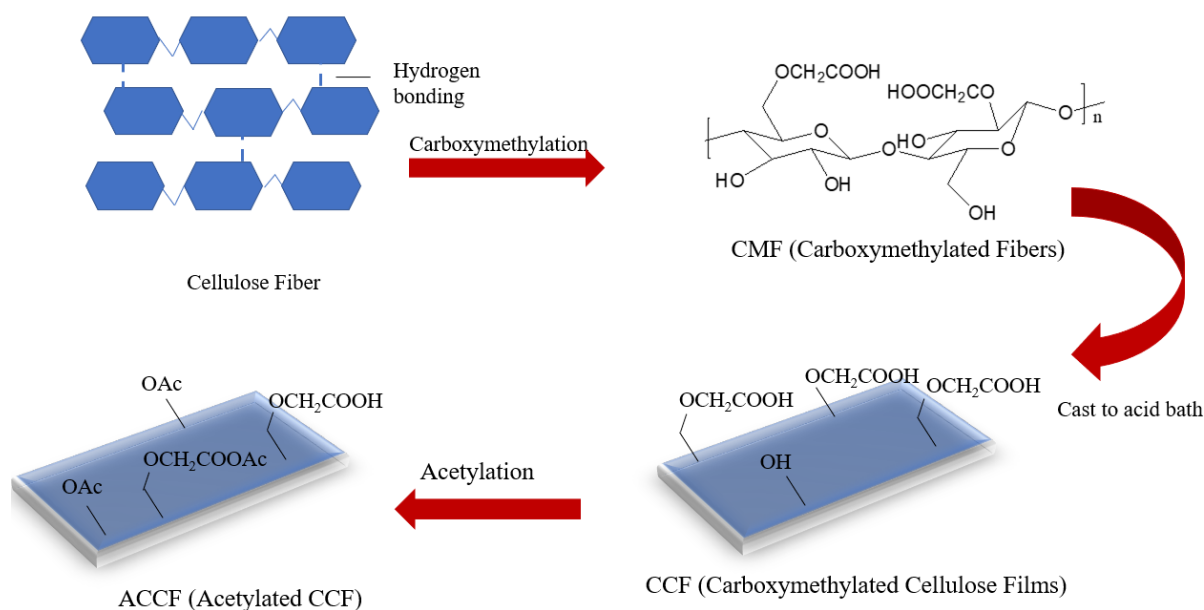
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A water-resistant cellulose-based film production for food packaging applications has been investigated. Previously, films made from mildly carboxymethylated cellulose fibers have been fabricated inexpensively with excellent mechanical properties and high-water absorption (WA) and water vapor permeation (WVP). This research is performed to limit WA and WVP of the carboxymethylated cellulose films (CCFs) by acetylation aimed at certain packaging utilizations. CCFs were prepared by a flow casting in an acid bath. Then films were acetylated by conventional acetylation methods done at room temperature for preparation of the water-resistant surface. The physical and chemical properties of the films were investigated. Fourier transform infrared (FTIR), X-ray diffraction (XRD) and nuclear magnetic resonance spectroscopy (NMR) demonstrated that acetylation was successful. Tests on water absorption, moisture absorption, and water contact angles have produced encouraging results. The water uptake is decreased from 60% to approximately 5% after acetylation. Although the loss of hydrogen bonding decreased the mechanical properties of acetylated CMF (carboxymethylated fibers) films slightly, it demonstrated a great wet-tensile after being submerged in water compared to the CMF films. Overall, the acetylation bestows CMF film a water-resistant surface that can be utilized in some food packaging areas.



ELECTRICALLY RESPONSIVE TRILAYER LIQUID CRYSTAL NETWORK ACTUATORS USING POLY(IONIC LIQUID)S

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LIQUID CRYSTAL NETWORK (LCN) ACTUATORS HAVE BEEN EXTENSIVELY STUDIED FOR THEIR POTENTIAL USE IN A WIDE RANGE OF APPLICATIONS SUCH AS OPTICS, SENSORS, AND SOFT ROBOTICS. IN THIS STUDY, WE PRESENT AN ELECTRICALLY RESPONSIVE TRILAYER LCN ACTUATOR USING POLY(IONIC LIQUID)S (PILS). THE ACTUATOR IS COMPOSED OF A TOP LAYER OF ALIGNED LIQUID CRYSTAL NETWORK (LCN), A MIDDLE LAYER OF PILS, AND A BOTTOM LAYER OF ALIGNED LCN AGAIN (FOR SYMMETRIC ACTUATION) OR KAPTON TAPE (FOR ASYMMETRIC ACTUATION). THE TRILAYER ACTUATOR PROVIDES BOTH ACTUATION AND SENSING FUNCTIONALITIES, WHERE THE LCN LAYER GENERATES THE ACTUATION FORCE, AND THE PIL LAYER SENSES THE DISPLACEMENT OF THE ACTUATOR AND THE CHANGE IN TEMPERATURE VIA THE CHANGE IN ELECTRICAL RESISTANCE. SYMMETRIC ACTUATORS ARE CAPABLE OF ELONGATION AND CONTRACTION DEFORMATION, WHILE ASYMMETRIC ACTUATORS UNDERGO BENDING DEFORMATION UNDER STIMULI. IN ADDITION, TRILAYER ACTUATORS CAN BE PROGRAMMED TO EXHIBIT OTHER DEFORMATION MODES, SUCH AS TWISTING AND WAVE PATTERNING. ALL THE AFOREMENTIONED DEFORMATIONS CAN BE MONITORED THROUGH CHANGES IN ELECTRICAL RESISTANCE. THE RESULTS DEMONSTRATE THAT THE ACTUATOR EXHIBITS LARGE ACTUATION STRAIN, HIGH IONIC CONDUCTIVITY, AS WELL AS ACTUATION AND SENSING STABILITY.