The 6th annual meeting on advanced materials

February 25-28th and March 1st 2022

Le 6e colloque annuel sur la recherche des matériaux fonctionnels

25-28 février et 1er mars 2022

LA **GRANDE** ENVERGURE PAR L'INFINIMENT PETIT

THINK **BIG** ON THE NANOSCALE

C'est avec une immense peine que nous annonçons le décès d'un membre chéri du comité étudiant du CQMF, Dan Petrescu. Dan a toujours été source d'une grande énergie et joie de vivre pour les gens qui l'entouraient. Il a, pendant ses années de doctorat, mené sur tous les fronts une vie de chercheur actif et ambitieux. Nous le regrettons amèrement et offrons nos plus sincères condoléances à sa famille et à ses amis. Qu'il repose en paix.

It is with great sadness that we share the death of a cherished committee member, Dan Petrescu. Dan had always been a source of positive energy and joy to the people around him. During his Ph.D., he led the life of a dynamic and ambitious researcher at every level. We will miss him dearly and would like to present our most sincere condolences to his family and his friends. May he rest in peace.

Table des matières / Table of Contents

CQMF QCAM

Platine/Platinum

PRIMA
Les matériaux pour avancer

BlueSolutions
BOLLORÉ

PHARMA IN SILICA INC

MERCI POUR VOTRE SOUTIEN! THANK YOU!

SFR
SYSTEMS FOR RESEARCH

cégep de Sherbrooke

CIC
SECTION MONTRÉAL
MONTREAL SECTION

Université de Montréal

UNIVERSITÉ DE SHERBROOKE

UNIVERSITÉ LAVAL

POLYTECHNIQUE MONTRÉAL
UNIVERSITÉ D'INGÉNIERIE

Mitacs

UNIVERSITÉ Concordia UNIVERSITY

UQÀM

UQAR

UQAC

UNIVERSITÉ DU QUÉBEC À TROIS-RIVIÈRES
UQTR

INRS
Institut national de la recherche scientifique

COLLÈGE MONTMORENCY

RAYMOR
NanoIntegris

AIM

McGill

ÉTS

CQMF
QCAM

Remerciements / Acknowledgements

Chemical Institute of Canada | ***For Our Future***
Institut de chimie du Canada | ***Pour notre avenir***

Materials Division (1st prize) Quebec City section (2nd prize)
Division Matériaux (1er prix) Section de Québec (2e prix)

Concours de vulgarization / Science Writing Competition

Cette année, les prix pour les meilleures présentations sont nommés à la mémoire de Dan Petrescu. Nous remercions la section montréalaise de l'Institut de Chimie du Canada et de SFR pour le généreux soutien financier qui rend possible cette initiative

This year's best presentation awards are named in memory of Dan Petrescu. We thank the Montreal Chapter of the Chemical Institute of Canada and SFR for the generous financial support that makes this initiative possible.

Comité Organisateur / Organizing Committee

Louis Cuccia (Concordia)
Noémie-Manuelle Dorval Courchesne (McGill)
Diego Mantovani (UL)
Dongling Ma (INRS)
Will Skene (UdeM)
Yasmine Benabed (UdeM)
Arnaud Laramée (UdeM)
Matteo Duca (QCAM)
Petr Fiurasek (QCAM)

Directeur / Director: Theo van de Ven (McGill)

Codirecteur / Co-director: Mohamed Siaj (UQAM)

Comité étudiant / Student committee:

Yasmine Benabed (présidente, Université de Montréal), Arnaud Laramée (vice-président, Université de Montréal), Nour Dissem (UQTR), Ilknur Eryilmaz (INRS), Mostafa Shagar (INRS), Chenghao Liu (McGill), Tom Liu (UQAM), Zongyi Liu (Université Laval), Victor Quezada (Concordia), Xiaomeng Wang (Université de Montréal), Tristan Perodeau (UdeM).

CQMF QCAM

Horaire

Vendredi, 25 février - Lien ZOOM			
10:00am	Mots de bienvenue		
10:15am	**Conférence plénière: Zhongwei Chen, U. de Waterloo**		
11:15am	Pause-café		
11:30am	**Présentation invitée: Yixiang Wang, Université McGill**		
12:00pm	**Présentation invitée: Yue Zhao, U. de Sherbrooke**		
12:30pm	Ajournement		
Lundi, 28 février - Lien ZOOM			
9:00	Bienvenue aux participants		
	Séance 1 - Polymères	**Séance 2 - Énergie**	**Séance 3 - Biomédical**
9:05am	Marie Mottoul	Simon Sprocq	Zongyi Liu
9:20am	Guillaume Chamelot	Elie HADDAD	Samila Leon Chaviano
9:35am	Lahbib Abenghal	Audrey-Anne St-Germain-Coderre	Abdali Zahra
9:50am	Hamid Lamoudan	Mohsen Fakourihassanabadi	Souheib Zekraoui
10:05am	Ilies Seddiki	Ouardia Touag	Erdem Cakmak
10:20am	Félix Gagnon		Taylor Hope
10:35am	**Remise des prix du concours de vulgarisation scientifique**		
10:50am	Pause-café		
11:10am	**Atelier Communication: Julia Del Re, AIM solder**		
11:45am	**Subventions et collaboration: Dimitri Ubersfeld, Mitacs**		
12:00pm	Lunch		
	Séance 4 - Nanosciences	**Séance 5 - Énergie**	**Séance 6 - Bio/Polymères**
1:00pm	Yuanfeng Wang	Jason Malenfant	Malama Chisanga
1:15pm	Ali Darvish	Xiaodan Zhu	Marilyne Bélanger-Bouliga
1:30pm	Diego Mendoza	Sébastien Néron	Nadjib Kihal
1:45pm	Jérémie Ouellette	Loveline Domingue	Mahdokht Akbari Taemeh
2:00pm	Tadeas Hanus	Vijay K. Jayswal	Guillaume Beaudoin
2:15pm	Heidi Jahandideh		Mostafa Eesaee
2:30pm	**Commandite Platine: Prima**		
2:45pm	**Commandite Platine: Pharma in Silica**		
3:00pm	Remise des prix des présentations		
3:15pm	Ajournement		
Mardi, 1 mars - lien ZOOM			
9:25am	Bienvenue aux participants		
9:30am	**Conférence plénière: Wim Noorduin, AMOLF**		
10:30am	Pause-café		
10:45am	**Présentation invitée: Georgios Kolliopoulos, Université Laval**		
11:15am	**Présentation invitée: Norma Mendoza, Raymor et Jefford Humes, NanoIntegris**		
11:45am	Mot de clôture		

QOMF QCAM

Schedule

Friday, February 25 - ZOOM LINK			
10:00am	Opening remarks		
10:15am	**Plenary talk: Zhongwei Chen, U. of Waterloo**		
11:15am	Coffee break		
11:30am	**Invited talk: Yixiang Wang, McGill University**		
12:00pm	**Invited talk: Yue Zhao, U. of Sherbrooke**		
12:30pm	Adjourn		
Monday, February 28 - ZOOM LINK			
9:00	Welcome to participants		
	Session 1 - Polymers	**Session 2 - Energy**	**Session 3 - Biomedical**
9:05am	Marie Mottoul	Simon Sprocq	Zongyi Liu
9:20am	Guillaume Chamelot	Elie HADDAD	Samila Leon Chaviano
9:35am	Lahbib Abenghal	Audrey-Anne St-Germain-Coderre	Abdali Zahra
9:50am	Hamid Lamoudan	Mohsen Fakourihassanabadi	Souheib Zekraoui
10:05am	Ilies Seddiki	Ouardia Touag	Erdem Cakmak
10:20am	Félix Gagnon		Taylor Hope
10:35am	**Award Ceremony: Science Writing Competition**		
10:50am	Coffee Break		
11:10am	**Communication Workshop: Julia Del Re, AIM solder**		
11:45am	**Grants and collaboration: Dimitri Ubersfeld, Mitacs**		
12:00pm	Lunch		
	Session 4 - Nanosciences	**Session 5 - Energy**	**Session 6 - Biomedical / Polymers**
1:00pm	Yuanfeng Wang	Jason Malenfant	Malama Chisanga
1:15pm	Ali Darvish	Xiaodan Zhu	Marilyne Bélanger-Bouliga
1:30pm	Diego Mendoza	Sébastien Néron	Nadjib Kihal
1:45pm	Jérémie Ouellette	Loveline Domingue	Mahdokht Akbari Taemeh
2:00pm	Tadeas Hanus	Vijay K. Jayswal	Guillaume Beaudoin
2:15pm	Heidi Jahandideh		Mostafa Eesaee
2:30pm	**Platinum sponsor: Prima**		
2:45pm	**Platinum sponsor: Pharma in Silica**		
3:00pm	Announcement of the best presentations		
3:15pm	Adjourn		
Tuesday, March 1 - ZOOM LINK			
9:25am	Welcome to participants		
9:30am	**Plenary talk: Wim Noorduin, AMOLF**		
10:30am	Coffee break		
10:45am	**Invited talk: Georgios Kolliopoulos, Laval University**		
11:15am	**Invited talk: Norma Mendoza, Raymor and Jefford Humes, NanoIntegris**		
11:45am	Closing remarks		

CQMF QCAM

Conférences plénières / Plenary lectures

The Future of Electric Vehicles: Batteries or Fuel cells

Zhongwei Chen

Department of Chemical Engineering and Mechanical and Mechatronics Engineering, University of Waterloo, Waterloo, Ontario

Résumé/Abstract

The increasing global consumption of fossil fuels, the consequent undesirable rapid growth of CO2 concentrations and environmental destruction are severe challenges to humankind. The electrification of the transportation sector has gained significant traction in the recent years to deal with these challenges. Two primary forms of vehicle electrification, battery and fuel cell electric vehicles (EVs) have received extensive attention and research. Comparatively speaking, battery seems to have won the first short-term race for green ascendancy, but the case for hydrogen fuel cells refuses to go away, even though its start date is receding into the distance. Some big built-in negatives such as battery production sustainability might undermine battery's long-term dominance, but renewable energy infrastructure still need more time to be sufficiently developed and able to facilitate a holistic hydrogen economy. In great anticipation, we are witnessing the pendulum swing in favor of battery or fuel cells in long-term race.

Herein, we will first present the technical comparison of batteries and fuel cells, then provide a comprehensive evaluation of emerging electric vehicle markets based on various batteries and hydrogen fuel cells, which have the greatest potential to succeed in commercial applications. Additionally, future prospects about batteries and fuel cells towards long-range, low-cost and high-utilization transportation markets will be proposed, the key points are the next-generation 3D solid-state battery with high safety and better production sustainability, high-efficiency non-precious electrocatalyst with low-cost and long-term stability, and the development of infrastructure for hydrogen transportation and distribution with larger scale and better economic feasibility. Beyond these, we will present our recent progress in advanced batteries and fuel cells by focusing on the aspects of low-cost and high-efficiency electrocatalysts for fuel cells, electrode innovation for batteries, electrolyte design towards high energy density and high safety solid-state batteries.

Bio

Dr. Zhongwei Chen is Canada Research Chair (CRC-Tier 1) Professor in Advanced Materials for Clean Energy at the University of Waterloo, Fellow of the Royal Society of Canada, Fellow of the Canadian Academy of Engineering, Director of Waterloo Center for Electrochemical Energy (WCEE), Associate Editor of ACS Applied Materials & Interfaces (ACS-AMI), and Vice President of International Academy of Electrochemical Energy Science (IAOEES). His research interests are in the development of advanced energy materials and electrodes for fuel cells, metal-air batteries, and lithium-ion batteries. He has published 3 books, 11 book chapters and more than 400 peer reviewed journal articles with over 38,000 citations with a H-index of 101. He is also listed as inventor over 60 US/international patents, with several licensed to companies internationally. He was the recipient of the 2016 E.W.R Steacie Memorial Fellowship, the member of the Royal Society of Canada's College of New Scholars, Artists and Scientists in 2016, the fellow of the Canadian Academy of Engineering in 2017, the Rutherford memorial medal from The Royal Society of Canada in 2017, which followed upon several other prestigious honors, including the Ontario Early Researcher Award, an NSERC Discovery Supplement Award, the Distinguished Performance and Research Award. Dr. Chen was ranked as the Global Highly Cited Researchers by Clarivate Analytics in 2018-2021. He was elected as Fellow of the Royal Society of Canada in 2019.

Self-organizing matter for functional materials

Wim Noorduin

Van 't Hoff Institute for Molecular Sciences, University of Amsterdam, Amsterdam, The Netherlands

Résumé/Abstract

Shaping, sculpting, and forging customizable compounds into arbitrary forms has the potential to revolutionize technologies for advanced functional materials. Current self-assembly strategies allow for impressive levels of control over either shape or chemical composition, but not both, as self-assembly inherently entangles shape and composition. Inspired by natural and biologically controlled mineralization processes, we here achieve independent control over shape and composition by performing chemical conversion reactions on nanocrystals which were first self-assembled in nanocomposites with programmable microscopic shapes. We show that these conversion reactions are surprisingly materials agnostic, allowing a large diversity of chemical pathways, and develop conversion pathways yielding a wide selection of shape-controlled compositions ranging from perovskites to transition metal chalcogenides. Finally, we introduce new strategies to control the self-assembly of the initial composite shapes using light, to direct the assembly process following exact user-defined patterns. Previously unimaginable customization of shape and composition is now achievable for assembling advanced functional components using bioinspired mineralization strategies.

Bio

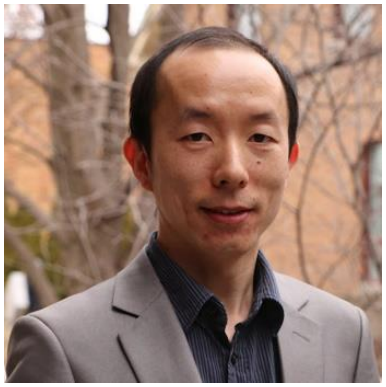
Dr. Wim Noorduin is a scientific group leader at the Dutch scientific institute AMOLF and professor at the University of Amsterdam. Noorduin's research focuses on the dynamic interplay between chemical reactions and crystallisation phenomena to control the emergence of complexity in the solid state.

In 2010, Noorduin received his PhD from Radboud University. From 2010 to 2013, he was at Harvard University as a postdoctoral researcher. From 2014 to 2015, he functioned as both a research associate at Harvard University and an assistant professor at Radboud University. From 2015 onwards, he has been leader of the Self-Organising Matter group at the NWO-Institute AMOLF in Amsterdam.

His papers have been published in a wide variety of prominent scientific journals, and he is the recipient of a various prestigious grants, including Veni, Vidi and KLEIN grants from the Netherlands Organization for Scientific Research.

Conférences invitées / Invited lectures

Functional materials derived from cellulose and plant proteins for value added applications



Yixiang Wang

Department of Food Science and Agricultural Chemistry, McGill University, Ste Anne de Bellevue, Québec

Résumé/Abstract

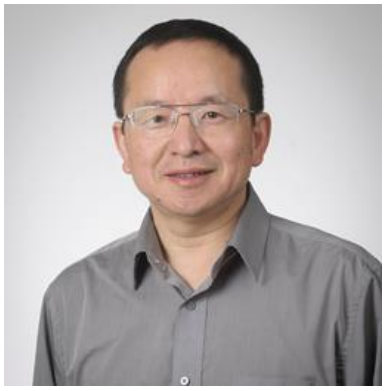
Natural polymers, such as cellulose, proteins, starch, chitin and chitosan, have been attracting increasing attention, primarily for two major reasons: environmental concerns generated from petroleum products and additional value to agricultural by-products. Nowadays, the non-degraded plastic materials have created the significant disposal and pollution issues threatening human health, development, and even survival. Recently, natural polymers have been applied as bio-renewable resources in the fabrication of biodegradable material. These natural polymers widely exist as by-products or waste, which have low value, and the disposal via landfill or incineration causes environmental problem and also represents a waste of useful resources. However, the processibility and mechanical properties of resultant materials derived from natural polymers are usually not comparable to those of synthetic polymers.

Therefore, based on the understanding of various structures, conformations and interactions of different natural polymers, a series of biodegradable functional materials with desirable properties have been developed from low-value biomass for food, medicine, and energy storage applications.

Bio

Dr. Yixiang Wang is an Assistant Professor in the Department of Food Science and Agricultural Chemistry at McGill University. Dr. Wang received his BSc in Chemistry and Doctoral degree in Polymer Chemistry and Physics from Wuhan University, China. Following a post-doctoral fellowship at University of Alberta, Dr. Wang worked there as a Research Associate from 2012 to 2017. Dr. Wang conducts research related to the fabrication of natural polymer based nano/micro particles, nano/micro fibers, composite films, and hydrogels, and the understanding of relationship between molecular structure and functional properties. The overall aim is to explore a systematic approach to develop value-added applications of natural polymers in functional food and biodegradable materials.

Deforming and Moving Polymers By Stimuli: One Step Towards Soft Robots



Yue Zhao

Département de chimie, Université de Sherbrooke, Sherbrooke, Québec

Résumé/Abstract

Crosslinked liquid crystalline and (some) semicrystalline polymers with aligned mesogens or chains can exhibit reversible shape change as they undergo a phase transition between ordered and disordered state. If the phase transition is triggered by a stimulus (heat, light, electric field) and made to go back and forth repeatedly (generally through stimulation on/off cycles), the macroscopic shape change can be translated into some sort of controlled motion to mimic robot-like locomotion or doing-work against an external load. In this talk, I will report our research in recent years on such phase transition-based shape-changing polymers and showcase examples of using stimuli to move solid polymer pieces. I will also discuss some related issues such as materials design, dynamic networks, complex shape morphing and autonomous motion under constant stimulation.

Bio

Yue Zhao received his BSc in 1982 from Chengdu University of Science and Technology (now Sichuan University), and his Ph.D. in 1987 from École Supérieure de Physique et de Chimie Industrielles de Paris (ESPCI). After postdoctoral studies at Université Laval, Canada, he joined the Chemistry Department of Université de Sherbrooke in 1991 and has been a Full Professor since 2000. Zhao's main research interests are the design, synthesis, study and exploitation for applications of self-assembled, nanostructured and stimuli-responsive polymers, liquid crystalline and hybrid materials. He has published over 230 papers in primary journals. He was awarded the Changjiang Scholar Chair Professorship at Sichuan University by the Ministry of Education of China in 2007, the Macromolecular Science and Engineering Award of the Chemical Institute of Canada (CIC) in 2013, and elected Fellow of CIC in 2014

Deep eutectic solvents as a sustainable alternative to water in advanced material processes

Georgios Kolliopoulos

Department of Mining, Metallurgical, and Materials Engineering,
Université Laval, Québec, Québec

Résumé/Abstract

Water is a rather eccentric compound: it sustains life on the planet and yet, its use in processing to-date is nothing but sustainable. Mineral and metal processing rely on aqueous chemistry, which involves vast amounts of water, and result in increasingly larger volumes of contaminated aqueous effluents that must be treated and disposed in tailings ponds. In this talk, I will present the path towards a sustainable transition towards green water-free solvometallurgical processing. Deep eutectic solvents (DESs) are eutectic mixtures of inexpensive, non-toxic, biocompatible salts. DESs can effectively replace water and aqueous solutions in processing be that in chemical or physical metallurgy. DESs have tunable properties, which enable us to tailor the liquid properties to make it selective to targeted metals or materials. Therefore, when properly selected, DESs offer an eco-friendly alternative to current state-of-the-art hydrometallurgical processes by minimizing waste generation as well as water and acid/base consumption whilst maintaining or improving the levels of selectivity in metal recovery. Finally, solvometallurgical processing promises to improve advanced material design processes by eliminating parasitic reactions during metal electrodeposition, such as H2 gas evolution, due to the absence of water from the system.

Bio

Dr. Georgios Kolliopoulos is an Assistant Professor in the Department of Mining, Metallurgical, and Materials Engineering at Université Laval since September 2019. He obtained his PhD from the Department of Chemical Engineering and Applied Chemistry, University of Toronto, in 2018, after completing his undergraduate studies in Mining and Metallurgical Engineering at the National Technical University of Athens, Greece, in 2013. His research focuses on the development of sustainable zero-waste extractive metallurgy processes that aim to minimize the use of water and acid/base reagents from process circuits and the overall environmental impact of mineral and metal processing. To-date, his research portfolio includes studies in platinum group metal recovery from spent automotive catalysts, solubility studies of rare earth sulphates in aqueous media, critical and strategic metal recovery from waste electronics, water recovery from industrial effluent streams via forward osmosis and freeze desalination, and adsorption of high impact inorganic pollutants from contaminated waters. His achievements so far have resulted in several scholarships and awards including the Metallurgy and Materials Society of CIM Doctoral Scholarship (2018), the Connaught Scholarship for International Doctoral Studies (2013-2018), and the Technical Chamber of Greece (2017) and the Limmat Foundation (2014) awards of academic excellence.

Overcoming the bottle neck of industrial production of high-purity single-walled carbon nanotubes and graphene at Raymor Industries/ NanoIntegris

Norma Mendoza

Modeling and Plasma Systems Specialist, Les Industries Raymor Inc, Boisbriand, Québec

Jefford J. Humes

Director of Research and Business Development, NanoIntegris Technologies Inc., Boisbriand, Québec

Abstract

The biggest challenge for carbon nanotubes and graphene commercialization is the production of industrial quantities with reasonable cost and high-volume supply.
Raymor Industries is a Canadian high-tech company using thermal plasma process to produce carbon nanostructures at large scale. Through their subsidiaries, NanoIntegris and Graphene LTD, Raymor also specializes in the production of enriched, single-walled carbon nanotubes and graphene dispersions. It has taken iterations between industrial

R&D, collaboration with academic researchers and industrial partners for Raymor to offer an affordable and optimized process with proven success in the integration of both carbon structures in different applications including electronics, energy and more.
In this talk, we will present the main products of Raymor-NanoIntegris, the high scale production of carbon nanotubes and graphene by using plasma and some examples of their current applications (including collaboration work with QCAM and GreEN Network and in the market of battery anodes).

Bio – Norma

Norma Mendoza is a modeling and plasma specialist at Raymor. She participates in the scale-up and optimization of plasma systems, product development such as graphene customized dispersions, materials characterisation, and technical customer service.

Before joining Raymor in 2018, she worked as a research associate at the Plasma Processing Laboratory of McGill University where she co-authored the patent: “Oxygen functionalized graphene nanoflake … nanofluid”.

Norma has 20 years of experience in plasma materials processing including CFD modeling, PVD coatings, CVD carbon nanotubes synthesis and nanomaterials characterisation. Norma received her B.A.S. in chemical engineering from University of Puebla BUAP (Mexico) and her M.Sc.A., and Ph.D. from University of Sherbrooke (Canada).

Bio – Jeff

At NanoIntegris, Mr. Humes has gained mastery in the purification and separation of single wall carbon nanotubes by electronic type along with graphene, BNNT, and MWNT production and purification. Jefford utilizes his technical mastery to seek new business opportunities for which NanoIntegris’ innovative technology can be applied. He has contributed to and been listed as a co-author within various articles from prestigious publications such as the American Chemical Society’s The Journal of Physical Chemistry Letters and Applied Physics Letters. Mr. Humes serves as a Visiting Scholar at Northwestern University within the Hersam Research Group and received his Bachelor of Science in Chemistry from Morehouse College, was a Merrill Scholar to the University of Leeds, and has performed Chemical and Medical research at numerous institutions such as the IBM Almaden Research Center, the University of Chicago, RUSH Medical College, Ohio State University, Unilever, and U.O.P.

Atelier Communication Workshop

Communiquer des sujets techniques à un auditoire non spécialisé

Communicating Technical Subjects to Non-Technical Audiences

Julia Del Re

Recherche et développement, AIM Solder, Montréal, Québec

Résumé

Communiquer est une compétence très recherchée dans un contexte professionnel. Selon un avis partagé par les recruteurs et les gestionnaires, cette compétence est un incontournable pour tout.e employé.e. L'aptitude à communiquer des idées complexes et des sujets techniques à des auditoires non spécialisés joue un rôle crucial pour toute personne qui envisage une carrière en industrie. Les employé.e.s affecté.e.s à des postes techniques auront souvent affaire à des parties prenantes sans formation technique. Dans cette situation, les employé.e.s doivent être en mesure de présenter leurs idées de manière persuasive. Communiquer de façon simple et facile à comprendre permet de renforcer la cohésion d'une organisation et de développer la collaboration entre collègues, tout en les encourageant à travailler à des objectifs communs. Cet atelier exposera les éléments saillants qu'il faut garder à l'esprit lors de la communication de sujets techniques à un auditoire non spécialisé.

Abstract

Communication is highly sought after skill in the professional world. Hiring managers and executives consistently rank it as the most important skill they look for in employees. The ability to communicate complex, technical ideas to non-technical audiences is one aspect of communication that is vital for anyone considering a career in industry. Technical employees will frequently find themselves dealing with non-technical stakeholders and they must be able to persuade them of their ideas. The ability to do this in a way that is simple and easy to understand unites the organization, fosters collaboration and inspires them to work towards a common goal. This workshop will explain the most important elements to consider when communicating technical content to general audiences.

Bio

Dr. Julia Del Re completed her PhD in the Department of Chemistry at McGill University in 2015 specializing in surface chemistry and characterization. During her degree she won numerous awards including the NSERC-CREATE ISS Student Exchange Award which provided funding for her to complete an internship at IBM Research in Almaden, California. Following her PhD she briefly worked for McGill University as a research associate before joining AIM Solder in 2017. In her work as a research scientist at AIM Solder she focuses on developing new solder pastes and understanding how their composition and processing affects their behaviour during application.

Subventions & collaboration & Grants (Mitacs)

Écosystème de subventions et collaboration de recherche avec le milieu universitaire

Dimitri Ubersfeld

Spécialiste et développement des affaires, Mitacs, Montréal, Québec

Résumé

Mitacs est un organisme national sans but lucratif qui, en partenariat avec le milieu universitaire canadien, l'industrie privée et le gouvernement, gère des programmes de recherche et de formation dans des domaines liés à l'innovation au Canada depuis 1999. Les partenaires admissibles comprennent les organismes à but lucratif et sans but lucratif (OBNL) et les sociétés d'État, pourvu que le projet de recherche proposé ait une orientation économique ou productive démontrable, comme la création d'emplois, la réduction des coûts ou l'augmentation de la productivité. En collaboration avec plus de 100 établissements universitaires, des milliers d'entreprises/ONG, hôpitaux, municipalités et les gouvernements fédéral et provinciaux, Mitacs établit des partenariats qui soutiennent l'innovation industrielle et sociale au Canada. Pour développer votre carrière grâce à de nouvelles connexions de recherche, l'expérience et la formation des compétences professionnelles, des financements sont disponibles pour toutes les disciplines.

Abstract

Mitacs is a national, not-for-profit organization that, in partnerships with Canadian academia, private industry and government, operates research and training programs in fields related to innovation in Canada since 1999. Eligible partners include for-profit organizations and not-for-profit (NFP) organizations and Crown corporations, as long as there is a demonstrable economic or productivity orientation of the proposed research project, such as creating jobs, reducing costs, or increasing productivity. Working with over 100 academic institutions, thousands of companies/ NGOs, hospitals, municipalities and both federal and provincial governments, Mitacs builds partnerships that support industrial and social innovation in Canada. To develop your career through new research connections, experience, and professional skills training, fundings are available for all disciplines.

Bio

Dimitri Ubersfeld a obtenu son PhD en Géosciences à l'Université de Lorraine, en France, en 2016. Après des premières études postdoctorales au Département de Génie Chimique de Polytechnique Montréal en 2017, il a poursuivi ses recherches postdoctorales de 2018 à 2020 au Département des génies civil, géologique et des mines de Polytechnique Montréal. Depuis fin 2020, en tant que spécialiste du développement des affaires de Mitacs à Polytechnique Montréal, Dimitri Ubersfeld est l'un des contacts officiels pour les étudiants et les professeurs de Polytechnique Montréal intéressés par les programmes de financement de Mitacs.

Commandite Platine/Platinum Sponsor

Prima Québec – Les Matériaux Pour Avancer

Sébastien Garbarino

Conseiller – Infrastructure et Innovation, Prima Québec, Montréal, Québec

Résumé

PRIMA Québec est reconnu comme l'acteur incontournable en matériaux avancés pour sa connaissance de l'écosystème et son expertise dans l'accompagnement des entreprises – pour un Québec plus compétitif à plusieurs égards grâce à la croissance soutenue de l'écosystème des matériaux avancés.

En tant que regroupement sectoriel de recherche industrielle (RSRI), PRIMA Québec compte sur le soutien financier du gouvernement du Québec et du secteur privé pour favoriser les relations recherche-industrie.

Des exemples de projets financés, les programmes disponibles pour le financement de vos projets d'innovation dans le domaine des matériaux avancés seront également présentés.

Bio

Spécialiste en recherche et développement de matériaux depuis plus de 15 ans, M. Garbarino est un expert dans le domaine de la chimie et des nanomatériaux pour les systèmes de stockage et de conversion de l'énergie.

Fort d'une maîtrise en Chimie organique, analytique et de l'environnement marin acquise en 2002 de l'Institut Universitaire Européen de la Mer (France), il décrochera, en 2007, au sein du réseau Européen « Surface Active Sites and Exhaust Fumes », un doctorat en Électrochimie de University College Cork (Irlande). Passionné par la structuration (de méso à nano) de matériaux dans le domaine de l'électrocatalyse, par les nanoparticules fonctionnalisées et par le développement de senseurs et de micro-supercondensateurs, il poursuivra sa formation post doctorale à l'Institut National de la Recherche Scientifique-Énergie Matériaux et Télécommunication (INRS-EMT). Associé de recherche à l'INRS dans le groupe de recherche du professeur Guay depuis 2011, il est co-inventeur de trois brevets et coauteur de 66 publications.

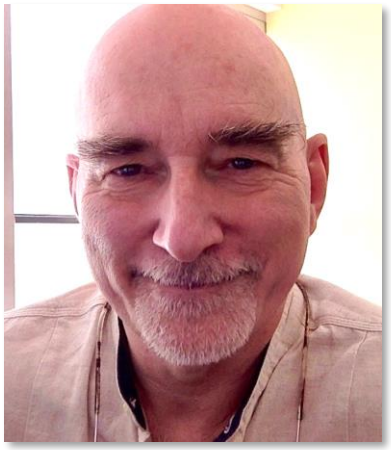
Il y a 3 ans, Sébastien Garbarino s'est joint à PRIMA Québec à titre de conseiller en infrastructures et innovation, et comme responsable de l'Infrastructure en Recherche et Développement du Québec (IRDQ) : un outil unique pour accompagner les entreprises québécoises et les chercheurs académiques dans leurs projets d'innovation dans le domaine des matériaux avancés.

Commandite Platine/Platinum Sponsor

Pharma in silica met la chimie de la nano silice au service des patients atteints de tumeurs solides

Myriam Laprise-Pelletier

Chercheure translationnelle, Pharma in silica, Québec, Québec



François Arcand

Président, Pharma in silica, Québec, Québec

Abstract

Pharma in silica élabore à Québec une nouvelle classe de traitements sécuritaires des cancers solides. Nous recrutons des scientifiques intéressés par le développement de la plateforme nanotechnologique OpKemo™, une minuscule particule de silice poreuse. L'émergence récente de technologies novatrices comme l'immunothérapie, les approches génétiques et le ciblage actif évoque que s'est produit un changement de paradigme dans la lutte contre le cancer. Or du point de vue du patient, les trente dernières années auront apporté des améliorations mitigées. On traite encore le cancer plus qu'on ne le guérit; les augmentations de durées de survie sont courtes; l'augmentation des taux de rémission est observée sur une minorité d'indications et de sous-groupes de patients. Un point crucial, de notre point de vue, est que la pratique de l'oncologie s'appuie encore largement sur des traitements qui malmènent le patient comme la chirurgie, la radiothérapie et la chimiothérapie, cela même en combinaison avec les nouveaux traitements.

La mise en œuvre de nanotechnologies est une des voies d'amélioration des traitements oncologiques. À ce jour, la majorité des nanomédecines développées en laboratoire concerne la livraison ou vectorisation de médicaments en intégrant un agent pharmacologique (ex. : un actif cytotoxique destiné au traitement d'un cancer) à l'intérieur de minuscules particules appelées nanovecteurs. Les caractéristiques de ces nanovecteurs (composition, taille, taux de chargement et chimie de surface) peuvent conduire à des pharmacocinétique et pharmacodynamique différentes de celles de l'actif pour, a) acheminer une plus grande quantité d'agent thérapeutique aux organes ou tissus à traiter et b) diminuer l'exposition des tissus sains à des substances irritantes ou délétères (solvants, médicament) pour générer un profil pharmacologique amélioré.

Pharma in silica a entrepris en juin 2019 le développement d'un nanovecteur dirigé contre le carcinome du poumon non à petites cellules (NSCLC), soit le plus mortel des cancers du poumon. Le nanovecteur OpPacliTM consiste en une nanosphère de silice dont la matrice poreuse est chargée de paclitaxel, un agent cytotoxique appartenant à la classe des taxanes. La nanomédecine OpPacliTM (OU la plateforme nanotechnologique OpKemo™) a pour ambition d'apporter deux contributions nouvelles à l'arsenal thérapeutique. D'abord améliorer la condition des patients subissant une chimiothérapie contre certains cancers solides. Ensuite augmenter l'efficacité de ces mêmes traitements. La polyvalence de la chimie de la silice est susceptible de procurer aux vecteurs thérapeutiques développés chez Pharma in silica des avantages distincts sur les nanomédicaments établis comme les liposomes et les actifs liés à des protéines.

Bio – Myriam

Dr. Myriam Laprise-Pelletier occupe le poste de chercheure translationnelle chez Pharma in Silica depuis 2020. Elle détient un B.Sc. en physique, une maîtrise et un doctorat en génie des matériaux de l'Université Laval. Elle a effectué ses études graduées dans le laboratoire du Pr. Marc-André Fortin (Université Laval), développant des nanoparticules de silice pour l'imagerie bimodale IRM/TEP et des nanoparticules d'or radioactives pour le traitement du cancer de la prostate. L'amélioration des traitements d'oncologie demeure le cœur de ses intérêts chez Pharma in silica.

Bio – François

Mr. François Arcand est le président de Pharma in silica (Québec), une société privée de stade préclinique. Il a obtenu un MBA de l'Université Concordia. Entrepreneur expérimenté en sciences de la vie, il a cofondé plusieurs compagnies (Medicago, Québec ; ERA Biotech, Barcelone ; Enemce Pharma S.L., Barcelone). Il a auparavant évolué dans le domaine des arts et de la culture.

Séances thématiques présentations étudiantes
Parallel student presentations

Séance 1 - Polymères/Session 1 - Polymers

Développement de revêtements auto-réparateurs pour les produits du bois d'intérieur

Marie Mottoul
Véronic Landry, Jean-François Morin
Université Laval
2325, rue de l'Université, Québec, G1V 0A6, Québec

Le bois est considéré comme un matériau chaleureux, intemporel, esthétique et noble pour les produits d'intérieur, mais son entretien et son usure précoce limitent son utilisation. Étant de dureté faible par rapport à d'autres matériaux utilisés pour des applications similaires, il peut être facilement endommagé lorsqu'il est soumis à des agressions mécaniques et ce, même s'il est protégé par des revêtements. Cette problématique peut notamment être résolue en améliorant les propriétés mécaniques des revêtements utilisés. Cette alternative a cependant déjà été largement étudiée et, malgré les améliorations atteintes, le bois demeure un substrat mou et des indentations peuvent toujours y être créées. Par conséquent, il est préférable de s'orienter vers les revêtements auto-réparateurs, qui permettent de traiter les égratignures et d'augmenter ainsi la durée de vie des produits du bois d'intérieur.

Parmi les stratégies d'auto-réparation disponibles, l'utilisation de ponts H se distingue grâce à leur caractère dynamique et leur faible température d'auto-réparation. Bien qu'ils soient faibles individuellement, ils sont additifs et permettent ainsi d'améliorer les propriétés mécaniques tout en apportant une auto-réparation. Dans le cadre de ce projet, des polyacrylates possédant des groupements urées dans leurs chaînes latérales ont été synthétisés et appliqués comme revêtements (Figure 1). Pour y parvenir, plusieurs monomères méthacrylates-urées ont été synthétisés à partir de différentes combinaisons d'amines et d'isocyanates, permettant ainsi de varier le nombre de donneurs et d'accepteurs de ponts H et les propriétés finales du revêtement. Dans cette présentation, la préparation des revêtements et ainsi que leurs propriétés seront exposées.

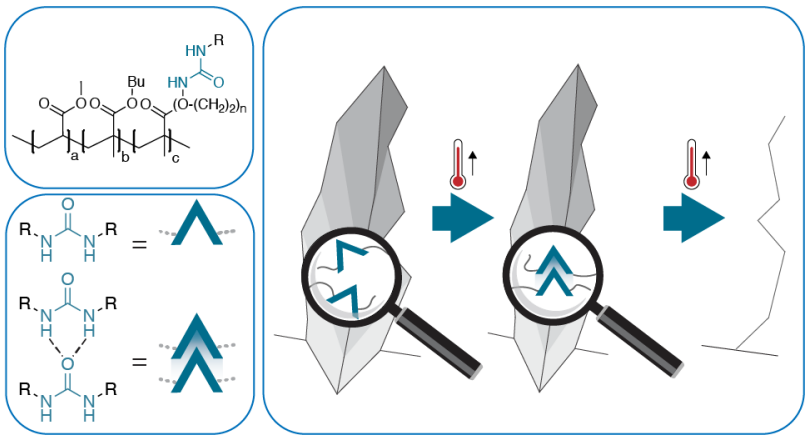


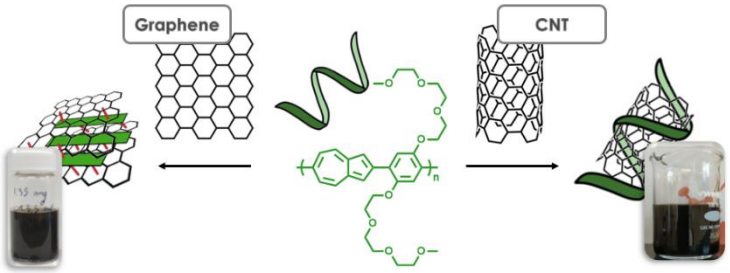
Figure 1: auto-réparation d'un polyacrylate possédant des groupements urées en chaîne latérale

Use of azulene based polymers and carbon materials for printed electronics

Guillaume Chamelot
Guillaume Chamelot, Jean-François Morin
Université Laval and Centre de Recherche sur les Matériaux Avancés (CERMA)
1045 Ave de la Médecine, Québec, G1V 0A6, QC, Canada

The rise of the Internet of Things (IoT) has led to a drastic increase in electronic devices production. Printed electronics (PE) can offer biodegradable and recyclable devices and thus is a promising technology to reduce e-waste. PE combines traditional printing techniques with conductive or semi-conductive ink to create flexible electronic devices. One of the most used materials for printed electrodes is silver nanoparticles due to their high conductivity and processability. However, silver nanoparticles have negative environmental impacts, toxicity, and high price. Thus, new materials for ink formulation are needed to make printed electronics a viable alternative to traditional fabrication methods. In this regard, carbon material inks, which consist of stable dispersions of graphene flakes or carbon nanotubes (CNT) in a solvent, offer several advantages such as good chemical stability and low environmental impact. However, the conditions used to prepare those dispersions are not ideal for printing as they often involved the use of high-boiling points, toxic solvents like NMP and DMF. When these solvents are replaced by low boiling point solvents, the use of a significant amount of non-conducting surfactants is necessary to stabilize the colloidal suspension, decreasing the conductivity values of the resulting printed film.

To overcome these issues, we propose to use π-conjugated polymers to stabilize carbon material in low boiling point solvents. More precisely, we aim to synthesize azulene-based polymers with different comonomers containing solubilizing side groups. We expect the enhancement of the π-π interactions to provide stable suspensions that exhibit, once printed, sufficient conductivity values to enable its use as electrode material in printed electronics.



Fabrication d'un revêtement antiadhérent sans silicone à base de fibres phosphorylées alkylées

Lahbib Abenghal, François Brouillette I2E3
Département de chimie, biochimie et physique
Université du Québec à Trois-Rivières
lahbib.abenghal@uqtr.ca

Les doublures antiadhésives sont des substrats à base de papier ou de film de plastique avec un ou deux côtés couchés par un matériau non collant. Ces doublures sont utilisées dans diverses applications, notamment les étiquettes, les fibres composites, les rubans adhésifs, les arts graphiques et les produits d'hygiène. La fonction principale de ce genre de papier est de protéger la couche adhésive du produit avant son utilisation. Actuellement, les silicones (ou polysiloxanes) sont universellement utilisés pour produire des revêtements antiadhésifs au niveau industriel. Le type le plus courant est le polydiméthylsiloxane linéaire (PDMS), une famille de polymères synthétiques liquides avec des chaînes principales de siloxane (-Si-O-) à haute stabilité thermique et chimique.

D'un point de vue chimique, la silicone est durcie et réticulée par la réaction d'hydrosilylation des groupes vinyle du squelette silicone avec les groupes silane ce qui permet de former de liaisons chimiques entre les molécules de PDMS. De plus, les réactions de condensation du polymère de silicone se produisent à surface des fibres de papier, qui donnent l'adhésion ou l'ancrage du film de silicone sur le substrat. Cependant, le recyclage de ces papiers n'est pas aisé en raison des liaisons covalentes entre les fibres du substrat et la silicone. Par conséquent, la plupart de ces revêtements sont brûlés et utilisés pour la production d'énergie.

Une solution adéquate pour surmonter ce problème consiste à utiliser un revêtement à base des fibres cellulosiques modifiées par les esters de phosphate en présence d'une base organique pour activer l'alkylation. À cette fin, nous avons opté d'utiliser ce genre de fibres comme des nouveaux matériaux de revêtement qui peuvent remplacer la silicone. Comme les fibres phosphorylées alkylées sont basées sur un biopolymère, elles peuvent être hydrolysées par un acide ou des enzymes. De plus, les fibres de cellulose et la chaîne alkyle peuvent être récupérées.

Les produits obtenus ont été caractérisés par les techniques suivantes: spectroscopie infrarouge à transformée de Fourier (IR-TF), microscopie électronique à balayage (MEB), analyse élémentaire par EDX et analyse par angle de contact. Les résultats préliminaires trouvés montrent bien que les dispersions de fibres phosphorylées permettent de réduire l'énergie libre de surface du papier support de 40,51 mJ/m^2 jusqu'à 26,73 mJ/m^2 condition nécessaire pour que le papier soit antiadhésif. Il a aussi révélé que le papier couché avait une faible valeur de résistance au pelage par rapport au papier siliconé ce qui rend la séparation du ruban adhésif très facile.

Mots-clés — Support antiadhésif, couchage, ancrage, papier, cellulose, fibres lignocellulosiques, ester de phosphate, phosphorylation, modification, force de pelage, adhésion résiduelle, recyclage.

AMÉLIORATION DES PROPRIÉTÉS MÉCANIQUES DES FIBRES LIGNOCELLULOSIQUES PAR LA RÉACTION DE PHOSPHORYLATION

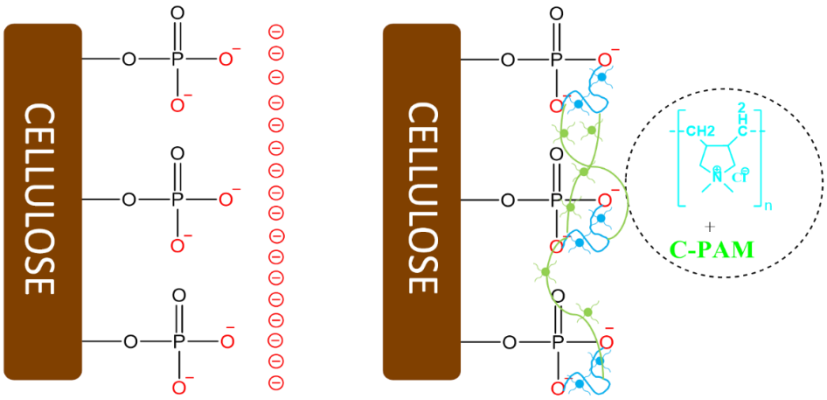
Hamid Lamoudan et François Brouillette
Institut d'innovation en écomatériaux, écoproduits et écoénergies (I2E3)
Université du Québec à Trois-Rivières

Il est bien connu que la phosphorylation des fibres lignocellulosiques permet de les rendre totalement ignifuges. Par contre, la transformation de groupements hydroxyles de la cellulose en groupements phosphates diminue le potentiel de liaison entre les fibres, ce qui réduit considérablement les propriétés mécaniques du papier.

Nous avons étudié la possibilité de former des feuilles en utilisant des agents de rétention classiques (coagulants et floculants cationiques) non pas pour améliorer la rétention de charges minérales ou de fibres de faibles dimensions, mais pour contrer la forte répulsion interfibres causée par la charge élevée des fibres phosphorylées. La pâte phosphorylée est alors comparée à une pâte kraft non modifiée avec laquelle du papier de très bonne qualité est obtenu. La forte charge anionique a été confirmée par la détermination de la charge totale par dosage conductimétrique. Les fibres phosphorylées sont 11 fois plus chargées négativement que les fibres kraft non modifiées qui sont pratiquement non chargées (2700 contre 230 méq/kg). La qualité de la formation a été évaluée par l'indice de formation Kaptra.

Les résultats démontrent que l'utilisation des agents de rétention possédant une charge positive permet d'améliorer significativement l'indice de formation de la feuille. On obtient une diminution de l'IFK de 133 à 17, une excellente valeur par rapport à celle des fibres de pâte kraft non modifiées qui ont un IFK de 35. Les mesures des propriétés physiques ont démontré que la réaction de phosphorylation, en utilisant 1 éq d'ester de phosphate/éq unité anhydroglucose, conduisait à une amélioration importante par rapport à la fibre de pâte kraft, environ 112% et 67% pour les indices d'éclatement et de rupture, jusqu'à 59% pour l'allongement et 177% pour l'absorption de l'énergie de rupture (TEA). Par contre, une diminution de 68% de l''indice de déchirure a été observée. Les feuilles composées de fibres phosphorylées et d'agents de rétention apportent donc une excellente formation et une meilleure résistance, allant même jusqu'à surpasser les feuilles composées uniquement de pâte kraft et de pâte phosphorylée sans agent de rétention.

Mots-clés : Fibre lignocellulosique, phosphorylation, indice de formation, coagulant, floculant, agent de rétention, résistance mécanique



Self-Healable Elastomers by Component Exchange

Ilies SEDDIKI and W. G. SKENE

Department of Chemistry, University of Montreal, Montreal QC, 1375 ave Thérèse-Lavoie-Roux

ilies.seddiki@umontreal.ca

Polymers have been extensively studied because of their properties that can be tailored such as mechanical, electrical, and optical. Polymers have the advantages of being both chemically and mechanically robust. While these are ideal properties for mechanically demanding applications, the polymers' properties cannot be modified post-polymerization. This is a severe limitation because the polymers cannot be restored after their mechanical failure. For example, once an elastomer is stretched beyond its breaking point, it is permanently damaged. In contrast, self-healing polymers have the capacity to autonomously restore their original properties after mechanical failure. Self-healing properties can be rationally designed into the polymer by using reversible bonds.[1] These bonds remain active post-polymerization, providing the means to perpetually restore and modify the polymer's properties. Imines are suitable reversible bonds for preparing self-healing polymers. These bonds are formed by the reversible condensation of an aldehyde and an amine.[2] The imine is also dynamic and it can undergo imine metathesis along with component exchange. The latter is the exchange of its constitutional components. Polymer component exchange can be leveraged for blending the unique properties of two discrete polymers to make polymers with hybrid properties: R_1- N=CH-R_1 + R_2-N=CH-R_2 gives R_2-N=CH-R_1 + R_1-N=CH-R_2.

We leveraged reversible imine formation to make polymers that can undergo component exchange. The benefit of these dynamic polymers is they are also self-healing. We used an amine functionalized copolymer (AA-PDMS)[1d] to prepare free-standing elastomeric films by cross-linking with various aldehydes. A fluorescent[3] and a colored[4] dyes were chosen as cross-linkers to visually track the self-healing and polymer exchanges. The polymer exchange could also be followed by FT-IR owing to the characteristic -N=CH- stretching at 1645 cm^{-1} and the amine and aldehyde vibrations ca. 1600 and 1700 cm^{-1}, respectively.[1c] The capacity of the films to heal after breaking will be demonstrated along with the cross-linking dependent stretching. It will be shown that films that can be stretched upwards of 3300 % strain contingent on the cross-linker and its density. The dynamic exchange of polymers will also be demonstrated as a means to modulate both the spectroscopic and mechanical properties.[5]

References

[1] a) H. Yan, S. Dai, Y. Chen, J. Ding, N. Yuan, *ChemistrySelect* **2019**, *4*, 10719-10725; b) P. Z. Baolin Zhang, Hanzhi Zhang, Casey Yan, Zijian Zheng, Biao Wu, You Yu, *Macromol. Rapid Commun* **2017**,*38*; c) P.-C. Zhao, W. Li, W. Huang, C.-H. Li, *Molecules* **2020**, *25*, 597; d) L. Y. Peng Wang, Bing Dai, Zhenhuai Yang, Shuai Guo, Gang Gao, Liangge Xu, Mingqi Sun, Kaili Yao, Jiaqi Zhu, *Eropean Polymer Journal* **2020**, 109382; e) Y.-B. R. Dong-Dong Zhang, Bao-Qing Zhang, Xin Qiao, Guohua Deng,Yongming Chen, Chen-Yang Liu, *Polymers* **2017**, 189-196. [2] B. T. Cho, S. K. Kang, *Tetrahedron* **2005**, *61*, 5725- 5734. [3] A. F. M. El-Mahdy, M. G. Mohamed, T. H. Mansoure, H.-H. Yu, T. Chen, S.-W. Kuo, *Chemical Communications* **2019**, *55*, 14890-14893. [4] M. Wałęsa-Chorab, W. G. Skene, *ACS Appl. Mater. Interfaces* **2017**, *9*, 21524-21531. [5] H. Wang, E. Zhao, J. W. Y. Lam, B. Z. Tang, *Materials Today* **2015**,*18*, 365-377.

LE VAT ORANGE, UNE NOUVELLE UNITE DANS L'ELECTRONIQUE ORGANIQUE

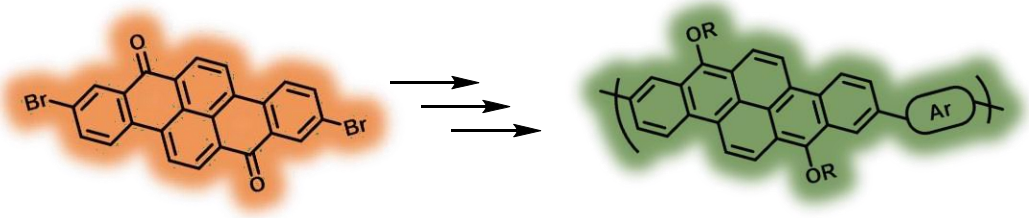
Félix Gagnon

Félix Gagnon, Vicky Tremblay, Armand Soldera, Michael Ocheje, Simon Rondeau-Gagné, Mario Leclerc et Jean-François Morin*

Département de Chimie et Centre des Recherche sur les Matériaux Avancés (CERMA)
Université Laval

LES NOUVEAUX MATÉRIAUX UTILISÉS EN ÉLECTRONIQUES DOIVENT DÉSORMAIS AVOIR UN IMPACTENVIRONNEMENTAL MOINDRE QUE L'EXPLOITATION DE TERRES RARES. AFIN DE RÉDUIRE NOTRE CONSOMMATION DE CES MATÉRIAUX INORGANIQUES ET PERMETTRE LE DÉVELOPPEMENT DE DISPOSITIFS FLEXIBLES, LÉGERS ET MOINS COÛTEUX, L'UTILISATION DE MATÉRIAUX SEMI- CONDUCTEURS ORGANIQUES EST DEVENU INÉLUCTABLE. CES MATÉRIAUX PEUVENT ÊTRE OBTENUS APRÈS UNE SÉRIE DE RÉACTIONS SUR DES DÉCHETS DE L'INDUSTRIE PÉTROCHIMIQUE OU DES PIGMENTS TEXTILES. CETTE MÉTHODE FOURNIT UNE NOUVELLE VOIE DE VALORISATION DE CES COMPOSÉS. DE PLUS, CES DÉRIVÉS SONT FLEXIBLES ET LÉGERS CE QUI ÉLARGIT L'ÉVENTAIL DE POSSIBILITÉ DANS LE DÉVELOPPEMENT DE DISPOSITIFS PORTABLES.

DANS LE CADRE DE CE PROJET, DE NOUVEAUX MATÉRIAUX SEMI-CONDUCTEURS ORGANIQUES À FAIBLE COÛT ONT ÉTÉ DÉVELOPPÉS AU DÉPART DU PIGMENT DE CUVE *VAT ORANGE 1*. LE PIGMENT A D'ABORD ÉTÉ ALKYLÉ AVANT D'ÊTRE AJOUTÉ DANS UNE RÉACTION DE BORYLATION DE MIYAURA. LE PRODUIT, AINSI, OBTENU A PU ÊTRE UTILISÉ DANS TROIS COPOLYMÉRISATIONS DE SUZUKI-MIYAURA AVEC LE *6,6'-ISOINDIGO*, LE *3,6-DI-2-THIENYL-PYRROLO[3,4-C]PYRROLE-1,4-DIONE* (DPP) ET LE *4,7-DITHIENO-2,1,3-BENZOTHIADIAZOLE* (TBT). LES POLYMÈRES OBTENUS, AVEC UNE LARGEUR DE BANDE INTERDITE (*EG*) ENTRE 1,61 ET 1,86 EV, ONT ÉTÉ TESTÉS AU SEIN DE TRANSISTORS ORGANIQUES À EFFET DE CHAMPS (OFET) AINSI QUE DE CELLULES SOLAIRES ORGANIQUES.



Séance 2 - Énergie/Session 2 - Energy

SYNTHÈSE ET CARACTÉRISATION DE COMPOSÉS GRAPHÈNE SOUFRE POUR LE DÉVELOPPEMENT D'UNE CATHODE DE BATTERIE LITHIUM-GRAPHÈNE SOUFRE DURABLE

Simon SPROCQ

Elie Haddad, Leonard Schué, Alain Rochefort, Richard Martel

Polytechnique Montréal – Université de Montréal

2900, boul. Édouard-Montpetit Campus de l'Université de Montréal 2500, chemin de Polytechnique Montréal (Québec) H3T 1J4

Un nouveau composé, basé sur la réaction entre le graphène et le soufre en phase gazeuse, a été synthétisé et caractérisé. Ce graphène fonctionnalisé par du soufre, nommé GS, est développé pour produire des encres pour l'électronique imprimable et pour l'élaboration de nouvelles cathodes durables inhibant la navette polysulfure dans les batteries Li-S. Les composés GS sont synthétisés selon un protocole simple à récipient unique, à température modérée, sans utilisation de solvant et de catalyseur. Pour optimiser ce procédé à plus grande échelle et d'améliorer le pourcentage d'atome de soufre lié de façon covalente au graphène, la réaction sur de fins flocons d'HOPG exfolié sur substrat SiO_2/Si et sur des monocouches de graphène obtenues par dépôt chimique en phase vapeur (CVD) a été étudiée. La caractérisation du GS repose sur un large éventail de techniques notamment la spectroscopie Raman, l'XPS et TEM-EELS. Les premiers résultats sur HOPG et graphène CVD sont encourageants, comme le montrent ces nouveaux pics en spectroscopie Raman, à 495, 1260, 1450, 2900 cm^{-1} représentatifs de liaisons covalentes entre le soufre et le carbone. Si tous les voyants sont au vert, l'étude se poursuivra ensuite sur le développement, l'étude de la performance et de l'inhibition de navette polysulfure d'une batterie Li-GS par voltammétrie cyclique (CV) et de cycles de charge/décharge galvanostatiques.

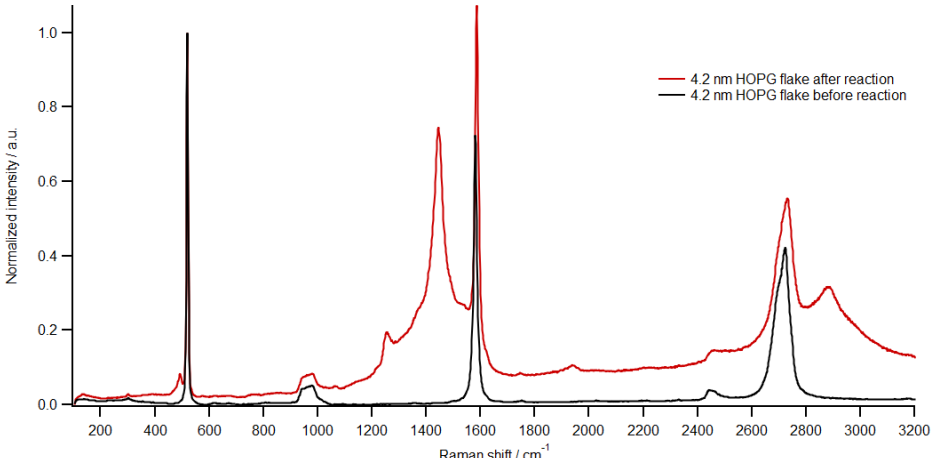


Figure: Flocons minces d'HOPG avant et après 24h de réaction

Modélisation des matériaux pour les technologies graphène soufre.

Elie HADDAD
Elie HADDAD, Alain ROCHEFORT
Polytechnique Montréal

Le graphène a fait le tour dans la communauté scientifique en raison de ses propriétés extraordinaires. Il est d'une grande importance de sonder les propriétés structurelles des matériaux synthétisés à base de graphène avant de les implémenter dans de nouvelles technologiques. Le présent projet porte sur la modélisation d'un nouveau matériau à base de graphène fonctionnalisé au soufre (GS) à l'aide d'outils numériques, avec comme objectif principal de trouver une cathode à base de soufre stable pour les piles Li-S. La caractérisation théorique des propriétés physico-chimiques du GS est essentielle pour permettre le développement de ce type de batteries. Dans ce cadre, la spectroscopie RAMAN est une méthode non-destructive de caractérisation des matériaux qui se base sur la diffusion inélastique de la lumière par la matière, elle est largement utilisée pour caractériser le graphène et ses dérivés. Un aperçu des méthodes de simulations basées sur les principes premiers pour la caractérisation RAMAN du graphène et des matériaux à base de graphène est effectuée. En particulier une emphase est mise sur l'utilisation de la théorie fonctionnelle de la densité (DFT) pour caractériser ce nouveau matériau GS. En effet, pour prédire les propriétés des matériaux à partir de principes premiers, la précision des calculs *ab initio* et la qualité des approximations utilisées pour relier les calculs aux propriétés spécifiques ont été disséquées afin de justifier correctement leur utilisation. Essentiellement, les techniques les plus appropriées pour étudier les systèmes GS ont été sélectionnées de manière *ad-hoc*. Le résultat est une description détaillée et exhaustive des spectres RAMAN des différentes itérations du matériau GS et une description détaillée des indices qui supportent le greffage du soufre au graphène.

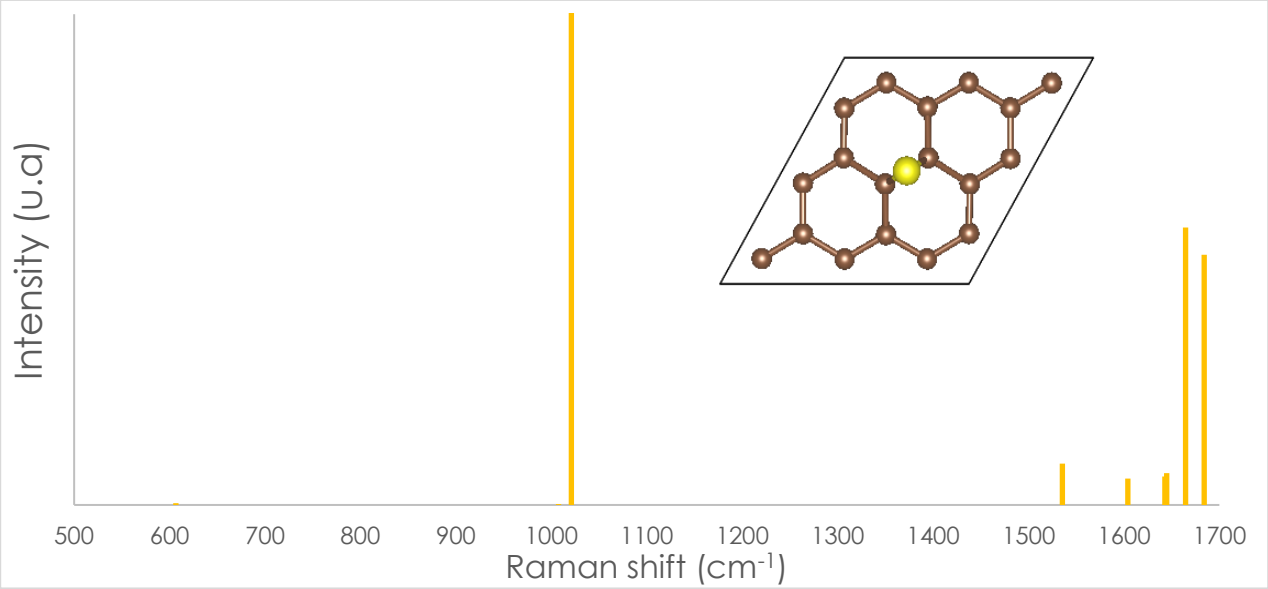


Figure 1 : Spectre Raman simulé d'une structure périodique de graphène fonctionnalisé au soufre. Le calcul a été effectué avec l'interface des codes PyNAO-SIESTA dans l'environnement de simulation atomique (ASE) en python.

MÉTALLOPORPHYRINES : SYNTHÈSE ASSISTÉE PAR MICRO-ONDES ET CARACTÉRISATION

AUDREY-ANNE ST-GERMAIN-CODERRE

Audrey-Anne St-Germain-Coderre, Mathieu Lepage et Mihaela Cibian

Université du Québec à Trois-Rivières

3351 Bd des Forges, Trois-Rivières, QC, G8Z 4M3

Les métalloporphyrines sont notamment étudiées pour leurs propriétés photophysiques et photo(électro)catalytiques comme photosensibilisateurs et/ou catalyseurs dans différents systèmes, comme ceux pour la photosynthèse artificielle (conversion de l'énergie solaire en énergie chimique). Cette dernière présente un potentiel élevé pour répondre aux changements climatiques auxquels nous sommes actuellement confrontés.

Dans le cadre de cette présentation, un projet en cours sur la synthèse des métalloporphyrines de cobalt et de nickel, assistée par micro-ondes, est présenté. L'intérêt envers l'utilisation d'un réacteur à micro-ondes pour la synthèse répond, en outre, au défi de recourir à des techniques dites vertes préférablement aux méthodes classiques, en permettant de réduire significativement la consommation d'énergie et la quantité de solvants utilisés. L'objectif de ce projet est de synthétiser et de caractériser des métalloporphyrines afin de les utiliser au sein de systèmes photo(électro)catalytiques pour des transformations telles que la valorisation de la biomasse et la production de carburants solaires.

Les étapes de synthèse pour les composés cibles, ainsi que des résultats préliminaires (synthèse et caractérisation de porphyrines) seront présentés. Les méthodes de caractérisation utilisées sont la spectrométrie de masse (ESI-TOF-MS), la spectroscopie infrarouge (FTIR), la résonance magnétique nucléaire (RMN-^{1}H) et la spectrophotométrie UV-visible.

An innovative approach to prepare porous Ni whiskers for the oxygen evolution reaction

Mohsen Fakourihassanabadi,
Somayyeh Abbasi, Julie Gaudet and Daniel Guay,
Institut national de la recherche scientifique
Énergie, Matériaux et Télécommunications (INRS-EMT)
1650 Lionel Boulet Blvd., Varennes, QC, Canada J3X 1P7
Daniel.Guay@inrs.ca

To reduce the cost of hydrogen production through water electrolysis, non-noble metal-based catalysts have been explored for the oxygen evolution reaction (OER). In recent years, nickel-based catalysts have drawn significant attention. Ni-based catalysts exhibits decent activity for the OER in alkaline electrolyte and high stability. In order to enhance further the activity of electrocatalysts for the OER, materials with high specific surface area should be prepared. In the present study we focused on the design of Ni-based materials with 3D structure. To achieve this, we have prepared a series of directionally solidified Ni-Al alloy on the surface of Ni plates. Then, Al was removed by immersion in an alkaline solution. The resulting structure is characterized by a very large number of long whiskers that can reach more than 1 mm in length. The effect of heat-treatment temperature and time on the size and surface density of these whiskers were assessed. The best sample showed an overpotential of 240 mV at 10 $mA.cm^{-2}$, and 350 mV at 500 $mA.cm^{-2}$. Also, this sample was able to perform the OER at 500 $mA.cm^{-2}$ during more than 6 days without any sign of degradation.

One-pot synthesis of $Al_2O_3/LiAlO_2$-coated $LiNi_{0.6}Mn_{0.2}Co_{0.2}O_2$cathode material for high performance lithium-ion battery

Ouardia Touag, Gaël Coquil, Mathieu Charbonneau, Denis Mankovsky, Mickaël Dollé.Laboratory of Chemistry and Electrochemistry of Solids (LCES)

The chemistry of lithium-ion batteries (LIBs) is an active area of research, notably through the increasingdemand for high energy and power density in LIBs, especially for application in electric vehicles (EVs)and hybrid electric vehicles (HEVs).

Among the various cathode materials, $LiNi_xCo_yMn_{1-x-y}O_2$ (NMC) intercalation compounds are the best candidates for applications in high performance LIBs. However, Ni-rich NMC suffers mainly from parasitic side reactions at the interface with the electrolyte, which leads to a lower thermal and electrochemical stability. Surface modification via coating is an effective concept to counter the capacity degradation of NMC and to improve the particles' structural stability for enhancing their cycle-life [1],[2]. Different processing techniques that usually requires several steps are presented in the literature. However, to facilitate the integration of a new product in the current battery market, it is preferable to reduce the number of steps during the synthesis process. In this work, we propose a one-pot synthesis of $Al_2O_3/LiAlO_2$-coated $LiNi_{0.6}Mn_{0.2}Co_{0.2}O_2$ particles, by using a continuous stirred-tank reactor (CSTR).

Firstly, the composition and morphology of the coated and uncoated cathode materials are characterizedby SEM, TEM, EDX and XPS. Then, the structural characterization of our materials is validated by XRD analysis. Consequently, we will compare the electrochemical performance and thermal stability of coated and uncoated NMC particles.

We will demonstrate that our approach provides an easy way to apply surface treatment onto Ni-rich NMC particles and simplifies the synthesis process at large scale production.

KEYWORDS: Lithium-ion battery, Ni-rich NMC cathode, $LiAlO_2$ coating, surface protection.

1. Negi, R.S., et al., *Enhancing the Electrochemical Performance of LiNi0.70Co0.15Mn0.15O2 Cathodes Using a Practical Solution-Based Al2O3 Coating.* ACS Applied Materials & Interfaces, 2020. 12(28): p. 31392-31400.
2. Kim, H.-S., et al., *Enhanced electrochemical properties of LiNi1/3Co1/3Mn1/3O2 cathode material by coating with LiAlO2 nanoparticles.* Journal of Power Sources, 2006. 161(1): p. 623-627.

Séance 3 - Biomédical/Session 3 - Biomedical

Development of a 3D-bioprinted Cancer Cell Architecture withApplication on the Chick Chorioallantoic Membrane

Zongyi LIU[1, 2]

John Oh [3], René C.-Gaudreault [4], Stephane Gobeil [4], Marc-André Fortin [1, 2]

[1] Laboratoire de Biomatériaux pour l'Imagerie Médicale (BIM), Axe Médecine Régénératrice, Centre de Recherche du Centre Hospitalier Universitaire de Québec -Université Laval, Québec, QC, Canada;

[2] Département de Génie des Mines, de la Métallurgie et des Matériaux, Université Laval, Québec, QC, Canada;

[3] Department of Chemistry, Concordia University, Montréal, QC, Canada;

[4] Département de Médecine Moléculaire, Faculté de Médecine, Université Laval, Québec, QC, Canada.

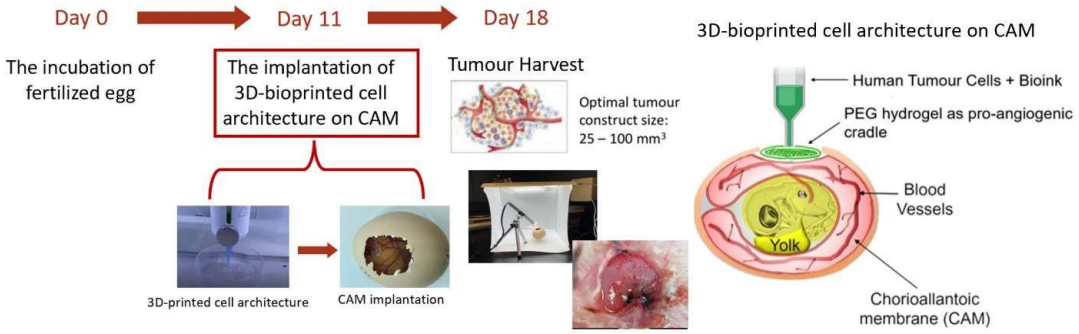
Introduction: To test the efficiency of anti-cancer drug delivery, it often involves the development of a "xenograft" tumor (e.g. with human cancer cells) on animals such as mice. However, mouse models are costly, time-consuming and require ethical approval. An attractive alternative is the chick chorioallantoic membrane (CAM) assay. CAM is a highly vascularized and nutrient-enriched extraembryonic membrane found in fertilized chick embryos. However, the main challenges in CAM assay are the short time window for tumour growth (only 8 days before hatching), and the limited selections of fast-growing cancer cell line on the CAM.

Objective: This project aimed at enhancing the size of tumors grown in the CAM assay, by using a 3D-bioprinted cell architectures. The development of this cell architecture could expand the experimental time window for tumour growth, allowing the increase of tumour size.

Methodology: A 3D-printed cancer-cells-containing hydrogel (alginate, hyaluronic acid, and collagen; previously measured for viscosity) was developed and implanted directly on the CAM. Different cancer cell lines (HT-1080, 92.1, SUM149, PC-3 and HT29) were selected for this optimized CAM assay, as well as for baseline experiments (without hydrogel). Cancer invasion and metastasis were monitored by histology/coloration assays, and the residual presence of polymers in the tumours was measured by FTIR.

Results: Tumours were harvested from CAM for all the cell lines during the 8-day time window. Optimized hydrogels were successfully printed with high reproducibility (n>20). FTIR provides a unique spectral signature of the hydrogel (O-H stretch: 3276 cm^{-1}, C=C stretch: 1528 cm^{-1} and C=O stretch: 1127 cm^{-1}).

Conclusion: Results confirmed the possibility to 3D-print hydrogel scaffolds for cancer cell encapsulation and CAM implantation. Overall, this 3D-printed cell architecture demonstrated its potential on expanding the experimental time window for tumour growth on CAM. Therefore, this new CAM assay could be used for evaluating the efficacy of anticancer drug delivery.



Contrast-enhanced hydrogels as cell scaffolds allowingMRI tracking after implantation in vivo

Samila Leon Chaviano[1,2]

Julie Fradette[3], Marc-André Fortin[1,2]

[1]*Laboratoire de Biomatériaux pour l'Imagerie Médicale, Axe Médecine Régénératrice, Centre de Recherche du Centre Hospitalier Universitaire de Québec - Université Laval, Québec, QC, Canada.* [2]*Département de Génie des Mines, de la Métallurgie et des Matériaux,Université Laval, Québec, QC, Canada. Département de Chirurgie, Centre de Recherche en Organogénèse Expérimentales (LOEX), Université Laval Québec, G1V 0A6, Canada*

Introduction: Cell-loaded hydrogels have many applications in regenerative medicine (e.g., adipose tissue implantation). These structures have low density, which makes it difficult to visualize them *invivo* with X-ray techniques. To resolve this issue in magnetic resonance imaging (MRI), a contrast agent must be incorporated into the hydrogel allowing the graft MRI tracking. Recently, ultrasmall iron oxide nanoparticles (USPION, core size <5 nm) have become an excellent "positive" contrast agent for signal enhancing in *T1*-weighted MRI.

Objective: This study aimed to develop and evaluate the magnetic properties of a COOH- functionalized USPION-PEG in alginate hydrogel for *in vivo* MRI tracking of adipose tissue grafts.

Materials&Methods: The USPION-PEG synthesis was performed through thermal decomposition method followed by phosphate-PEG(5K)-COOH ligand exchange. COOH-functionalization will allow to attach USPION to the hydrogel (leakage prevent) or other molecules (e.g., dyes). Nanoparticle- containing hydrogels were formed by mixing alginate (aqueous solutions) and USPION-PEG at certain concentrations, using CaCO3/D-(+)-gluconic acid δ-lactone (GDL) for alginate crosslinking.Nanoparticle size was measured by TEM and DLS, whereas the physicochemical properties were determined by FTIR, TGA, and XPS. Relaxivity measurements of the solutions were performed in aNMR relaxometer.

Results: USPION-PEG were successfully synthesized (DLS hydrodynamic diameter = 35.1 ± 3.9 nm; mean TEM core size 4.8 ± 0.6 nm). The presence of PEG ligands at the surface of the nanoparticle core after ligand exchange was confirmed by FTIR, TGA and XPS. Transverse (r2)/longitudinal (r1) relaxivity ratios were measured for both the USPION-PEG solution (r2/r1=3.6) and USPION-PEG in the alginate hydrogel (r2/r1=5.3), and both systems confirmed USPIONprovided positive contrast enhancement for *T1*-weighted imaging.

Conclusion: The synthesized COOH-functionalized USPION-PEG showed to be a potential positivecontrast agent for *T1*-weighted MRI. Overall, this study demonstrated preliminarily that the obtainedMRI contrast-enhanced hydrogel could help monitoring the outcomes of adipose tissue implantationsin regenerative medicine.

BACTERIAL COLLAGEN-TEMPLATED SYNTHESIS AND ASSEMBLY OF INORGANIC PARTICLES

ZAHRA ABDALI[1]

Masoud Aminzare[1], Amy Chow[1], Noémie-Manuelle Dorval Courchesne[1]

[1]Department of Chemical Engineering, McGill University, Montréal, QC, Canada

Collagen has been used as a common template for mineralization and assembly of inorganic nanoparticles, due to the special arrangement of its fibrils and the presence of charged residues. There is a group of bacterial collagen-like proteins, which is inherently secreted on the surface of *Streptococcus pyogenes* and rich in charged amino acids. Therefore, this type of collagen can be a potential substrate for the nucleation and growth of inorganic particles. Here, we show that through different interactions with these charged residues, bacterial collagen can be used to nucleate three different inorganic materials: hydroxyapatite, silver nanoparticles, and silica. After incubation in precursor solutions, all three minerals are distributed evenly along the collagen fibers with a more homogenous size, compared to the ones that were formed without a collagen template. The even distribution of the particles is an important parameter for the physicochemical and biological properties of the composites. Furthermore, the gelation of silica occurring during mineralization represents a means to produce processable collagen composites into the hydrogels and xerogel forms, which is challenging to achieve with bacterial collagen alone. Overall, we highlighted the advantage of simply conjugating bacterial collagen (biocompatibility, providing a proper mineralizing template) as the organic template, with minerals, as the inorganic component (mechanical properties and antibacterial properties), to expand their applications in the field of biomaterials and tissue engineering, such as antibacterial bone scaffold.

Development of anatomically relevant brachytherapy implants of complex shapes optimized for the treatment of uveal melanoma

Souheib Zekraoui[1,2], Théophraste Lescot [1,2], Marc-André Fortin[1,2], Solange Landreville[1,3], Luc Beaulieu[1,4] , Claudine Bellerive [5]

[1]Laboratoire de Biomatériaux pour l'Imagerie Médicale, Axe Médecine Régénératrice, CR du CHU de Québec_U.Laval; [2] Département de Génie des Mines, de la Métallurgie et des Matériaux, Faculté des Sciences et de Génie, U.Laval; [3] Département d'Ophtalmologie et d'ORL-CCF, Faculté de Médecine, U.Laval; [4] Département de Physique, de Génie Physique, et d'Optique, U.Laval; [5] Département d'Ophtalmologie, CHU de Québec_U.Laval

Introduction: Uveal melanoma (UM) is the most common type of eye cancer in adults, and episcleral plaque brachytherapy (EPB) is the gold standard to treat this cancer. However, episcleral plaques are available in limited geometries, that do not consider the specific anatomy of a patient. As a result, there is often a poor conformity between dose patterns and tumor contours, leading to side effects on the healthy tissues (e.g., damagesto the optical nerve). Episcleral plaques made by additive manufacturing (3D printing) withbiocompatible polyether ether ketone (PEEK), could improve the precision of the treatment. To enable this, PEEK filaments must be produced by extrusion, including certain additives, prior to their insertion in the 3D printer. In this context, it is of prime importance to study the potential impact of the extrusion process on the polymer quality.

Materials & Methods: Medical grade PEEK powder (Goodfellow, UK) was used in thisstudy. The extrusion was performed using a single screw extruder (FM1, 3Devo Inc.) at atemperature profile between 390 and 400°C. Purging compounds (3Devo Inc.) were usedfor cleaning as well as thermo-transition materials allowing the PEEK extrusion (400°C).The PEEK polymer was analyzed before and after extrusion using XPS, FTIR and TGA. **Results**: A high quality PEEK filament (Ø=1.75 ± 0.05 mm) was successfully extruded.The FTIR spectra show similar functional groups in the PEEK before and after extrusion.XPS spectra showed no evidence of major structure changes, except for a decrease inoxygen on the filament surface. The TGA analysis confirmed the absence of moisture and polymer contamination.

Conclusion: A PEEK filament was produced by high-temperature extrusion from a PEEKpowder, without significantly altering the chemical structure of the polymer. The next stepwill be the production of PEEK filaments containing nanostructures, for biomedical 3D printing applications.

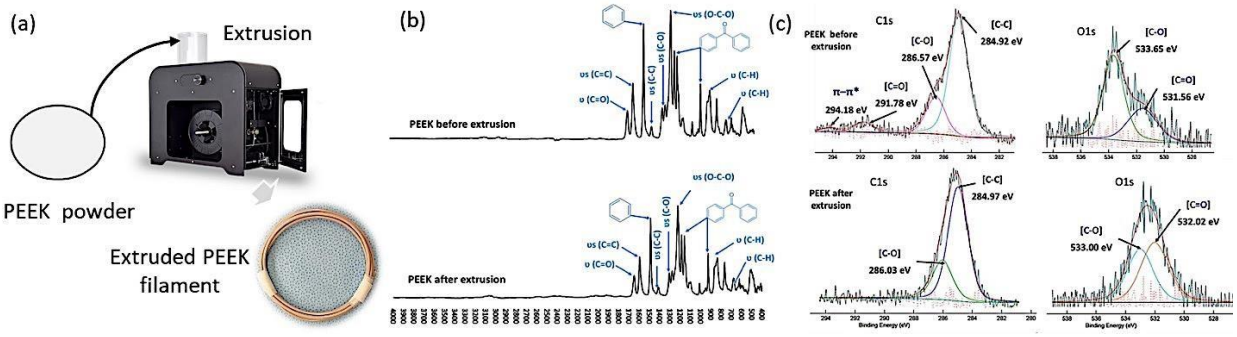


Figure 1 : a) PEEK filament extrusion process

b) FTIR spectra of the PEEK polymer before and after extrusion c) XPS High resolution spectra

ENGINEERED CELL-MIMICKING MICROBEADS TOSTUDY CAPTURE EVENTS UNDER FLOW

Erdem Cakmak Hugo Level, Corinne Hoesli
McGill University

Despite continuous scientific advancements, cardiovascular diseases continue to dominateas the biggest cause of death worldwide. Coronary artery disease is a major factor that contributes to the death toll by directly causing heart muscle tissue death and heart arrest.Stent implantation is the sole available treatment to reinstate blood flow but also causes damage to the endothelium during the operation, thus requiring subsequent interventions. Rapid stent endotheliazation can be achieved by capturing endothelial colony-forming cells (ECFCs) under flow on oriented antibody immobilized surfaces, allowing to promote tissuegrowth. A 2D computational model was developed to study the behavior of endothelial progenitor cell (EPC) adhesion on stent surfaces under flow conditions. To study cell adhesion events, highly customizable peptide-modified polystyrene beads were developed. The novel approach employed to fabricate these microparticles allows for a complex and flexible surface chemistry capable of immobilizing a wide range of antigens and antibodies, for the purpose of engineering microbeads to display cell-like properties. Microbead capture by surface-immobilized antibodies was studied by flowing RGD-TAMRAfunctionalized beads over an anti-rhodamine surface. Increased frequency of bead tethering events visualized through real-time imaging was observed on regions functionalized with anti-rhodamine antibodies. This novel experimental platform could serve as powerful and versatile tool to study and optimize surfaces for cell capture, and tomodel mechanical forces involved in flowing cell tethering.

MECHANISTIC INSIGHT INTO FLAVIN BIOPHOTOCATALYSIS FOR PROTEIN TAGGING AND PHENOL PHENOL COUPLING

Taylor Hope, Nicole Removski, Jacinthe Maisonneuve and Mathieu Frenette
Département de Chimie, Université du Québec à Montréal
Case postale 8888, succursale *Station Centre-ville. Montréal, Québec H3C 3P8*

The field of photoredox catalysis is expanding into novel territory. In collaboration with Merck's Exploratory Science Center in Cambridge Massachusetts, we are investigating a method to tag proteins using a naturally occurring photocatalyst: riboflavin. This blue light absorbing dye can oxidize phenols in the triplet excited state leading to persistent phenoxyl radicals that can couple via radical-radical dimerization. This surprisingly efficient process has been used to tag proteins in vitro and in vivo with the spatial and temporal control afforded by light-activated processes.

A growing number of researchers have been searching for a photochemical method to tag proteins, however, there is an important need to understand the processes at play before accepting this tool as a simple "click process".

We investigated the mechanism of this biophotocatalytic reaction using density-functional theory calculations, cyclic voltammetry, transient absorption, Stern-Volmer quenching, and kinetics studies. The combination of experimental and computational results suggest that the mechanism is a radical-radical recombination pathway rather than the radical addition mechanism commonly proposed for this type of reaction.[1-2]

1. Li BX, Kim DK, Bloom S, Huang RY, Qiao JX, Ewing WR, Oblinsky DG, Scholes GD, MacMillan DW. Site-selective tyrosine bioconjugation via photoredox catalysis for native-to-bioorthogonal protein transformation. Nature chemistry. 2021, 13(9), 902-908.
2. Ryu KA, Kaszuba CM, Bissonnette NB, Oslund RC, Fadeyi OO, Interrogating biological systems using visible-light-powered catalysis. Nature Reviews Chemistry. 2021, 5(5), 322-337.

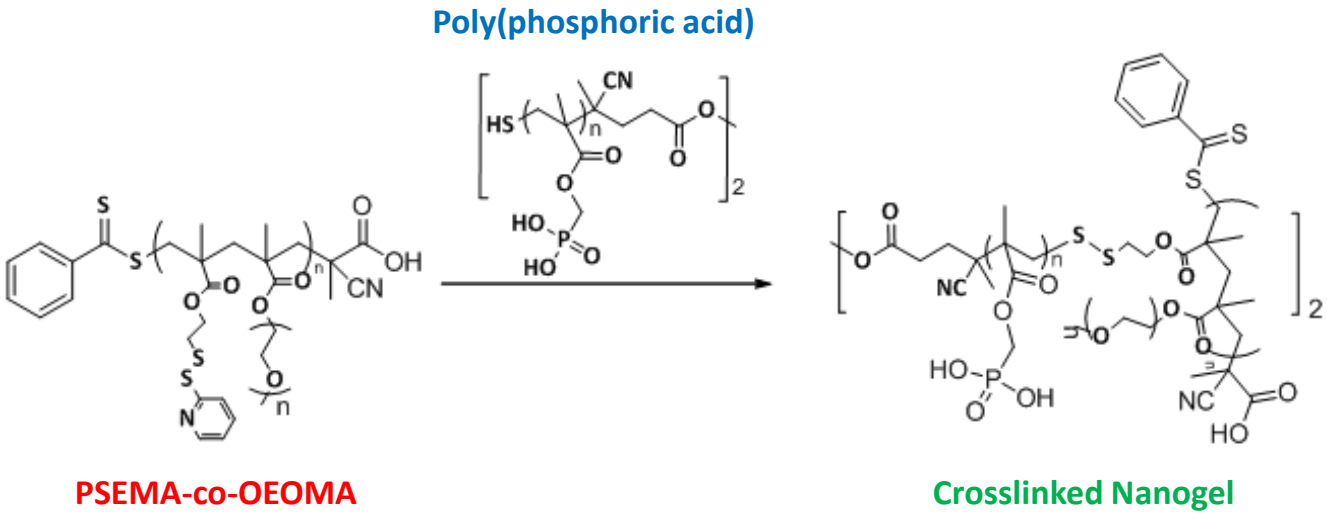
Séance 4 - Nanosciences/Session 4 - Nanosciences

Synthesis of Reductive Nanogels Crosslinked with Polyanion Mimic to Oligonucleotides

Yuanfeng Wang, Christopher J. Wilds, Jung Kwon Oh,

Department of Chemistry and Biochemistry, Concordia University, Montreal, Quebec, Canada H4B 1R6

Gene therapy with nucleic acid-based therapeutic agent has emerged as a promised strategy to treat various human diseases. However, the efficient delivery of nucleic acids has to face a critical challenge as the nucleic acids are susceptible to hydrolytic and enzymatic degradation during blood circulation and in the body. The conventional delivery strategy based on cationic polymers that enable the formation of polyplexes through ionic complexation has been explored. The polyplexes are well-designed for effective endosomal escape of nucleic acids through proton-sponge effect, and then finally transfer to nuclei leading to excellent gene transfection. However, the polyplex-based nanocarriers present critical drawbacks including the cytotoxicity by cationic polymers, the degradation of nucleic acids in polyplexs, and the propensity to aggregate with serum proteins during blood circulation. Here, a new paradigm for nucleic acid delivery explores the design of reactive, but neutral hydrophilic copolymers and the use of genes as therapeutics and crosslinkers. The poly(phosphoric acid) terminated with thiol groups is synthesized severing as mimic to oligonucleotides; consequently, the poly(phosphoric acid) is covalently conjugated with a water-soluble random copolymer (PDSEMA-co-OEOMA) bearing pendant pyridyl-disulfide functional groups through thiol-disulfide exchange reactions in aqueous solutions, resulting in the formation of crosslinked nanogel with the mimic to therapeutic nucleic acids. Consequently, the reductive cleavage of disulfide linkages from the fabricated nanogel has the potential to prompt the detachment of therapeutic nucleic acids from the nanogel cores and enable the enhanced release of nucleic acids through degradation (or destabilization) of nanogel cores in the presence of glutathione inside cells.



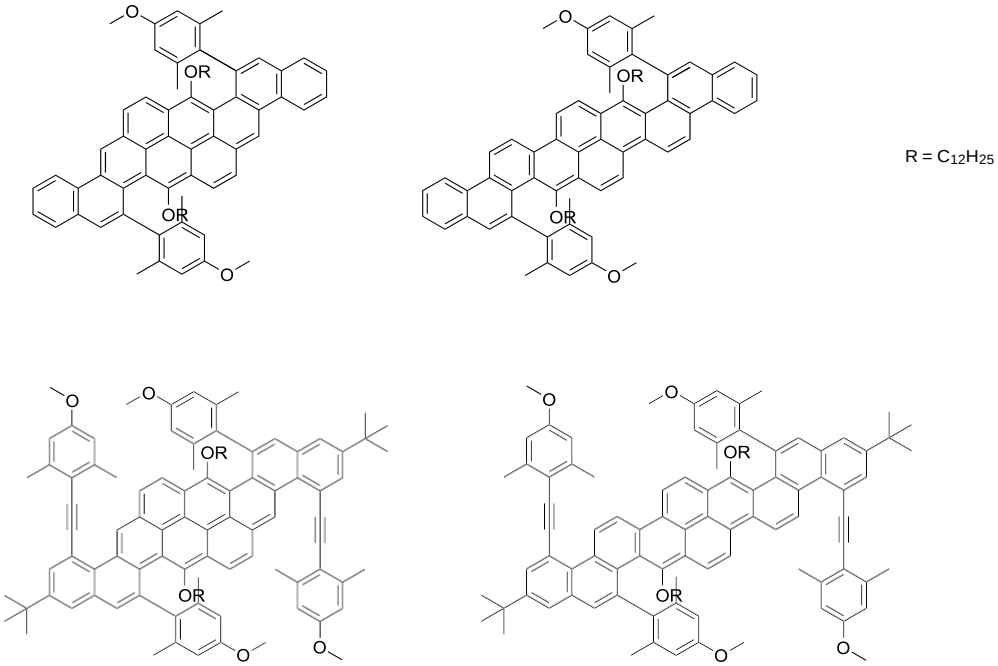
Vat orange 1&3 as precursors for preparation of organic semiconductors

Ali Darvish Supervisor: Jean-François Morin

UNIVERSITÉ LAVAL

Semiconductors are the cornerstone of modern electronics. The advantages of organic semiconductors such as low-cost production, mechanical flexibility, lightweight and low- temperature processing compared to inorganic semiconductors announce them as interestingmaterials in the different types of optoelectronic devices.

Recently, we used commercially available vat orange 1 and 3 as precursors for the preparation of stable, soluble, and low bandgap organic semiconductors. These dyes are particularly suitable as building block for organic electronics as they possess an extended pi- conjugated surface, synthetic handles allowing chemical modification and are very low-cost. Inthis presentation, we will show our strategy to increase the size of the pi-conjugated system through annulation at different positions of the polycyclic aromatic hydrocarbon (PAH) backbone. We accomplished that by using the alkyne-benzannulation reaction using either Brønsted acids or metal catalysts as the electrophile. Interestingly, low bandgap, chiral and contorted PAHs have been obtained in few synthetic steps. Characterization of the optical and electronic properties will also be presented.



CQMF QCAM

DEVELOPMENT OF MULDIMODAL IMAGING PROBES USING CARBON DOTS

DIEGO MENDOZA
Concordia University
7141 Sherbrooke O, Montreal, QC H4B 1R6, Canada

Molecular imaging techniques have a significant role to monitor human health. However, these techniques possess some limitations. In this context, the design of probes that can be suitable for multiple molecular imaging techniques has been proposed as a new approach to address the issue.Most recently, carbon dots (CDs) have attracted significance in the medical field because of their biocompatibility, an important characteristic for clinical applications. This class of nanoparticles has demonstrated to improve the efficiency of molecular imaging techniques and help diagnose diseases even at early stages.

Herein, a dual-modal carbon-based nanomaterial functionalized with a transition metal ion, Mn^{2+}, is presented. The intrinsic fluorescent properties of the carbon dots, attributed to the functional groups on their surface, make them suitable as fluorescence imaging probes while the coupling of metals using a chelating agent, diethylenetriaminepentaacetic acid, (DTPA), and a cross-linker, (1-ethyl-3-(3-dimethylaminopropyl) carbodiimide hydrochloride) (EDC), will tailor them as magnetic resonance (MR) imaging probes.

NOUVEAUX SYSTÈMES CATALYTIQUES

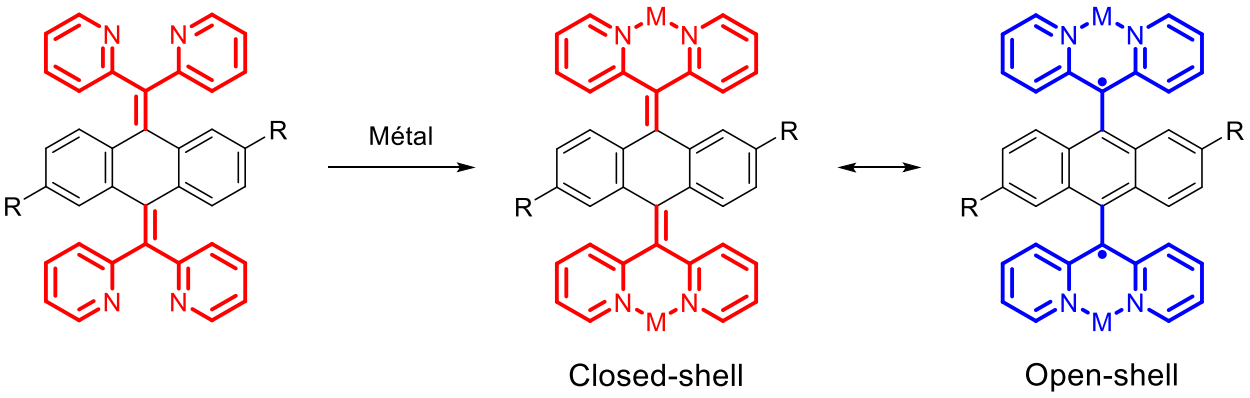
JÉRÉMIE OUELLETTE

Jérémie Ouellette, Jean-François Morin

Département de Chimie and Centre de Recherche sur les Matériaux Avancés (CERMA), Université Laval

Les réactions formant des liaisons carbone-carbone sont d'une importance capitale en chimie organique. Elles permettent de synthétiser des molécules complexes utilisées dans de nombreux domaines, tels que la chimie pharmaceutique, l'électronique organique et la chimie des matériaux. La manière la plus classique de former de tels liens est l'utilisation de réactions de couplages organométalliques impliquant des catalyseurs métalliques contenant des métaux de la famille du platine. Malgré l'importance que ces catalyseurs organométalliques occupent en synthèse organique ainsi que dans les procédés industriels, ceux-ci sont rares, dispendieux et ont une toxicité élevée, même en petites quantités. Une solution pour pallier ce problème est d'utiliser des métaux plus répandus et moins coûteux tels que le nickel, le fer ou encore le cuivre. Cependant, les réactions de couplage carbone-carbone impliquant ces espèces sont peu développées et moins efficaces. Il faut donc développer de nouveaux systèmes catalytiques afin de contourner ce problème et d'offrir une alternative crédible à ces métaux.

Une des manières envisagées serait l'utilisation de nouveaux ligands non-innocents. Ces composés participent dans le cycle catalytique comme puits d'électrons ouvrant la perspective de nouvelles réactions de couplage moins dispendieuses et moins toxiques. Dans le laboratoire du Professeur Morin, nous développons des composés diradicalaires stables à partir de systèmes π-conjugués d'anthraquinone et d'anthanthrone qui sont des molécules peu coûteuses et commercialement disponibles afin de former des ligands non-innocents applicables à des réactions de couplages carbone-carbone utilisant des métaux de transitions peu dispendieux tels que le nickel, le fer et le cuivre.



GRAPHENE ENGINEERING BY PLASMA ENABLES THE GROWTH OF SINGLE CRYSTALLINE SEMICONDUCTORS

T. Hanuš[1,2], T. M. Diallo[1,2], A. Boucherif[1,2]

[1]*Institut Interdisciplinaire d'Innovation Technologique (3IT) Université de Sherbrooke, 3000 Boulevard Université, Sherbrooke, J1K 0A5, Québec, Canada*

[2]*Laboratoire Nanotechnologies Nanosystèmes (LN2), CNRS IRL-346*

Email : tadeas.hanus@usherbrooke.ca

The graphene and its integration with semiconductor materials (Si, Ge, III-V, etc.), have attracted overwhelming scientific and technological interest in electronics, quantum devices, and optoelectronics. [1] The epitaxial growth of 3D semiconductor materials on 2D materials (Si, Ge, III-V, etc.) has sparked interest in a new generation of detachable heterostructures made possible by direct integration of 3D/2D materials. Even though the basics of Van der Waals epitaxy are already established, the growth of single-crystalline semiconductor materials (3D) on 2D graphene substrate is still very challenging. This is mostly caused by weak Van der Walls bonding as well as the low surface energy of graphene. [2] Although, remote epitaxy has successfully demonstrated the growth of single-crystalline layers of various materials on a graphene substrate, [3,4] its use is limited only to polar materials and excludes applications involving Si and Ge. Therefore, we have implemented engineering of the surface energy of graphene by plasma treatment, to address the aforementioned challenges.

In this study, we investigate the surface engineering of single-layer graphene (SLG) using plasma treatment and its influence on the nucleation of Ge on SLG. Moreover, the effects of plasma treatment duration on the quality and chemical bonding of plasma treated SLG are studied by Raman spectroscopy and X-ray photoelectron spectroscopy (XPS), respectively. The presence of induced defects is demonstrated by the increasing nuclei density during the nucleation of Ge on the treated SLG. These observations provide a clear insight regarding the role of induced defects in the nucleation process and the surface reactivity of the graphene. These findings provide a new understanding of plasma induced defects in SLG and their application in the growth of functional hybrid heterostructures.

[1] Novoselov, K., Fal′ko, V., Colombo, L. et al. Nature 490, 192–200 (2012)

[2] Alaskar, Y., et al., Adv. Funct. Mater. (2014).

[3] Kim, Y., et al., Nature 544, 340–343 (2017)

[4] Kong, W., et al., Nature Mater 17, 999–1004 (2018)

Emulsion-Templated Reduced Graphene Oxide-Cellulose Nanocrystal Hybrid Sponges for Water Treatment

Heidi Jahandideh

Heidi Jahandideh, Nathalie Tufenkji

McGill University

3610 University Rue, Montreal, Quebec

Removal of pollutants from contaminated water remains a challenge as the world's population is increasing rapidly and new pollutants are constantly introduced to the environment due to medical and technological advances. Therefore, the demand for new materials as efficient pollutant adsorbents is greater than ever. In this work, emulsion-templated graphene-based hybrid sponges have been fabricated and utilized in removing different types of contaminants. Mixtures of graphene oxide (GO) and cellulose nanocrystals (CNCs) are first used to stabilize oil-in-water emulsions. The emulsion is then mixed with vitamin C (VC), which is a green reducing agent, to form the hybrid sponge. Incorporating CNCs in the GO emulsions improves their mechanical properties while hindering the stacking of GO sheets during GO self-assembly. The porosity of rGO-CNC sponges comes from the emulsions' droplets and interlayer spacing of GO sheets due to intercalation of CNCs and is a function of GO/CNC loading as well as oil/water ratios. Polydispersed oil droplets lead to formation of a hierarchical porous material while monodispersed droplets result in fabrication of a uniformly porous sponge, each being more suitable in removing different types of contaminants. We further show that the sponges can remove a wide variety of contaminants such as dyes and emerging contaminants from water.

Séance 5 - Énergie/Session 5 - Energy

TOWARDS ROUTINE ORGANIC STRUCTURE DETERMINATION USING RAMAN MICROSCOPY

Jason Malenfant

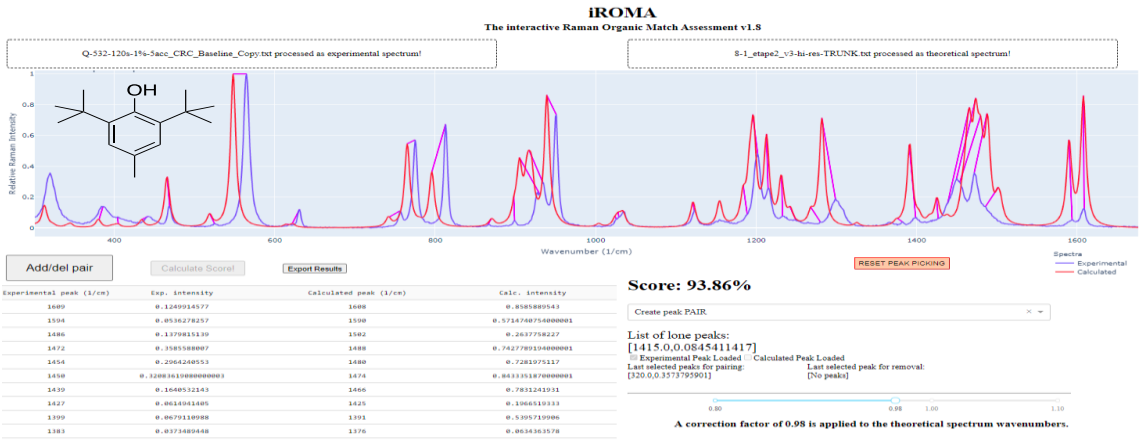
Lucille Kuster, Chloé Samard, Maxime Denis, Sylvain Canesi, Mathieu Frenette

Département de chimie, Université du Québec à Montréal

Montréal, Québec

Raman microscopy is a non-destructive characterization method that we hope to develop into a routine structure determination technique to assist organic structure determination. As little as a few micrograms are needed to obtain high resolution spectra on modern Raman microscopes. The data obtained offers a “fingerprint” of polarizable vibrational modes specific to each molecule and their particular configuration. Known molecules are routinely matched with spectra from databases, however, novel structures are more challenging. Their spectra are sometimes difficult to interpret visually, however, high-level DFT calculations can very precisely model the peak positions and confirm or deny a proposed structure.

We developed a software to quantify the match between a proposed structure and the experimental Raman spectrum obtained. The software, called iROMA (see below for a screenshot), takes as input two Raman spectra: the experimental spectrum and the one predicted by DFT. The user is then asked to assign pairs of predicted and observed peaks using a graphical user interface. Our algorithm will then calculate a match score based on three parameters: (1) match of peak positions, (2) match of peak intensities and (3) number of unassigned peaks. Overall, we find the software will assign good match percentages for small molecules with known structures and will reject matches for known negatives. We encountered problems in spectral matching for molecules with strong intermolecular forces—for these systems, DFT modeling requires the exact packing structure of the crystal which is prohibitive for high level calculations. One solution to reduce intermolecular interactions is to solubilize in tetrahydrofuran (THF) where spectra can be more accurately modeled. With good results for small molecules, we are looking to expand the application with more complex organic products.



Piezo-Elasticity and Stability Limits of Monocrystal Methane Gas Hydrates: Atomistic-Continuum Characterization

Xiaodan Zhu
Authors : Xiaodan Zhu; Alejandro Rey; Phillip Servio
McGill University
845 Rue Sherbrooke O, Montréal, QC H3A 0G4

Increasing energy demand for sustainable and lower greenhouse gas (GHG) emissions is driving the continued interest in gas hydrates. These materials have a guest-host structure, which is created by water cages and gas guest molecules. The water molecules form the host cages and the gas molecules are encapsulated as the guests, such as methane and carbon dioxide (CO2). With this unique guest-host structural feature,gas hydrates can be used for gas storage and carbon dioxide (CO2) sequestration. In addition, gas hydrates pose challenges in flow assurance in various industries as they interrupt normal flows. Some of these challenges are related to material instabilities causedby changing external conditions. Thus, we seek to determine the theoretical pressure stability limits of monocrystal defect-free sI methane gas hydrates at 0 K using accurate density functional theory (DFT) to simulate the hydrate's thermodynamic and elastic responses under varying pressures. The pressure stability limits are determined by Born stability criteria and piezo sensitivity factors. The important brittle-to-ductile transitions of gas hydrates are established. Taken together the piezo-sensitivity of a complete set of elastic properties of sI methane gas hydrates and material stability limits determined by atomistic calculations provide new data and fundamental understanding for technological applications.

DIPHENOQUINONES REDUX

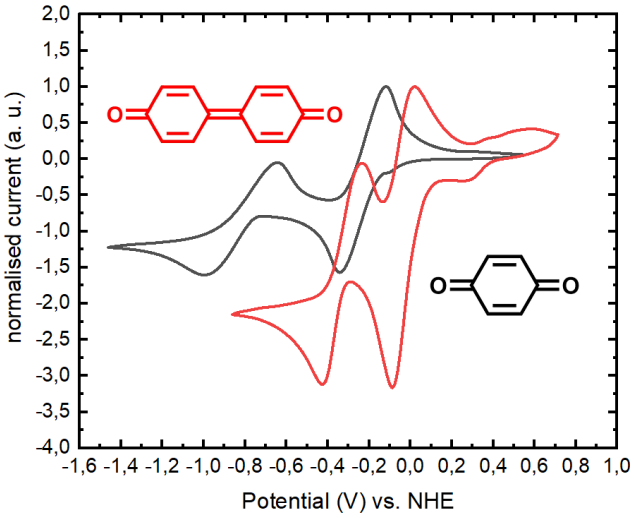
Sébastien Néron

Sébastien Néron, Mathieu Morency, Liguo Chen, Thierry Maris, Dominic Rochefort, Radu I. Iftimie, and James D. Wuest

Université de Montréal

Montréal, Québec, Canada, H2V 0B3

Benzoquinones can undergo reversible reductions and are attractive candidates for use in carbon-based batteries. Related compounds of potential utility include 4,4'-diphenoquinones, which have extended quinonoid structures with two carbonyl groups in different rings. Diphenoquinones are a poorly explored class of compounds, but we have found that even highly reactive examples such as unsubstituted parent diphenoquinone **2** can be synthesized, isolated, crystallized, and fully characterized. Experimental and computational approaches have established that typical 4,4'-diphenoquinones have nearly planar cores with weak interannular C=C bonds. Derivatives unsubstituted at the 3,3',5,5'-positions react readily by hydration, dimerization, and other processes. Association of diphenoquinones in the solid state normally produces chains or sheets held together by multiple C–H···O interactions, giving structures that differ markedly from those of the corresponding 4,4'-dihydroxybiphenyls. Electrochemical studies show that diphenoquinones are stronger oxidants than analogous benzoquinones, can be reduced reversibly in favorable cases, and can be incorporated as solids in composite electrodes for use in batteries. Together, these results help bring diphenoquinones into the mainstream of modern chemistry and provide a foundation for developing redox-active derivatives for use in green carbon-based batteries and other electrochemical devices.



DESIGNING CONDUCTING REDOX POLYMERS FOR BATTERIES APPLICATIONS

Loveline Domingue

Loveline Domingue, Ali Nazemi and Steen B. Schougaard

Université du Québec à Montréal

2101 Jeanne-Mance, Montreal, Québec H2X 2J6, Canada

Batteries are omnipresent in our modern world. They are currently used in multiple electronic devices such as phones, laptops and power tools. They are also used in transportation and for energy storage.[1] However, most batteries are metal based which causes environmental issues relating to wastes management. [2] In this presentation, organic polymer-based electrode material for battery applications will be discussed. This polymer-based electrode is inspired from metal-based electrodes and contain a redox, a conductive and an ionic segment. The composite material is formed of poly(3,4-ethylenedioxythiophene) (PEDOT) which is a highly conductive and stable compound, poly(benzoquinone) or poly (naphtoquinone) which are known for their high energy density and poly (styrenesulfonate) a strong electrolyte. These compounds are linked together on a polymeric scaffold by RAFT polymerization and electrochemically to form a polymer film with promising electrochemical properties. [3] Techniques such as XPS, XRD, EQCM, UV spectroscopy and AFM are used to characterize this new material. This provides a promising approach towards better, safer, and more ecologically-friendly batteries.

References:

[1]. Ding, Y., Cano, Z.P., Yu, A., and *al*. Electrochem. Energ. Rev. 2019, 2, 1–28.

[2]. Liang, Z., Cai, C., Hu, J., and *al*. ACS Sustain. Chem. Eng. 2021, 9(17), 5750–5767.

[3]. Chhin, D., Nazemi, A., & Schougaard, S. B., and *al.* ACS Appl. Energy Mater. 2019, 2, 7781−7790.

Synthesis of Fluorescent Carbon Nanoparticles by Dispersion Polymerization of Acetylene

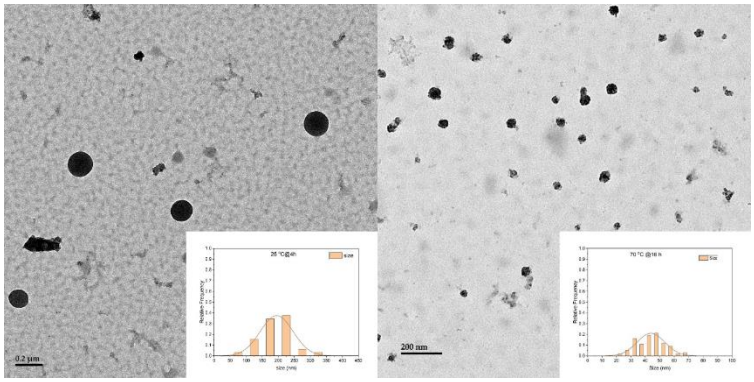
VIJAY K. JAYSWAL

Anna M. Ritcey and Jean-François Morin

Département de Chimie et Centre de Recherche des Matériaux Avancés (CERMA), Université Laval,

1045, de la Médecine, Québec City, Quebec, Canada G1V 0A6

Carbon nanoparticles (CNPs) have emerged as one of the most promising nanomaterials due to their distinct optoelectronic properties for a diverse range of applications in the area of electronics, energy conversion/ storage, and bio-imaging. The uniqueness in terms of functions and properties of the CNPs gets more interesting as it changes distinctly with a change in the shape, size, and dimensionality of these nanoparticles. The synthetic methods reported until now involves high-temperature (>100 °C) processes, which often results in uncontrolled shape, size, and polydispersity. In this work, we focus on the development of a low-temperature synthetic method for the preparation of fluorescent carbon nanoparticles allowing precise control over the shape, size, and properties by dispersion polymerization of acetylene as a precursor. The shape- and size-tunable nanoparticles were synthesized in a single step with dispersion polymerization by Glaser-Hay coupling. The shape and size of the resulting carbon nanoparticles are controlled by changing different reaction parameters such as temperature, reaction time and pressure. The control over the different reaction parameters allows us to obtain monodisperse CNPs in spherical (and tubular) shape with a size in the range of 25 nm to 250 nm. The use of low-temperature methods (RT < T < 70 °C) also allows us to overcome the limitations associated with current methods. After isolation, CNPs were characterized by microscopy techniques to analyze their shape and size. The nanoparticles were further characterized to by various techniques for chemical composition, structure, morphology, and optical properties. The residual alkynes in the CNPs' structure were exploited for further post-functionalization/graphitization to yield multifunctional CNPs, which were fluorescent in the blue region.



Séance 6 – Biomédical/Polymères
Session 6 – Biomedical/Polymers

Using microfluidics-integrated SERS assay for multiplex detection of seroconversion and cross-reactivity of antibodies in non-hospitalised adults

Malama Chisanga† and Jean-Francois Masson

Department of Chemistry, Quebec Centre for Advanced Materials (QCAM), Regroupement Québécois sur les Matériaux de Pointe (RQMP), and Centre interdisciplinaire de recherche sur le cerveau et l'apprentissage (CIRCA), Université de Montréal, CP 6128 Succ. Centre-Ville, Montreal, Québec, H3C 3J7, Canada.

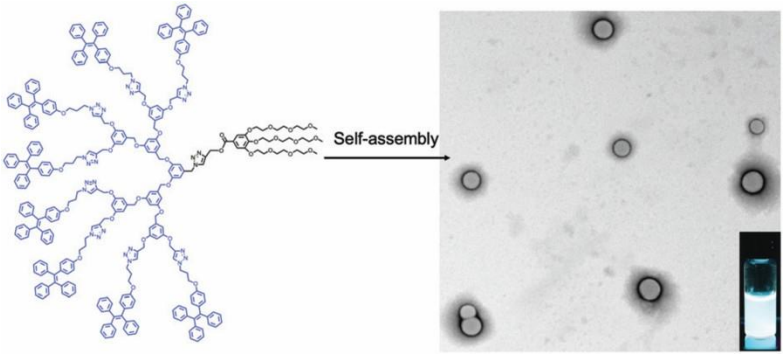
The ongoing pandemic caused by the novel coronavirus 2019 disease (COVID-19) has led to the deathof >5.7 million people out of >390 million clinically confirmed COVID-19 cases globally[1]. Although polymerase chain reaction (PCR) plays a key role in the detection of active infections with SARS-CoV-2 virus, it has become absolutely essential to understand antibody response to SARS-CoV-2 in order totrack and mitigate the efficacy of humoral immunity over time. This is especially vital currently, given that the emergence of highly transmissible SARS-CoV-2 variants of concern (VOCs) has raised serious concerns about the potency of antibodies acquired from past COVID-19 infections against re-infectionswith dominant VOCs. Development of assays that allow rapid detection of antibody response dynamicsis urgently needed to measure seroprevalence among human populations. Herein, we demonstrate the applicability of microfluidics-integrated multiplexed SERS assay for simultaneous analysis of multipleantibody-spike cross-reactivities and durability of antibodies recognising the full-length spike proteinsof the native, P.1 and B.1.617.2 SARS-CoV-2 strains in a single serum sample. We screened for bindingantibody responses in twenty-four non-hospitalised adults who returned PCR-confirmed SARS-CoV-2positive infection and fully recovered before the P.1 and B.1.617.2 VOC emerged. By using multiplexed SERS assay to measure multiple immunity profiles, we will report simultaneous seroconversion and cross-protection of anti-spike IgG, IgA and IgM antibodies with seropositivity rates of up to >97%. Thepersistence of spike-specific antibodies up to 8 weeks post-infection will be highlighted, including the correlation between antibody responses and patient age. Our findings build on current evidence which aim to inform effective and timely intervention of vaccination strategies.

1. Johns Hopkins University and Medicine ─ Coronavirus Resource Center (https://coronavirus.jhu.edu), (Accessed 4th February, 2022)

Size-Tunable Fluorescent Dendrimersomes via Aggregation-Induced Emission

Marilyne Bélanger-Bouliga
Brandon Andrade-Gagnon, Diep Thi Hong Nguyen and Ali Nazemi*
Université du Québec à Montréal (UQAM)
C.P. 8888, Succursal Centre-ville, Montréal (Qc), H3C 3P8, Canada

Dendrimers are a class of macromolecules which are recognized by their branched, 3- dimensional globular, monodisperse chemical structure.[1] Amphiphilic Janus dendrimers (AJDs) are a sub-class of dendrimer compose of a hydrophilic and hydrophobic counterpart brought together at a centerpoint in which both dendritic blocks can be independently tunedto reach the wanted generation number.[2] AJDs are known to undergo self-assembly in aqueous media forming a variety of nanostructures such as micelles, tubules, cubusomes,ribbons and vesicles depending on their hydrophilic-hydrophobic balance.[3] Dendrimer- derived vesicle-based material are of particular interest due to their resemblance to biological membranes. Fluorescent dendrimersomes have the ability to couple imaging withdrug/gene delivery for in vivo studies opening the field to a new class of theranostic materials. Although fluorescent dendrimersomes have been previously reported using common chromophores, such materials suffer from aggregation-caused quenching limitingtheir scope of application.[4] In this context, molecules such as tetraphenylethylene (TPE) with Aggregation-induced emission (AIE) property can help overcome these drawbacks. Herein, we report the synthesis of TPE-functionalized AJDs up to third generation. Their self-assembly under kinetic and thermodynamic control is studied yielding fluorescent dendrimersomes of tunable size (□ 60–200 nm) and quantum yields (5.7%-17.4%), depending on the dendrimer's generation number and the self-assembly condition.



References:

1. Walter, M. V.; Malkoch, M., *Chem. Soc. Rev.* **2012**, *41*, 4593-4609.
2. Caminade, A.-M.; Laurent, R.; Delavaux-Nicot, B.; Majoral, J.-P., *New J. Chem.* **2012**, *36*, 217-226.
3. Percec, V.; Wilson, D. A.; Leowanawat, P.; Wilson, C. J.; Hughes, A. D.; Kaucher, M. S.; Hammer, D. A.; Levine, D. H.; Kim, A. J.; Bates, F. S.; Davis, K. P.; Lodge, T. P.; Klein, M. L.;DeVane, R. H.; Aqad, E.; Rosen, B. M.; Argintaru, A. O.; Sienkowska, M. J.; Rissanen, K.; Nummelin, S.; Ropponen, J., *Science* **2010**, *328*, 1009-1014.
4. Liu, X.; Zhou, J.; Yu, T.; Chen, C.; Cheng, Q.; Sengupta, K.; Huang, Y.; Li, H.; Liu, C.; Wang, Y.; Posocco, P.; Wang, M.; Cui, Q.; Giorgio, S.; Fermeglia, M.; Qu, F.; Pricl, S.; Shi, Y.; Liang, Z.; Rocchi, P.; Rossi, J. J.; Peng, L., *Angew. Chem. Int. Ed.* **2014**, *53*, 11822-118

MANIPULATING THE SELF-ASSEMBLY OF PERYLENE DIIMIDEINTO FUNCTIONAL SUPRAMOLECULAR STRUCTURES BY HARNESSING CROSS-ß-SHEET PEPTIDES

NADJIB KIHAL

Ali Nazemi, Steve Bourgault

Université du Québec à Montréal Département de Chimie 2101, rue Jeanne-Mance Montréal, Québec, H2X 2J6

Owing to their chemical and thermal stability as well as their unique physicochemical and optoelectronic properties, perylenediimides (PDIs) are one of the most relevant organic dyes that have been largely exploited for various biomedical and nanotechnological applications.[1,2] However, the precise control of their molecular self-assembly into highly ordered supramolecularnanomaterials using various PDI-containing hybrid materials remains problematic. In this study, wetook advantage of the high aggregation propensity of the amyloidogenic domain of the islet polypeptide, the segment 20-29, to design ordered nanofilaments functionalized with PDI. PDI-$[Leu]_2$derivative was prepared from perylenetetracarboxylic dianhydride before being conjugated, via a flexible hexyl spacer, on the N-terminal amine of the elongated protected peptidyl-resin. Symmetric and asymmetric hybrid peptides were obtained, and their self-assembly was initiated by theirsubsequent dispersion in aqueous buffer with constant stirring. Self-assembly process was periodically followed by UV-vis absorbance and fluorescence emission measurements of PDI, by circular dichroism spectroscopy and by atomic force microscopy. The analyses revealed that both PDI-peptides self-assembled into long, unbranched, and linear filaments with a cross-β-sheet quaternary organization. The UV-vis absorbance spectra exhibited a clear signature of H-aggregates for both assemblies. Overall, this study exposes that defined nanostructures functionalized with PDIcan be obtained from amyloid peptide building blocks, opening the possibility to novel applications in bioimaging and photodynamic therapy.

Keywords— Self-assembly; perylenediimide; peptides; supramolecular; amyloid assemblies.

References

1. Würthner et al., Chem. Rev. 2016, 116 (3), 962–1052.

2. Chen et al., Chem. Rev. 2015, 115 (21), 11967–11998..)

PHYSICOCHEMICAL STUDY OF RADIOCHROMIC GEL BEHAVIOUR UPON EXPOSURE TO LIGHT AND OXYGEN

Mahdokht Akbari Taemeh[1,2]

Sophie Lemay[1,2], Marc-André Fortin[1,2], Solange Landreville[1,3]

[1]*Laboratoire de Biomatériaux pour l'Imagerie Médicale, Axe Médecine Régénératrice, Centre de Recherche du Centre Hospitalier Universitaire de Québec – Université Laval,Québec, QC, Canada*

[2]*Département de Génie des Mines, de la Métallurgie et des Matériaux, UniversitéLaval, Québec, QC, Canada*

[3]*Département d'Ophtalmologie et d'ORL-CCF, Faculté de Médecine, Université Laval,Québec, QC, Canada*

Introduction: Methacrylic acid (MAA)-based (MAGIC) gels are dosimetric tools measuringabsorbed dose in medical physics and oncology. They contain radiosensitive material thatpolymerizes under exposure to radiation. The polymerized material can be visualized by MRI, providing a 3D dose distribution before administration on patients, confirming the entirely coverage of the tumor. This technology is widely used in high-energy external radiotherapy, but less adapted to brachytherapy (internal radiotherapy with radioactive object), specifically low dose rate because of small doses and longtime irradiation needed. Recent developments in 3D printing of brachytherapy devices require the optimization of MAGIC gels to enhance their sensitivity. Thus, a careful optimization of components and preparation must be performed.

Objective: This study aimed at physicochemical characterization of MAGIC gel after exposure to light and oxygen, prior to studies involving radioactive materials.

Methodology: MAGIC gels were prepared with MAA, gelatin, copper sulfate, L- Ascorbicacid, hydroquinone and deionized water using a previously described procedure[1].After being jellified at 4°C, a sample was exposed to light and oxygen for 14 days to be compared with an unexposed sample. SEM (cryo-prepared), FTIR and XPS analysis wereperformed to analyze the structural and physicochemical evolution in MAGIC gels.

Results: After exposure to light and oxygen, the clear hydrogel turned brownish. From SEMimages of the exposed sample, the dispersion of small holes is attributed to the evaporationof nitric oxide, and surface roughness is an indication of MAA and gelatin degradation. FTIRanalysis showed that a certain fraction of MAA was not polymerized, whereas XPS resultsshowed a significant decrease in nitrogen contribution in carbon-nitrogen bond confirmingoxidation of nitrogen and emission of nitric oxide during the light and oxygen exposure.

Conclusion: MAGIC gels must be kept out of light and protected from oxygen (sealed andopaque vessels) during their exposure to brachytherapy objects.

UN COPOLYMÈRE HYDROPHILE RENDU THERMOSENSIBLE: L'UCST DU COPOLYMÈRE D'ACRYLAMIDE ET ACIDE ACRYLIQUE

GUILLAUME BEAUDOIN

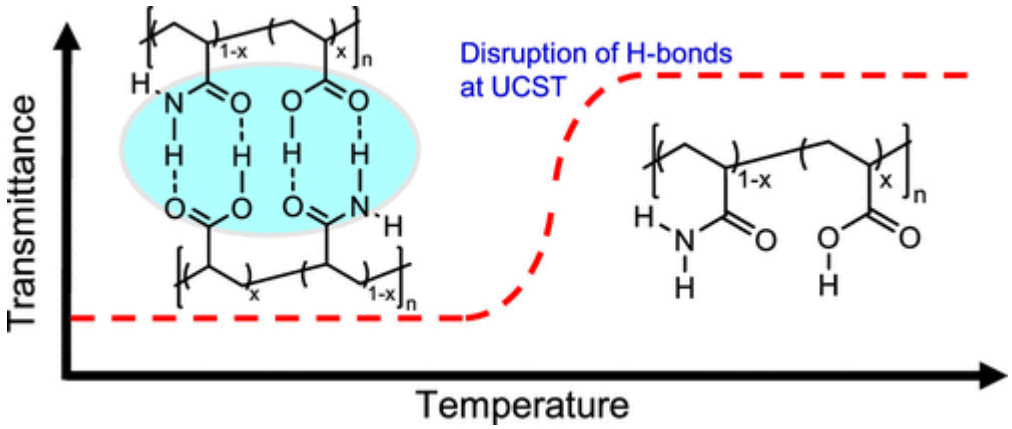
Guillaume Beaudoin, Anne Lasri, Chuanzhuang Zhao, Benoît Liberelle, Gregory De Crescenzo, and Xiao-Xia Zhu

Université de Montréal et École Polytechnique de Montréal

2900 Bd Edouard-Montpetit, Montréal, QC H3T 1J4

2500 Chem. de Polytechnique, Montréal, QC H3T 1J4

Les homopolymères d'acrylamide et d'acide acrylique sont connus pour être hydrophiles et solubles dans l'eau. Leurs copolymères sont solubles dans l'eau à pH neutre mais peuvent être transformés en polymères possédant un comportement à température critique supérieure de solution (UCST) lorsque les groupements acides carboxyliques sont protonés (pH < 3). A des températures inférieures à l'UCST, la formation de liaisons hydrogène entre les chaînes de polymère entre les groupes acides et amides rend le copolymère insoluble. Ces liaisons hydrogène sont rompues lorsque la température est chauffée au-dessus de la température critique (T_c), présentant un comportement UCST. Dans cette étude, des copolymères aléatoires hydrosolubles linéaires d'acrylamide et d'acide acrylique de différentes compositions et masses molaires ont été synthétisés. Les propriétés thermosensibles des copolymères ont été étudiées pour élucider les effets de leur composition, de leur masse molaire et de leur concentration en mesurant leurs températures de point de trouble (T_{cp}) dans des solutions de tampons acides pour maintenir les groupements d'acides carboxyliques à l'état protoné. Les effets du pH et des sels ajoutés ou de l'urée ont également été étudiés.



INCREASED HYDROPHILICITY AND DEGRADATION RATE OF POLYCAPROLACTONE FOR BIOMEDICAL APPLICATIONS

MOSTAFA EESAEE

Mostafa Eesaee, Phuong Nguyen-Tri

Université du Québec à Trois-Rivières (UQTR), Laboratory of Advanced Materials for Energy and Environment,

3351 Boulevard des Forges, Trois-Rivières, Quebec G8Z 4M3, Canada

Poly(ε-caprolactone) (PCL) is a biocompatible, nontoxic, and biodegradable polymer making it an ideal candidate for various pharmaceutical and biomedical applications. However, PCL degrades at a slower rate than most biopolymers that limits its biomedical applications. In this study PCL was blended with L-ascorbic acid (LAA) to achieve increased hydrophilicity and shorter degradation period as a candidate for specific biomedical applications such as bio tissue engineering scaffolds where a good level of hydrophilicity and a short degradation time is needed. It has been demonstrated through microscopic observations that PCL and LAA form immiscible blends where LAA tends to be distributed in the from of small particles. At low percentages of AA (1 and 2 wt%), while not interacting with the lamellar growth, LAA caused a minor nucleating effect on PCL, resulting in smaller average spherulitic size. On the other hand, 5% of LAA left behind micrometric crystals, and the PCL spherulites tend to grow from the surface of LAA microcrystals. The natural evaporation of solvent resulted in aggregates of LAA; however, when given time and at elevated temperatures, LAA crystals were nucleated and grown in the form of needle-like crystals at random directions. AFM observation revealed that LAA particles were present on the surface of the blend which has increased the polymer's hydrophilicity, evidenced by a drop in the water contact angle of blends compared to PCL. Short-term hydrolytic degradation has been conducted the samples and resulted in the removal of AA particles from the surface of PCL/AA blends. As a result, a porous structure of PCL remained with a higher surface area and more chance of surface degradation. The addition of a small amount of LAA into PCL is a cheap and effective way of increasing PCL's hydrophilicity and degradation rate.