



Conférence annuelle sur la recherche des
matériaux fonctionnels

Advanced Materials

Annual Conference

3 et 4 mai, 2018 / May 3 and 4, 2018

Université de Montréal

Pavillon 3200, rue Jean-Brillant

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Mohini Ramkaran (McGill University)

Horaire/Schedule

Jeudi, 3 mai / 2018 / Thursday May 3

MATIN

8h30 - 9h30	Accueil des participants avec café/thé et viennoiseries et installation des affiches	
9h30 - 9h45	Mots de bienvenue du doyen Frédéric Bouchard et directeur Michel Lafleur	B-2285
9h45 - 10h45	Jacques Lefebvre, National Research Council Canada Nanomaterials for Printed Electronics <i>Introduction: Richard Martel</i>	B-2285
10h45 - 11h15	Pause-café	
11h15 - 12h15	Steven Bloembergen, GreenMark Biomedical Inc. Targeted Biobased Nanomaterials for Minimally Invasive Healthcare Applications <i>Introduction: Theo van de Ven</i>	B-2285

MIDI

12h30 - 13h30	Diner	Cafétéria Chez Valère
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Séances thématiques

SÉANCE 1 : MATÉRIAUX POLYMÉRIQUES 'A' ET ENERGIE / POLYMER MATERIALS 'A' AND ENERGY

PRÉSIDENTS / CHAIRES

Julian Zhu (13h30 - 15h10)

Steen Schougaard (15h40 - 17h00)

13h30 - 13h50	Jaana Vapaavuori, Université de Montréal Taming Macromolecules with Light - Supramolecular Photoresponsive Materials at Three Different Length Scales	B-2305
13h50 - 14h10	Amélie Auge, Yue Zhao, Université de Sherbrooke Réticulation par l'intermédiaire d'un monomère colorant d'auto-assemblages de copolymères tribloc à base de poly(acrylamide-co-acrylonitrile) démontrant un comportement de type nanogels UCST par exposition à une source NIR	B-2305
14h10 - 14h30	Arman Moini Jazani, Jung Kwon Oh, Concordia University Synthesis of well-defined, multi stimuli responsive degradable amphiphilic block copolymer via combining ATRP and RAFT polymerization: Toward dual reduction and acidic pH labile shell-sheddable micelles	B-2305
14h30 - 14h50	Faraz Rajput, Milan Maric, Phillip Servio, McGill University Using Molecularly Tailored Amphiphilic Block Copolymers as Methane Kinetic Hydrate Inhibitors	B-2305
14h50 - 15h10	Pierre Ovlaque, Mathieu Robert, Saïd Elkoun, Université de Sherbrooke Enhancement of PLA/milkweed floss biocomposites properties using fiber surface modifications	B-2305
15h10 - 15h40	Pause-café	B-2305
15h40 - 16h00	Eric McCalla, McGill University Consequences of engaging oxygen in the redox of high energy Li-ion positive electrodes	B-2305
16h00 - 16h20	Yasmine Benabed, Mickaël Dollé, Université de Montréal Synthesis, structure and electrochemical properties of new lithium iron vanadates	B-2305
16h20 - 16h40	Malak Dayeh, Janine Mauzeroll, Steen Schougaard, McGill University, UQAM Extending Scanning Micropipette Contact Method to Investigate High Energy Cathode Materials Using Ionic Liquid	B-2305
16h40 - 17h00	Mengyang Fan, Daniel Guay, INRS-EMT Pb nano-dendrites for highly-selective CO₂ electrochemical reduction	B-2305

SÉANCE 2 : AUTO-ASSEMBLAGE ET NANOMATÉRIAUX / SELF-ASSEMBLY AND NANOMATERIALS

PRÉSIDENTS / CHAIRES

Louis Cuccia (13h30 - 15h10)

Christine DeWolf (15h40 - 17h00)

13h30 - 13h50	Rafik Naccache, Concordia University Carbon Dot Nanomaterials and their Applications	B-2325
13h50 - 14h10	Linda Reven, McGill University Liquid Crystal Nanocomposites	B-2325
14h10 - 14h30	Anna Ritcey, Université Laval Self-assembled plasmonic nanostructures	B-2325
14h30 - 14h50	Hu Zhu, C. Géraldine Bazuin, Jean-François Masson, Université de Montréal Monolayer Arrays of Nanoparticles Using Block Copolymer Brush Templates	B-2325
14h50 - 15h10	Qingzhe Zhang, Dongling Ma, Mohamed Chaker, INRS-EMT Plasmonic Photocatalysts toward Broadband Solar Harvesting for Efficient Photocatalysis	B-2325
15h10 - 15h40	Pause-café	B-2325
15h40 - 16h00	Emanuele Orgiu, INRS-EMT Polymeric 2D van der Waals Heterostructures	B-2325
16h00 - 16h20	Chaoying Fu, Emanuele Orgiu, Dmitrii Perepichka, INRS-EMT, McGill University Face-on vs edge-on: tuning the structure of tetrathiafulvalene monolayers with solvent	B-2325
16h20 - 16h40	Yuan Fang, Dmitrii Perepichka, McGill University Alkyl Chain Length Effects on Double-Deck Assembly at the Liquid/Solid Interface	B-2325
16h40 - 17h00	Ahmad Al Shboul, Jérôme Claverie, Mohamed Siaj, UQAM A selective process to extract high-quality Reduced Graphene Oxide (RGO) leaflets and large diameter of semiconducting SWNTs	B-2325

ÉVÉNEMENTS SPÉCIAUX EN PARALLÈLE

17h00 - 18h00	Assemblée générale annuelle des membres	B-2305
17h00 - 18h00	Assemblée générale du comité étudiant	B-2325

SOIRÉE

18h00 - 21h00	Session d'affiches scientifiques - cocktail dînatoire avec service et bar	B-2-15 à B-2-23
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Vendredi, 4 mai / 2018 / Friday May 4

ATELIER SPÉCIAL

8h30 - 9h30	J.F. Masson and F. Rosei Atelier spécial: Publier dans des journaux scientifiques	B-2285
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MATIN

9h15 - 9h30	Accueil des participants	
9h40 - 10h40	Luis M. Campos, Columbia University Materials Design for 3rd-Generation Solar Cells <i>Introduction: Dmitrii Perepichka</i>	B-2285
10h40 - 11h10	Pause-café	
11h10 - 11h20	David Polcari (SFR, Commendite Or) How can SFR help you do better research?	
11h20 - 12h20	Alain Vallée, Blue Solutions Canada Blue Solutions, lithium metal polymer battery and supercapacitor. From materials science and design, to energy storage solutions <i>Introduction: Antonella Badia</i>	B-2285

MIDI

12h30 - 13h30	Diner	Cafétéria Chez Valère
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Séances thématiques

SÉANCE 3 : MATÉRIAUX POLYMÉRIQUES 'B' / POLYMER MATERIALS 'B'

Président / Chaire : Will Skene (13h30 - 15h10)

13h30 - 13h50	Ali Nazemi, UQAM Nanomaterials via Block Copolymer Living Crystallization-Driven Self-Assembly in One- and Two Dimensions	B-2305
13h50 - 14h10	Amélie Robitaille, <i>Mario Leclerc</i> , Université Laval Polymères à base de naphthalène diimide et de perylène diimide préparé par Poly (hétéro)arylation directe pour des cellules solaires tout polymère efficaces	B-2305
14h10 - 14h30	Alberto Guerrero, <i>Suzanne Giasson</i> , Université de Montréal Multi-Responsive Hierarchical Coatings: Synthesis and Characterization	B-2305
14h30 - 14h50	Ricardo Zednik, ETS Electrowriting: a new tool for high-resolution additive manufacturing of smart polymer materials?	B-2305
14h50 - 15h10	Phuong Nguyen-Tri, <i>Robert Prud'homme</i> , Université de Montréal Nanoscale characterization of miscible and immiscible blends upon crystallization by AFM-IR	B-2305

SÉANCE 4 : ENVIRONNEMENT, DÉVELOPPEMENT DURABLE AT APPLICATIONS BIOMÉDICALES ENVIRONMENT, SUSTAINABLE DEVELOPMENT AND BIOMEDICAL APPLICATIONS

Présidente / Chaire : Nathalie Tufenkji (13h30 - 15h10)

13h30 - 13h50	Véronic Landry, Université Laval Developing the next generation of interior wood products	B-2325
13h50 - 14h10	<i>Ricardo Brandes, Bruno Chabot, François Brouillette</i> , UQTR Development of Electrospun Chitosan/Phosphorylated Nanocellulose Sorbent Nanocomposite for the Removal of Metal Ions from Aqueous Solutions	B-2325
14h10 - 14h30	Nariman Yousefi, <i>Nathalie Tufenkji</i> , McGill University Hierarchically porous, ultra-strong graphene oxide-based sponges for exceptional adsorption of water contaminants	B-2325

SÉANCE 4 : ENVIRONNEMENT, DÉVELOPPEMENT DURABLE AT APPLICATIONS BIOMÉDICALES
ENVIRONMENT, SUSTAINABLE DEVELOPMENT AND BIOMEDICAL APPLICATIONS

Présidente / Chaire : Nathalie Tufenkji (13h30 - 15h10)

14h30 - 14h50	Richard Lincoln, <i>Gonzalo Cosa</i> , McGill University Mitochondria Alkylation and Cellular Trafficking Mapped with a Lipophilic BODIPY-Acrolein Fluorogenic Probe	B-2325
14h50 - 15h10	Fan Yang, <i>Dongling Ma</i> , INRS-EMT An Integrated Multifunctional Nanoplatform Based on Superparamagnetism and Near-Infrared to Near-Infrared Photoluminescent Nd³⁺-doped NaYF₄ Nanoparticles for Deep-tissue Dual-mode Imaging	B-2325

APRÈS-MIDI		
15h10 - 16h10	T. Randall M. Lee, University of Houston Photonic and Magnetic Nanoparticles and Nanoscale "Teflon" Coatings <i>Introduction: Jérôme Claverie</i>	B-2285
16h15 - 16h30	Remise des prix étudiants et mot de clôture du colloque	B-2285

Présentations Orales / Lectures

Conférences plénières/Plenary lectures

Photonic and Magnetic Nanoparticles and Nanoscale "Teflon" Coatings

T. Randall M. Lee (University of Houston)

This presentation will describe an emerging class of photonic nanoparticles having systematically tunable absorptions ranging from visible to near infrared (NIR) wavelengths. These nanoparticles serve as versatile nanoscale tools, where the particles can be optically detected/modulated by irradiation with NIR light. Highlighted here will be the preparation, characterization, and applications of these hollow "nanoshell" particles, which possess a variety of dimensions, chemical compositions, and optical properties. In particular, current synthetic strategies allow the preparation of NIR-active nanoshells that possess diameters as small as 40 nm, which opens the door to new medical diagnostics and therapies, as well as unique opportunities in the energy sector, where such nanoshells offer unique benefits in plasmon-enhanced solar-to-fuel energy conversion. Separate studies targeting the development of cubic and spherical magnetic nanoparticles for biosensing will also be described; importantly, our studies have found cubic magnetic nanoparticles to offer a variety of advantages when compared to the more widely utilized spherical magnetic nanoparticles. A third topic will focus on fluorinated organic thin films, with an emphasis on understanding the minimum degree of fluorination required to give nanoscale "Teflon-like" coatings.

Materials Design for 3rd-Generation Solar Cells

Luis M. Campos (Columbia University)

The ability to generate multiple excitons from a single photon has the potential to significantly enhance the photocurrent in single-junction solar cells. This talk will provide an overview on our approach to the design, synthesis, and evaluation of materials for next-generation photovoltaics. The presentation will most likely begin with a joke, a mildly funny one to test the waters. If it all goes well, other hilarious remarks will be peppered throughout the talk. If the reference to "stable genius" is not too old by then, it could appear in one of the slides. By the end of the talk, one can only dream that a standing ovation will erupt. A rose landing on the stage will certainly be welcomed, or the slow clap... yeah, that would be cool too.

Nanomaterials for Printed Electronics

Patrick Malenfant (National Research Council Canada)

This presentation covers conductive molecular ink development as well as semiconducting SWCNT (sc-SWCNT) enrichment and transistor fabrication via solution based processes. I will highlight our recent progress in understanding sc-SWCNT enrichment using conjugated polymers, with special consideration given to the effect of doping on the mechanism and purity of the final product. Developments in sc-SWCNT-based electronics will also be described, with an emphasis on the performance of transistors utilizing random networks of sc-SWCNTs as the semiconducting channel material. Challenges and advances associated with using polymer-based dielectrics will also be discussed. Such transistor packages have enabled the realization of fully printed transistors as a result of the unique and excellent electrical and mechanical properties of sc-SWCNTs. A demonstration of a fully additive process to make TFT backplanes via R2R printing will also be described.

Blue Solutions, lithium metal polymer battery and supercapacitor. From materials science and design, to energy storage solutions

Alain Vallée (Blue Solutions Canada)

Blue Solutions is an acknowledged specialist in energy storage and aims to become a world leader in energy management and storage solutions. Blue Solutions has successfully introduced batteries and electricity storage solutions based on a unique Lithium Metal Polymer (LMP®) technology, while also exploring the potential of supercapacitors. The LMP® batteries are used in mobile applications, such as car sharing and electric vehicles, but also in stationary applications, including electricity storage for individuals, companies and local authorities. The first part of the talk will focus on the LMP batteries technology, its chemistry, actual performances and challenges to improve performances. The second part of the talk will focus on the supercapacitor technology that is under development. The dielectric material used in this new class of capacitor is based on molecules and polymers with polyaromatic core, that allows π - π stacking within the material, with high polarizability and comprising insulating subunits for leakage prevention within the capacitor.

Targeted Biobased Nanomaterials for Minimally Invasive Healthcare Applications

Steven Bloembergen (GreenMark Biomedical Inc.)

We enjoy taking lessons from Nature in designing new intelligent, safe and environmentally responsible materials. Building on past learnings in designing new polymeric materials for high volume commodity applications, such as paper and wood binder systems, this presentation will review several targeted biobased nanomaterials that are being developed for minimally invasive dental and medical applications including some of the fundamental science, development work and steps to commercial implementation.

Conférences invitées/Invited lectures

Consequences of engaging oxygen in the redox of high energy Li-ion positive electrodes

Eric McCalla (McGill University)

In the on-going massive amount of research and development invested in trying to increase the energy density of Li-ion batteries towards meeting electric vehicle targets, one very promising route is to engage oxygen reversibly in the redox process in the positive electrodes. This occurs in Li-rich layered oxides, but it usually occurs along with a number of other processes which hinder battery performance including irreversible oxygen loss, massive migration of transition metals during charging, and various reactions taking place with the electrolyte (particularly once oxygen gas is present in the cell). Here, the key results of a survey study examining model systems will be presented. Materials were selected for study such that each of these processes can be de-coupled from the others. The materials studied include $\text{Li}_4\text{FeSbO}_6$, $\text{Li}_4\text{Fe}_{0.56}\text{TeO}_6$, Li_2IrO_3 (two polymorphs). Direct observations by TEM of key transformations taking place on the atomic scale will be shown (e.g. oxygen dimers forming when oxygen is oxidized, and columns of vacancies forming upon oxygen release). Finally, principles guiding the design of materials that engage oxygen redox will be elucidated.

Taming Macromolecules with Light - Supramolecular Photoresponsive Materials at Three Different Length Scales

Jaana Vapaavuori (Université de Montréal)

When noncovalently bonded to macromolecules, photoresponsive azobenzene derivatives can be harnessed for controlling the properties of materials at length scales spanning at least three orders of magnitude. In this presentation, I will discuss our recent work seeking fundamental understanding of how the nanometer-scale photoinduced changes in azobenzene geometry can be translated into different applications involving polymers. First, starting with the length scale of 10-100 nm, I will show how the morphology of self-assembled diblock copolymers can be switched by supramolecularly attaching azobenzene molecules selectively to one of the blocks. Second, by using a novel IR method, molecular-level origins of photoinduced surface patterning, in which azobenzene motion is converted into micron-scale material motion, will be elucidated. Third, stimuli-induced (light and humidity) changes visible at macroscopic scales will be discussed, by introducing supramolecular polymer-azobenzene humidity memories and light-switchable polymer wrinkles at the scale of approximately 10-100 μm . This presentation highlights that the key to achieving high-tech applications of these materials is to first understand the delicate balance of supramolecular interactions in soft condensed materials, and then develop methods for controlling them.

Carbon Dot Nanomaterials and their Applications

Rafik Naccache (Concordia University)

In recent years, nanomaterials (defined as materials < 100 nm in a single dimension) have garnered a significant interest for the development of novel applications in the physical and life sciences. This is especially true for luminescent nanoparticles, which have been investigated for the development of sensors, imaging/diagnostic probes, display and solar cell applications. Recently, a relatively new class of luminescent nanomaterials, namely carbon dots has come to light. Carbon dots, sometimes known as carbogenic dots, are carbon, oxygen, nitrogen and hydrogen containing materials with the first two elements typically accounting for $\sim 90\%$ of their elemental composition and contributing to their low chemical toxicity profile. Moreover, they are typically water dispersible and can be prepared from an abundant number of inexpensive sources. While they are small in size (typically 1-5 nm), they can offer a high quantum yield of emission, a process that is controlled through passivation of the surface with an organic reagent. Combined with their small size and versatile optical properties, developing CDs as multifunctional probes can be achieved. We focus on tailoring the physico-chemical and optical properties of carbon dots via temperature-mediated synthesis routes and investigate the development of fluorescent probes for sensing and bimodal optical and magnetic resonance imaging applications.

Nanomaterials via Block Copolymer Living Crystallization-Driven Self-Assembly in One- and Two Dimensions

Ali Nazemi (UQAM)

The solution self-assembly of block copolymers yields nanomaterials that have attracted considerable attention with respect to a variety of applications over the past few decades. Poly(ferrocenyldimethylsilane) (PFS) is a crystallizable polymer. Block copolymers with a PFS core-forming block undergo a process termed "crystallization-driven self-assembly (CDSA)" in selective solvents to yield well-defined micellar structures.[1] The termini of these micelles remain active and the addition of further polymer solution (commonly called unimer) results in the formation of well-defined, spatially segmented block co-micelles. Using this method, multifunctional one- and two-dimensional structures as well as hierarchical materials can be prepared.[2] In this talk, recent advances in the development of functional one-dimensional micelles as well as heteroepitaxial growth in two dimensions via block copolymer CDSA will be discussed

1. Gilroy, J. B.; Gädt, T.; Whittell, G. R.; Chabanne, L.; Mitchels, J. M.; Richardson, R. M.; Winnik, M. A.; Manners, I. *Nature Chem.* 2010, 2, 566
2. Qiu, H.; Boott, C. E.; Gould, O. E. C.; Harniman, R. L.; Miles, M. J.; Webb, S. E. D.; Winnik, M. A.; Manners, I., *Science* 2016, 352, 697.

Polymeric 2D van der Waals Heterostructures

Emanuele Orgiu (INRS-EMT)

Solution processable semiconducting polymers with excellent film forming capacity and mechanical flexibility are emerging as alternatives to conventional inorganic semiconductors. However, the required optimization of the charge transport within conjugated polymers can be obtained only through a full control of the molecular assembly at the different length scales.

Here, we present a general strategy, based on Langmuir-Schäfer deposition, to control the polymer organization to form uniaxially aligned architectures at the water-air interface prior to their transfer onto a flat substrate. In particular, we demonstrate that the hole mobility of isoindigo-based conjugated polymer,[1] in our films processed in air is comparable with those previously reported for films prepared under N₂ atmosphere.

Interestingly, the charge transport in such ordered films is highly anisotropic as also confirmed by optical, structural (GIXD) and morphological (AFM) characterizations. By using Langmuir-Schaefer deposition, the layer-by-layer growth of 2D polymer structures possessing different electronic properties was made possible for the first time. On a fundamental side, this approach allows to obtain polymer layers where charge, spin, and heat transport could be confined in two dimensional films. On a more applied side, our work opens up new avenues towards ultra-thin devices with tailored optical and electronics properties.

1. S. Bonacchi, M. Gobbi, L. Ferlauto, M.-A. Stoeckel, F. Liscio, S. Milita, E. Orgiu, P. Samori, *ACS Nano*, 2017, 11, 2000-2007

Electrowriting: a new tool for high-resolution additive manufacturing of smart polymer materials?

Ricardo Zednik (ETS)

Electrospinning and additive manufacturing have recently been identified as new alternative polymer processing techniques. In electrospinning, an electric field is applied to a polymer source that can be in solution or in the molten state; the electrostatically charged polymer is stretched into fibers, with diameters in the nano- to macroscale, which are collected on a grounded target. Additive manufacturing of polymers is often plagued by poor resolution and uncontrollable material properties that are particularly detrimental to smart materials. However, electrowriting is a near-field electrospinning technique that combines exceptional control of material properties with accurate fiber placement, thereby promising a high-resolution additive manufacturing technique with particular potential for smart polymers, including piezoelectric PVDF.

Developing the next generation of interior wood products

Véronic Landry (Université Laval)

NSERC/Canlak Industrial Research Chair in interior wood-product finishes (CRIF) aims to develop densification and finishing solutions to increase the use of wood in both residential and non-residential applications. Increasing the use of wood is closely related to enhanced surface mechanical performance and, incidentally, reduced wear and maintenance challenges. Improving fire performance is another major challenge, which is expected to become increasingly important in the coming years. CRIF's mission is to improve the performance (mechanics, fire and appearance) of wood products so that they appear as obvious choices for building decision-makers. CRIF's research program will focus on the densification of wood products (DENSIFY axis), on the development of high-performance mechanical and fire-resistant finishes (PROTECT axis) and, to a lesser extent, on the modification of the appearance of wood surfaces (DECORATE axis). As part of CRIF's research program, strategies based on the use of low volatile organic compound (VOC) compounds, photochemistry, cure-on-command polymerization and stimuli-sensitive materials will be employed. This presentation will provide an overview of CRIF's research program.

Présentations orales / Contributed Lectures

1. Liquid Crystal Nanocomposites

Linda Reven, McGill University

Nanoparticles (NPs) and liquid crystals (LCs) can be combined to enhance the liquid crystal electro-optical properties as well as to create dynamic nanoparticle assemblies. In addition to creating different nanoparticle assemblies with common thermotropic liquid crystals, our group is developing stable LC nanocomposites based on hydrogen bonded supramolecular liquid crystals. We have systematically tuned the nanoparticle ligand shells to vary the density and strength of hydrogen bonding groups so as to optimize the miscibility in simple mesogenic acids. We have also explored the effect of polymer functionalized NPs on the stability of a hydrogen-bonded "blue phase" LC mixture.

2. Multi-Responsive Hierarchical Coatings: Synthesis and Characterization

Alberto Guerron, Université de Montréal (Suzanne Giasson)

Stimuli-responsive polymer coatings enable surface properties to be tuned by external stimuli (i.e., changes in environmental conditions) via changes in their physical conformation, surface chemistry or both. However, such coatings usually suffer from major shortcomings such as lack of selectivity and rapidity in responsiveness or poor environmental stability. The present work aims to overcome some of these limitations by investigating a new generation of responsive hierarchical coatings whose physical properties and surface chemistry can be tuned independently and reversibly using different external stimuli. The hierarchical coatings consist of two-dimensional functionalized-microgel arrays whose characteristic dimensions and surface properties can be independently controlled using different stimuli. Results show that it is in fact possible to obtain independent physical and chemical responses by functionalizing the surface of thermo-responsive microgels with pH-responsive polymer brushes. These systems are very promising as functional elements in nanotechnologies such as microfluidics.

3. Mitochondria Alkylation and Cellular Trafficking Mapped with Lipophilic BODIPY-Acrolein Fluorogenic Probe

Richard Lincoln, McGill University (Gonzalo Cosa)

Protein and DNA alkylation by endogenously produced electrophiles, is associated with the pathogenesis of neurodegenerative diseases, to epigenetic alterations, and to cell signaling and redox regulation.[1] In this presentation, I will show how we have exploited the sensitivity of BODIPY fluorescence intensity to the presence of an unsaturation at the meso-position[2] toward reporting on Michael addition reactions between cellular proteins and an electrophile warhead. We have prepared a fluorogenic BODIPY-acrolein probe, AcroB,[3] which undergoes a >350-fold fluorescence intensity enhancement concomitant with protein adduct formation. AcroB enables a direct quantification of single post-translational modifications occurring on cellular proteins via recording fluorescence bursts in live-cell imaging studies. In combination with super-resolution imaging,[4] protein alkylation events may be registered and individually counted, yielding a map of protein-electrophile reactions within the cell lipid milieu, occurring predominately in the mitochondria. AcroB further enables tracing alkylated proteins through the cell endo- and exocytic pathways, and may help elucidate key aspects of mitochondria electrophile adduct excretion and recycling.

1. Rudolph, T. K.; Freeman, B. A.; *Sci. Signaling* 2009, 2, re7.
2. Lincoln, R.; Greene, L. E.; Bain, C.; Flores-Rizo, J. O.; Bohle, D. S.; Cosa, G.; *J. Phys. Chem. B*, 2015, 119, 4758-4765.
3. Lincoln, R.; Greene, L. E.; Zhang, W.; Louisia, S.; Cosa, G.; *J. Am. Chem. Soc.*, 2017, 139, 16273-16281.
4. Roeffaers, M. B.; et al; *Angew. Chem. Int. Ed. Engl.*, 48, 2009, 9285-9289.

4. Using Molecularly Tailored Amphiphilic Block Copolymers as Methane Kinetic Hydrate Inhibitors

Faraz Rajput, McGill University (Milan Maric, Phillip Servio)

Under appropriate conditions, formation of gas hydrate plugs in pipelines becomes problematic due to damaging pipelines as well as the equipment in the process downstream. In these cases, the prevention of gas hydrate formation becomes crucial. To investigate the inhibition potential of kinetic hydrate inhibitors (KHI) on a methane-water gas hydrate system, amphiphilic block copolymers, acting as macrosurfactants, were synthesized to include both hydrophobic and hydrophilic properties using RAFT polymerization with a switchable RAFT agent.

A PVA-PS block copolymer inhibited hydrate growth comparable to the industrially used PVP inhibitor. By substituting PS with a more hydrophobic PPFS as the short end group, the methane hydrate growth rate further decreased from the PVA-PS system, resulting in greater inhibition than the PVP homopolymer. Similar trends were observed with PVP based amphiphilic KHI with added hydrophobic caps. Increased hydrate inhibition with increasingly hydrophobic head groups further emphasizes the role of the structure of the KHI on its inhibition potential. The synthetic scheme and characterization allows the precise molecular tailoring of KHIs and marks one of the first times that controlled radical polymerization is being targeted to design KHIs based on block copolymer motifs. The results from these alternative KHI designs can either improve current KHIs used industrially or lead to new KHIs to safely handle gas hydrates in situations where their formation is thermodynamically favourable.

5. Polymères à base de naphtalène diimide et de pérylène diimide préparé par Poly (hétéro)arylation directe pour des cellules solaires tout polymère efficaces

Amélie Robitaille, Université Laval (Mario Leclerc)

Depuis la découverte des propriétés électroniques des polymères π -conjugués par les professeurs MacDiarmid, Heeger et Shirakawa en 1977 beaucoup de développements ont été réalisés afin d'améliorer les performances électroniques de ces plastiques. Ces semi-conducteurs offrent maintenant d'excellentes performances comparables au silicium amorphe, par exemple, en cellules solaires. De plus, les polymères π -conjugués offrent un avantage majeur face aux matériaux inorganiques, car il est possible de solubiliser ces polymères pour formuler des encres permettant la fabrication de dispositifs électroniques flexibles et légers par impression continue, une méthode simple et peu dispendieuse.

Durant des années, la cible des cellules solaires organiques était de convertir 10% de l'énergie solaire en électricité. Les scientifiques travaillaient principalement au développement de nouveaux polymères donneurs qu'ils jumelaient à des matériaux accepteurs dérivés du fullerène comme le Phenyl-C71-Butyric-Acid-Methyl Ester (PC70BM). Cela a récemment permis d'atteindre des taux de conversion énergétique surpassant les 10%. Malheureusement, les matériaux accepteurs d'électrons dérivés du fullerène possèdent plusieurs inconvénients comme un faible coefficient d'absorptivité molaire ainsi qu'une modification limitée de leurs propriétés optoélectroniques. Finalement, ces matériaux possèdent une faible stabilité et tendent à s'agglomérer pour former des domaines cristallins au sein de la cellule solaire diminuant ainsi les performances des dispositifs au fil du temps.

Le nouveau défi est donc de développer de nouveaux matériaux accepteurs d'électrons plus stables et possédants des propriétés optoélectroniques plus modulables continuer d'améliorer les performances des cellules solaires organiques. Le naphtalène diimide (NDI) et le pérylène diimide (PDI) sont des unités pauvres en électrons fréquemment rencontrées dans la littérature lors du développement d'accepteurs d'électrons. Ces unités sont généralement polymérisées par couplage de Stille qui nécessite l'utilisation d'intermédiaires organométalliques peu stables et toxiques rendant ces polymères moins attrayants pour l'industrie. La polymérisation par hétéroarylation directe (PHAD) est une méthode qui permet d'éviter ces intermédiaires diminuant du même coup le nombre d'étapes de synthèse et le coût de ces matériaux. Cette présentation portera sur le développement de nouveaux polymères accepteurs d'électrons à base de NDI et PDI polymérisés par PHAD avec des unités pauvres en électrons pour obtenir des polymères accepteurs avec des propriétés optoélectroniques intéressantes pour les cellules solaires organiques. Afin de vérifier l'efficacité de conversion énergétique de ces nouveaux matériaux, des prototypes de cellules solaires ont été réalisés et seront présentés.

6. Hierarchically porous, ultra-strong graphene oxide-based sponges for exceptional adsorption of water contaminants

Nariman Yousefi, McGill University (Nathalie Tufenkji)

Porous materials such as graphene oxide (GO) sponges have been recently shown to be an effective class of advanced materials for water and wastewater treatment. Use of nanosheets with exceptionally high specific surface area and a high degree of porosity are key to achieving sponges with remarkable adsorption capacity for various contaminants; however, in most cases self-assembly of nanosheets into these 3D structures results in a significant loss of surface area due to their restacking, and most importantly, formation of isolated pores with no interconnectivity. We report here a novel and green method for rational assembly of GO nanosheets into 3D porous structures with interconnected hierarchical pore architecture. We use computed X-ray tomography (CT) at both micron- (microCT) and nanoscales (nanoCT) as a non-destructive imaging method to investigate the internal pore architecture of the sponges. We demonstrate that the unique architecture of the sponges provides an ultra-high specific surface area, which subsequently translates into an exceptionally high adsorption capacity for a variety of classical (dyes, heavy metal ions, organic compounds) and emerging contaminants (pharmaceuticals, toxins). The sponges also successfully remove contaminants from multicomponent waters that better mimic real wastewaters.

7. Development of Electrospun Chitosan/Phosphorylated Nanocellulose Sorbent Nanocomposite for the Removal of Metal Ions from Aqueous Solutions

Ricardo Brandes, UQTR (Bruno Chabot, François Brouillette)

Water contamination is a growing worldwide concern. Toxic contaminants cause serious problems for the environment and human health. Heavy metals are considered toxic and dangerous contaminants. Humans are exposed to heavy metals by consuming contaminated water, resulting in effects, such as cancer and in extreme cases, death. Adsorption is a tertiary wastewater treatment technology with excellent efficiency and low-cost. Activated carbon is the most widely used material in adsorption, however, its high cost is a major constraint. Chitosan (CS) and phosphorylated nanocellulose (PNC) are alternative low-cost adsorbents known for their high ability to adsorb heavy metals. Electrospinning technique is an excellent choice for the production of adsorbent membranes because it is a process able to produce nanofibers with the high specific surface area. Thus, the main objective of this work was to develop electrospun membranes based on CS/PNC in order to produce an adsorbent with the highest adsorption capacity of heavy metals. Electrospinning solutions and nanocomposite membranes were characterized in relation to morphological and chemical properties. The membranes were tested for the removal of cadmium ions from aqueous solutions. The batch adsorption experiments were employed to investigate the contact time. The nature of the adsorption was evaluated by the kinetic models. This low-cost bioadsorbent may contribute to water sustainability as an excellent alternative to existing technologies. The initial results have shown a great potential of cadmium ions removal by the nanocomposite membranes produced.

8. Nanoscale characterization of miscible and immiscible blends upon crystallization by AFM-IR

Phuong Nguyen-Tri, Université de Montréal (Robert Prud'homme)

We report here an investigation of the crystallization and phase separation at sub-micrometer scale of two different binary blends: i) an immiscible polycaprolactone/polyethylene glycol (PCL/PEG)[1] blend characterized by a small ΔT_m and ii) a miscible polyhydroxybutyrate/polyethylene glycol (PHB/PEG)[2] blend by using mainly an AFM-IR. It was found that, at higher temperatures, the PEG is dispersed into PCL, with inclusions of several hundred nanometers in diameter, but smaller than the micron, while, at lower temperatures, the PEG is rejected outside the PCL spherulites, before its crystallization. In the case of PHB/PEG blends, there is no phase separation and PHB crystallizes first due to the large difference in ΔT_m . This blend forms banded spherulites in which the PEG is mainly found in the valleys while the PHB is mainly located in the ridges; simultaneously, the lamellae are oriented flat-on in the valleys and edge-on in the ridges.

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9. Synthesis of well-defined, multi stimuli responsive degradable amphiphilic block copolymer via combining ATRP and RAFT polymerization: Toward dual reduction and acidic pH labile shell-sheddable micelles

Arman Moini Jazani, Concordia University (Jung Kwon Oh)

Development of stimuli responsive degradable (SRD) amphiphilic block copolymer (ABP) nanoassemblies has seen an enormous surge over the past decades, owing to the escalating demand in drug delivery application. Progress in controlled radical polymerization (CRP) techniques has created new opportunities for developing ABP labeled with a degradable linkage at the junction of hydrophilic and hydrophobic block. Our group has investigated new strategies utilizing atom transfer radical polymerization (ATRP) and reversible addition fragmentation chain transfer (RAFT) polymerizations to synthesize dual cleavable, asymmetrical, fully polymethacrylate backbone-based amphiphilic block copolymer. The block copolymer comprises of hydrophilic poly(oligo ethylene glycol methacrylate) (POEOMA) block and a hydrophobic polymethacrylate block having pendant disulfide linkages (PHMssEt). Both blocks are covalently connected with an acetal linkage and disulfide bond at the junction, thus forming reduction and acidic pH degradable block copolymer of POEOMA-AC-SS-PHMssEt. The synthesis of block copolymer via different routes with individual and concurrent mechanism as well as studies of their SRD property and self-assembly into dual reduction and acidic pH labile shell-sheddable micelles are presented.

10. Extending Scanning Micropipette Contact Method to Investigate High Energy Cathode Materials Using Ionic Liquid

Malak Dayeh, McGill University, UQAM (Janine Mauzeroll, Steen Schougaard)

With the ever-growing demand for energy storage devices, rechargeable lithium ion batteries (LIBs) are being considered as the leading candidates in the fields of portable electronics, and in hybrid, plug-in hybrid, and all electrical vehicles[1]. They are a commercial success offering uniquely high volumetric and gravimetric energy density, as well as, longer lifetime than comparable battery technologies[2]. Lithium ion batteries are used in portable electronics and recently in automotive vehicles, however, the capacity and charge/discharge rates of the electrode materials require improvements. Cathode fabrication for lithium ion batteries involves a combination of conductive material (e.g. carbon), binder (e.g. polyvinylidene fluoride), and active material. The cathode film is cast onto a metal foil before use in the battery. The performance of the battery however, is dependent on the ratio of the film components, the casting and drying procedure, and the coin cell assembly.

Here we present scanning micro-pipette contact method[3] as a technique for probing lithium ion battery materials. The proposed technique allows small substrate areas ($\sim 10\ \mu\text{m}$ in diameter) decorated with battery active material[4] to be probed within a lithium electrolyte solution in protic ionic liquid. The ionic liquid 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide was used to extend the electrochemical window and enable the study of lithium-ion battery materials with high oxidation potential. As a proof-of-concept, localized electrochemical measurements were first performed on lithium iron phosphate active particles, and then on the higher energy density lithium nickel manganese cobalt oxide $\text{Li}[\text{Ni}_{1/3}\text{Co}_{1/3}\text{Mn}_{1/3}]\text{O}_2$ particles drop cast on a glassy carbon substrate. The investigation of isolated particles of active material enables the determination of the oxidation and reduction potentials, peak currents, and charge capacity of the material. Complementary scanning electron microscopy and atomic force microscopy images of the scanned area allow particle sizes to be measured and related to the electrochemical signal. Our studies showed that the new SMCM probe was stable and could be used to analyze high energy lithium-ion battery materials in the range of 2.5 to 5.1 V vs. Li/Li^+ with a coulombic efficiency $> 90\%$, a marked improvement compared to previous studies.

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11. A selective process to extract high-quality Reduced Graphene Oxide (RGO) leaflets and large diameter of semiconducting SWNTs

Ahmad Al Shboul, UQAM (Jérôme Claverie, Mohamed Siaj)

The discovery of carbon materials (CMs), graphene and carbon nanotubes (CNTs), has triggered a revolution in nanoscience and nanotechnology fields. Indeed, CMs exhibit extraordinary physical and chemical properties for a vast range of potential applications. However, their deployment is limited by various limiting steps, such the quality and purity of the material, the cost and scalability of their production techniques. Chemical oxidation and reduction of graphite is a well-known mass-production process of graphene. However, such technique leads to Reduced Graphene Oxide (RGO) which can be viewed as a mixture of small clusters of sp^2 domains distributed in a disordered carbon structure. Thus, a material with inferior properties is obtained than the pristine graphene. Similarly, production techniques of Single Wall Carbon Nanotubes (SWNTs) generate heterogeneous mixtures of nanotubes. Such mixtures contain SWNTs with different chiralities, diameters, lengths, and electrical conductivities (i.e. metallic or semiconducting). In order to harvest the desirable electronic properties of such CMs, one must devise an efficient process to sort and purify these CMs. Therefore, in this work we have developed a separation process named Double Liquid-Phase Extraction (DLPE). We used DLPE to selectively sort RGO flakes and SWNTs in isooctane. Interestingly, the colloidal stability is influenced by the pH of the aqueous phase, temperature and polymer concentration. Thus, we evaluated the intricate balance between the colloidal stabilization of RGO and operational parameters. The near neutral pH, room temperature and 0.25 mg/mL of polymer were chosen as the optimal operational parameters for the best colloidal stability. Remarkably, RGO flakes with high quality are collected in isooctane, leaving destroyed leaflets in water. Furthermore, the DLPE has been found efficient to selectively extract the large diameter of semiconducting SWNTs in isooctane, while excluding other materials such as catalytic and carbonaceous impurities, metallic tubes and small diameter of semiconducting SWNTs.

12. Pb nano-dendrites for highly-selective CO₂ electrochemical reduction

Mengyang Fan, INRS-EMT (Daniel Guay)

Electrochemical reduction of CO₂ (ERC) into fuels and other value-added products is one of the most prospective ways to remediate to excess CO₂ emitted at point source.[1, 2] Using renewable electricity as a source of energy, ERC process constitutes a promising alternative to reduce the atmospheric CO₂ levels while storing at the same time intermittent and renewable energy into chemical bonds. Among earth-abundant ERC electrocatalysts, Sn, Pb and Bi are known to be highly selective for formate production, with faradic efficiency (FE) > 90%. However, several challenges still need to be addressed for these materials to become viable alternatives for industrial applications. In particular, issues related with large overpotential and low current densities need to be addressed, along with the long term stability of electrodes.[3,4]

In this study, Pb films with a porous honeycomb primary structure and a dendrite-like secondary structure were prepared by Dynamic Hydrogen Bubble Template (DHBT). Detailed physicochemical characterization revealed that the thickness (up to 70 μm) and electrochemically active surface area (up to 2700 cm^2) of the porous Pb films could be tuned through the deposition current density and deposition time. The ERC activity and stability of the electrodes were investigated by linear sweep voltammetry and potentiostatic electrolysis in 1 M KHCO₃ electrolyte at standard pressure and room temperature. Formate production was quantified by UV-visible spectrophotometry. It was shown that porous Pb films, which are made of dendrites growing along the [100]-axis, are highly active and stable, with a partial current density (j_{formate}) of -7.5 mA cm^{-2} and a formate Faradaic efficiency of 97% upon 6 hours of electrolysis.

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13. Monolayer Arrays of Nanoparticles Using Block Copolymer Brush Templates

Hu Zhu, Université de Montréal (C. Géraldine Bazuin, Jean-François Masson)

Block copolymer (BCP) thin films self-assembled on surfaces are good templates for 2D patterning of metal and semiconductor nanoparticles. Previous research relied on relatively thick BCP films having microphase-separated nanostructures with distinctive surface patterns for guiding the deposition of phase-selective nanoparticles. We show that ultrathin BCP films formed from an adsorbed brush layer are also suitable templates for producing dense nanoparticle arrays. To achieve this, polystyrene-block-poly(4-vinylpyridine) (PS-*b*-P4VP) thin films were dip-coated on silicon substrates and used to template 15-nm gold nanoparticles (AuNPs). The effect of polymer solution concentration on template thickness, surface morphology and AuNP pattern, determined by ellipsometry, AFM and SEM, respectively, was investigated. For high BCP solution concentrations, film formation was dominated by BCP deposition upon substrate withdrawal, leading to P4VP surface micelles (dots) in a PS matrix. For low BCP concentrations, it was dominated by adsorption of a featureless brush layer during substrate immersion in solution. Both film types yield dense AuNP deposition, but differing in surface pattern, the former producing AuNP clusters on the P4VP dots and the latter individual AuNPs. Dense individual AuNP deposition also occurs on 1- μ m diameter fibers coated by a BCP brush layer after dip-coating in concentrated BCP solutions, where increasing curvature parallels the effect of decreasing solution concentration. This enables the development of surface-enhanced Raman scattering (SERS) optophysiology probes capable of detecting multiple targets.

14. Synthesis, structure and electrochemical properties of new lithium iron vanadates

Yasmine Benabed, Université de Montréal (Mickaël Dollé)

Iron vanadates have been widely explored as possible electrode material for Li batteries. Up to now, the ternary $\text{Li}_2\text{O}-\text{Fe}_2\text{O}_3-\text{V}_2\text{O}_5$ phase diagram only displays two lithium iron vanadium oxides with a similar spinel structure. Our recent investigations allowed us to identify two new phases in this system. One of the two compounds will be discussed in this presentation starting with its synthesis and thermal properties. Its structure characterization was conducted from a single crystal XRD data collection; the structure was successfully solved and refined. Mossbauer and magnetic measurements were performed to verify the oxidation state of iron ions, to support the obtained crystal structure and to explore any possible structural/magnetic transitions. A specific emphasis will be given to the interesting electrochemical properties of this new phase.

15. Self-assembled plasmonic nanostructures

Anna Ritcey, Université Laval

Molecular-scale phase separation in block copolymers leads to the formation of periodic nanostructures. In the case of amphiphilic block copolymers spread at the air-water interface, this is manifested in the formation of surface micelles, composed of circular hydrophobic domains surrounded by coronas of hydrophilic segments. We have employed surface micelles as templates for the preparation of ordered assemblies of metal nanoparticles (NPs). Particle size, capping ligand length, and particle loading all influence the precise spatial distribution of the particles within the template, leading to a variety of assemblies, including clusters, lines and rings. This talk will focus on the plasmonic properties of these nanostructures and their potential application in chemical sensing.

16. Enhancement of PLA/milkweed floss biocomposites properties using fiber surface modifications

Pierre Ovlaque, Université de Sherbrooke (Mathieu Robert, Saïd Elkoun)

Milkweed floss is a natural fiber that shows great opportunities to enhance mechanical properties of plastics thanks to its unique structure. Milkweed floss presents a tube-like geometry with a 20 μ m diameter and a wall thickness of 2 μ m. Thus, milkweed floss exhibits a very large surface per volume unit compared to conventional bast natural fibers. Therefore, good mechanical reinforcement can be achieved in polymeric matrices thanks to pipe geometry.

However, like other natural fibers, milkweed floss exhibits a strong lack of adhesion with biomatrices such as polylactic acid (PLA). The lack of adhesion can mainly be attributed to the high ratio of lignin, hemicellulose, and wax reported for milkweed floss chemical composition. Therefore, in order to enhance the mechanical reinforcement of PLA, two distinctive treatments (alkaline treatment and silanol coupling agents) were applied on the milkweed floss surface.

Prior to biocomposites molding, focus was placed on the effect of treatments on milkweed floss properties. Influence of both treatments on the tensile properties of the fiber was studied. Also, modification of the roughness of milkweed floss was assessed with atomic force microscopy (AFM). Finally, scanning electron microscopy (SEM) was performed on treated fibers to evaluate modifications of geometry induced by both treatments.

Afterwards, PLA biocomposites with a fiber ratio of 1%w were produced using an injection molding process. Mechanical properties of biocomposites reinforced with treated fibers were characterized in the tensile solicitation and single cantilever in the dynamic mechanical analysis (DMA). Dynamic scanning calorimetry (DSC) was also conducted on biocomposites to study thermal properties modification. As a final point, SEM observation was performed on fractured samples to evaluate the improvement of the adhesion between milkweed floss and PLA.

Results tend to prove that both methods of surface modification induced strong alteration of the milkweed floss mechanical properties. However, both methods seem effective to promote higher mechanical properties in biocomposites. Indeed, surface treatments induce strong improvement of adhesion between fiber and matrices that compensate diminution of mechanical properties.

17. Face-on vs edge-on: tuning the structure of tetrathiafulvalene monolayers with solvent

Chaoying Fu, INRS-EMT, McGill University (Emanuele Orgiu, Dmitrii Perepichka)

Tetrathiafulvalene (TTF) is one of the most widely used building blocks for organic conductors and redox-active materials. The ability to control the supramolecular structure of these materials, particularly at interfaces, is critical for application in device. In this work, we show how the structure of N-alkylated tetrathiafulvalenecarboxamide TTFAm18 films on graphite can be tuned between edge-on and face-on orientation, depending on the choice of the solvent. The former orientation is realized in non-polar solvents and results in formation of 1D π -stacks of TTF moieties that are hold together by H-bonding of carboxamide substituents. The latter orientation is enforced by the use of polar H-bonding solvents (alkanoic acids) which break intermolecular H-bonding and maximize the interaction of TTF molecules with the surface. In both cases, the surface density of TTFs is precisely defined by the length of the alkyl chain. Using Scanning Tunneling Microscopy and Atomic Force Microscopy, we show how the supramolecular assemblies observed at the liquid-solid interface can be transferred to growing dry films, thus paving the way for application of such periodically structured materials in devices.

18. Alkyl Chain Length Effects on Double-Deck Assembly at the Liquid/Solid Interface

Yuan Fang, McGill University (Dmitrii Perepichka)

Alkyl chains can unexpectedly be missing when imaging molecular self-assembly using Scanning Tunneling Microscopy (STM). Herein, by carefully tuning the STM tunneling conditions, 'missing' alkyl chains in the self-assembly of aminoquinone derivatives were unambiguously visualized at the liquid/solid interface. Consequently, a double-deck packing model was proposed where a double layer is formed at the alkyl chain region while the head group region remains as a single layer. Specifically, we report the first systematic study of double-deck assembly at the liquid-solid interface. A series of alkylated aminoquinone derivatives with chain lengths varying between 6 and 22 were synthesized, and their self-assembly was investigated by STM. The competition between the fraction of alkyl chains adsorbed on the surface and the optimal conformational bending of alkyl chains near the head group leads to a quantized structural transformation from complete double-deck assembly to complete monolayer packing. The effect of molecular symmetry and metal complexation on the formation of the double-deck assembly was also explored.

19. An Integrated Multifunctional Nanoplatfrom Based on Superparamagnetism and Near-Infrared to Near-Infrared Photoluminescent Nd³⁺-doped NaYF₄ Nanoparticles for Deep-tissue Dual-mode Imaging

Fan Yang, INRS-EMT (Dongling Ma)

Dual-mode imaging, which combines optical and magnetic resonance (MR) imaging, as a diagnosis tool for cancer at early-stage has been shown to be particularly attractive because it will allow retrieving both macroscopic and subcellular information of bio-species, and thus leading to improved diagnostic accuracy. To this end, a variety of multifunctional multifunctional (superparamagnetic and photoluminescent) nanoparticles (NPs) have been specifically designed for dual-mode imaging. However, most of these hybrid NPs show shallow tissue penetration and low signal contrast in optical imaging due to the tissue-induced extinction and autofluorescence since their photoluminescent components based on organic dyes, upconversion nanoparticles (UCNPs) and quantum dots (QDs) are operated in the visible range. In this work, we prepare a biocompatible core/shell/shell sandwich structured Fe₃O₄@SiO₂@NaYF₄:Nd³⁺ nanoplatfrom possessing excellent superparamagnetic and near-infrared (excitation) to near-infrared (emission), i.e., NIR-to-NIR photoluminescence properties. This NIR-to-NIR feature enables deep-tissue penetrated optical imaging with high signal-to-noise ratio which was demonstrated by the ex vivo experiment of chicken samples with thickness of 13 mm. Meanwhile, owing to the superparamagnetic Fe₃O₄ core inside, this nanoplatfrom can be rapidly confined under an external magnetic field and exhibited a significant darkening effect in T2-weighted images in MR imaging. More importantly, the developed NPs are much less toxic than semiconductor QDs, which usually contain Pb and/or Cd. These results including excellent photostability, fast magnetic response, significant T2-contrast enhancement and negligible cytotoxicity suggest that Fe₃O₄@SiO₂@NaYF₄:Nd³⁺ nanoplatfrom can be extremely suitable for use in high resolution, deep-tissue dual-mode (optical and magnetic resonance) imaging in vivo and magnetic-driven applications.

20. Plasmonic Photocatalysts toward Broadband Solar Harvesting for Efficient Photocatalysis

Qingzhe Zhang, INRS-EMT (Dongling Ma, Mohamed Chaker)

Photocatalysis is considered to be one of the most promising technologies for tackling the energy crisis and environmental pollution by directly harvesting and utilizing solar energy. However, most of the photocatalysts are only able to capture photons in the ultraviolet (UV) and blue ranges, with a large portion of solar energy remaining unutilized. Plasmonic Au nanoparticles (NPs) have been extensively incorporated with semiconductor for efficient photocatalysis, benefiting from their unique size-tunable localized surface plasmon resonance effect. Herein, we will present some of our recent development in Au plasmonic NPs and their applications in photocatalytic environmental remediation. One example is about our recent synthesized nanocomposites based on plasmonic Au NPs, in-situ synthesized lanthanide-doped NaYF₄ (NYF) on graphitic carbon nitride (g-C₃N₄) with high NYF yield and high coupling efficiency between NYF and g-C₃N₄. It shows excellent stability, and enhanced UV-, visible- and near infrared-light photocatalytic activity in the degradation of organic pollutants in wastewater.[1] Furthermore, compared with our previously reported results,[2] this work renders a much more facile approach to realize the concept of combining photocatalysis, plasmonic and upconversion. Another example is the latest subtly designed Au NP-loaded hierarchical TiO₂ spheres, which exhibit both strikingly high activity and selectivity in 4-Nitrophenol reduction to 4-Aminophenol under visible light irradiation. In addition to yielding novel and interesting materials and properties, the current work also provides physical insights that can contribute to the future development of plasmon-enhanced broadband photocatalysts and their applications in energy and environmental areas.

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21. Réticulation par l'intermédiaire d'un monomère colorant d'auto-assemblages de copolymères tribloc à base de poly(acrylamide-co-acrylonitrile) démontrant un comportement de type nanogels UCST par exposition à une source NIR

Amélie Auge, Université de Sherbrooke (Yue Zhao)

Les nanogels photosensibles démontrant une variation de volume médiée par l'exposition aux rayonnements proche-infrarouge (NIR) attirent de plus en plus l'attention notamment pour la libération contrôlée de médicaments. Jusqu'à présent, les principales études reportent des systèmes à base de polymères LCST (transition de volume négative) ou de polymères semi-cristallins (transition état vitreux-caoutchoutique). Dans cette étude, nous reportons pour la première fois la synthèse de nanogels photosensibles à base de copolymères UCST et particulièrement de poly(acrylamide-co-acrylonitrile) (PAAm-co-AN). Le choix du PAAm-co-AN s'explique surtout par la possibilité de contrôler sa température de transition de phase par ajustement du ratio molaire AAm/AN. Toutefois, il a été démontré que les rapports de réactivités varient significativement par variation des conditions de copolymérisation. Ainsi, le contrôle du ratio AAm/AN permettant l'observation de propriétés thermosensibles devient difficile lors de la synthèse de nanogels par les méthodes classiques telles que la polymérisation par précipitation ou par dispersion. La réticulation post-polymérisation s'avère donc une méthode pertinente pour l'obtention de nanogels à base de PAAm-co-AN. Tout d'abord, un copolymère tribloc de poly(diméthylacrylamide)-b-poly(acrylamide-co-acrylonitrile)-b-poly(diméthylacrylamide) (PDMA-b-PAAm-co-AN-b-PDMA) a été obtenu par polymérisation RAFT. Le caractère hydrophile du PDMA confère au copolymère une stabilité colloïdale, tandis que le PAAm-co-AN est responsable des propriétés thermosensibles. La réticulation s'effectue ensuite par réamorçage de la polymérisation grâce à la présence de la fonction trithio toujours présente au centre du copolymère. La réticulation s'opère par l'intermédiaire d'un monomère colorant multi-vinyle qui est capable d'absorber le rayonnement à 980nm et de réémettre cette énergie sous forme de chaleur. Le comportement thermosensible des nanoparticules avant et après réticulation a été étudié par différentes méthodes lors des deux mécanismes de transfert de chaleur, par conduction et radiation.

Affichages/Posters

Infrastructures

A. Centre de recherche sur les matériaux avancés (CERMA)

Joël Boismenu-Lavoie (Université Laval)

Le Centre de recherche sur les matériaux avancés (CERMA) regroupe 18 membres dont la recherche s'inscrit dans l'un ou plusieurs de ses principaux axes :

- Les macromolécules naturelles et artificielles;
- Les nanomatériaux;
- Les biomatériaux.

Nos chercheurs et leurs équipes possèdent une grande expertise dans la conception, la synthèse, la fabrication et la mise en œuvre de matériaux de nature très diverse. Nous comptons parmi nous des professeurs provenant des domaines de la pharmacie, du génie électrique, chimique ou des matériaux, de la chimie, de la médecine ainsi que des sciences de bois.

Cette diversité fait la force du CERMA, puisqu'elle permet un partage de connaissance plus étendu et un accès à de l'équipement de pointe diversifié. Les groupes de recherches étant présents à la fois sur le campus de l'Université Laval et dans divers hôpitaux de la région font en sorte que les étudiants ont accès à des outils très utiles dans leurs projets de recherche.

Cet exposé mettra en valeur les différentes expertises trouvées au sein du Centre, ainsi que les équipements étant accessibles aux membres ainsi qu'à de potentiels collaborateurs.

B. McGill Chemistry Materials Characterization Facility (MC2) - MILab & TASLab

Mohini Ramkaran (McGill University)

The McGill Chemistry Materials Characterization (MC2) facility regroups expert personnel and state-of-the-art instrumentation for the investigation of materials in a wide range of disciplines. The MC2 is staffed by scientists with expertise in these areas and serve both the experienced and novice investigators by providing training, measurements and/or data interpretation. Our infrastructures are accessible to both the internal and external researchers at affordable rates. Here, we describe two of our facilities: the Microscopy and Imaging Lab (MILab) equipped with various scanning probe microscopes (SPM) and electron microscope and the Thermal Analysis and Spectroscopy Lab (TASLab) with multiple DSC, TGA, UV-Vis and FTIR platforms.

C. SynLab part of the MC2

Violeta Toader (McGill University)

SynLab offers organic synthesis services that help those who do not have chemical manufacturing capabilities to create new functional materials. In a state of the art laboratory we perform chemical custom synthesis of known and new compounds - on the milligram to gram scale - in a timely and cost effective manner. We are committed to provide high quality materials that are fully characterized using modern techniques (NMR, DSC, UV-Vis, MS, etc.). Our expertise covers the field of functionalized polymers and small organic molecules for surface modification and/or as building blocks for bottom-up self-assembling materials. We also perform the synthesis of stable labeled (2H , 13C) compounds. The diversity of the research topics of QCAM members is mirrored in the diversity of the synthetic projects. The poster will highlight some of our achievements over the past 14 years.

D. Réseau Québécois pour la microscopie électronique des matériaux/ Quebec Network for Electron Microscopy of Materials

Nadi Braidy (Université de Sherbrooke)

The Quebec Network for Electron Microscopy of Materials (QNEMM) was created in 2018 by seven institutions (Université de Sherbrooke, Polytechnique Montréal, Université de Montréal, McGill University, Université Laval, Concordia University and École de Technologie Supérieure) to support Québec's R&D in advanced materials community using state-of-the-art electron microscopy.

The QNEMM will oversee and coordinate the access and operation of the high performance electron microscopes that were funded by the Canada Foundation for Innovation (CFI) 2017 competition. In addition, the QNEMM will (i) promote and create awareness of the potential of electron microscopy to support advanced materials R&D among academia and industry in Québec (ii) create and consolidate expertise in Québec academia and industry in the field of materials characterization by electron microscopy and interpretation of data and (iii) develop innovative methods for materials analysis by advanced microscopy and interpretation of imaging data and microanalysis.

E. Vibrational Spectroscopy & Scanning Probe Microscopy (SPM) At The Laboratory of Characterization Of Materials (LCM)

Patricia Moraille (Université de Montréal)

Since January 2001, the Laboratory for the Characterization of Materials (LCM) offers Quebec's research community access to a variety of state-of-the-art instruments. Research professionals provide training as well as technical support. We describe here, the various scanning probe microscopy (SPM) & vibrational spectroscopy (IR & Raman) options that are available at the LCM. The expertise and savoir-faire of this platform makes it one of Quebec's specialized infrastructures for the imaging and characterization of nanostructured materials and thin films on the nanometer to micron length scales. Our facilities are used by more than 100 scientists yearly and open to all researchers from both academia and industry at affordable rates.

F. NanoQAM

Gwenaél Chamoulaud (UQAM, Mohamed Siaj)

Le Centre de recherche NanoQAM est constituée de quatre laboratoires de l'Université du Québec à Montréal qui regroupent, chacun, une large série d'appareils scientifiques de haute performance et de routine permettant la synthèse ainsi que la caractérisation de nanomatériaux et systèmes nanométriques.

G. LAMP: Laboboratoire d'analyse de molécules et matériaux photoactifs

Daniel Chartrand (Université de Montréal, Will Skene)

Les équipements et les méthodes disponibles au laboratoire seront présentés. Le service se divise en trois grands axes:

- La caractérisation robotisée de dispositif solaire (I/V, EQE/IQE, EIS)
- Le suivi de photo-réaction ou d'électrolyse (production H₂, CO, CH₄)
- La caractérisation électrochimique et photophysique transitoire ou à l'équilibre de systèmes moléculaires (spectroscopie UV-vis-NIR, FTIR, fluorescence).

Pour plus d'info consulter la page web : <http://132.207.196.24/welcome/>

Recherche / Research

1. Chiral Amplification of Tri-o-Thymotide Clathrates

Thao Nguyen, Concordia University (Louis Cuccia)

A branch of inclusion compounds that crystallizes as guest molecules are encapsulated inside the host molecule lattice is called clathrate. The chemistry of clathrates dates from the middle of the twentieth century including the discovery of new inclusion compounds and hosts, and their pragmatic applicabilities in chemical analysis and molecular separation process. Our compound of interest, tri-o-thymotide (ToT), exhibits a remarkable propensity to complex with more than 100 of guest molecules on crystallization thanks to its uniquely flexible chirality. The 12-member-ring molecule constrained by a rotation around a single bond adopts a three-propeller shape configuration (either M or P) which is dynamically racemizing in solution, but preserved during conglomerate crystallization. In light of the rich research history of ToT, we would like to present a novel approach to its synthesis using a simple one-pot mechanochemistry and revisit the study of chiral amplification and discrimination using a wet abrasion method known as *Viedma ripening*.

2. Component exchange for property tailoring

Abdel Al Ahmad, Université de Montréal (Will Skene)

Component exchange is the switching of constitutional components within a given a compound. The exchange is enabled by reversible bonds. These can either be supramolecular or covalent bonds. Component exchange involving dynamic bonds can be triggered with external stimuli such as heat, catalyst or mechanical forces. It will be shown that dynamic component exchange can occur with covalent imine bonds. Property tailoring by component exchange such as fluorescence and electrochemistry will be demonstrated.

3. Evidence of hydrocarbon nanodrops in highly ordered Stratum Corneum model membranes

Adrian Paz Ramos, Université de Montréal (Michel Lafleur)

The stratum corneum (SC), the top layer of skin, dictates both the rate of water loss through the skin, and absorption of exogenous molecules into the body. The crystalline organization of the lipids in the SC is believed to be a key feature associated with the very limited permeability of the skin. In this work, we characterized the organization of SC lipid models that include, as in native SC, cholesterol, a free fatty acid series (saturated with C16-C24 chains), as well as a ceramide bearing an oleate linked to a very long saturated acyl chain (Cer EOS). The latter is reported to be essential for the native SC lipid organization. Our ²H-NMR, infrared and Raman spectroscopy data reveal that Cer EOS leads to the formation of highly-disordered liquid domains in the solid/crystalline matrix. The lipid organization imposes steric constraint on Cer EOS oleate chains in such a way that these hydrocarbon nanodroplets remain in the liquid state down to -30 °C. These findings modify the structural description of the SC substantially, and propose a novel role of Cer EOS as this lipid is a strong modulator of SC solid/liquid balance.

4. Supramolecular photochemistry towards artificial photosynthesis: Ir and Ru photosensitizers with Co Hydrogen Evolving Catalyst

Olivier Schott, Université de Montréal (Garry Hanan)

The following work is focused on the reduction of protons. Here, the study highlights the intrinsic properties of photosensitizers for efficiency and photo-redox stability, the supramolecular interaction between photosensitizers and catalysts for the enhancement of electronic transfers and the tuning of cobaltoximes and polypyridyl Co derivatives for robustness and efficiency. Ir[1] and amide polypyridine based Ru[2] photo-sensitizers in association with Co catalysts are investigated in different conditions (various wavelengths of irradiation[3], various concentration, different solvent) and their photo-catalytic activities are discussed.

1. (a) C. Lentz, O. Schott, T. Auvray, G. Hanan, B. Elias, *Inorg Chem* 2017, 56, 10875-10881; (b) A. Jacques, O. Schott, K. Robeyns, G. S. Hanan, B. Elias, *European Journal of Inorganic Chemistry* 2016, 2016, 1779-1783.
2. G. S. Hanan, A. K. Pal, O. Schott, D. Chartrand, *ChemSusChem* 2017.
3. E. Rousset, D. Chartrand, I. Ciofini, V. Marvaud, G. S. Hanan, *Chem Commun (Camb)* 2015, 51, 9261-9264.

5. Unraveling the kinetics and dynamics of reversible DNA nanotube opening using single molecule fluorescence imaging

Casey Platnich, McGill University (Gonzalo Cosa, Hanadi Sleiman)

DNA nanotubes (NTs) have recently gained popularity as potential biophysical probes and drug delivery vehicles due to their many attractive qualities, such as rigidity and site-specific addressability. While DNA nanomachines, including NTs, have been shown to be capable of controlled opening and closing behaviours, the dynamics and kinetics of these molecular movements remain poorly understood, in part due to a lack of analytical tools appropriate for their study. We report here the adaptation of single-molecule fluorescence methodologies to observe the reversible switching between double- and single-stranded forms of DNA nanotubes. Specifically, we have employed total internal reflection fluorescence microscopy (TIRFM) to examine, in real time, the removal and re-hybridization of fluorescently labeled linking strands from surface-bound DNA NTs. This allowed for the direct observation of the conformational changes DNA NTs can undergo while switching from the more rigid double-stranded form to a more flexible single-stranded analog, and back. In particular, we were interested in understanding to what degree the repeat units of the NT exhibit cooperativity during these structural changes. Additionally, our work addressed the robustness of these DNA assemblies using single-molecule two-colour co-localization analysis. We also used the polydispersity of our NT synthesis to our advantage, studying a range of NT sizes in each experiment in order to understand how the number of repeat units in each structure dictates its behaviour. In doing so, we showcase how SMF methodologies are uniquely poised to understand the vexing kinetics and dynamics of DNA nanostructures

6. Mapping Redox Activity in Supported Lipid Bilayers

Aya Sakaya, McGill University (Gonzalo Cosa)

Supported lipid bilayers (SLB) have gained wide attention as assembly scaffolds, owing to their ability to self-assemble into well-defined fluid structures, allowing the compartmentalization and direct assembly of components of interest in a fluid platform. An excellent model of cellular membranes, supported lipid bilayers offer the opportunity to mimic and study processes occurring across these fluid mosaics such as respiration, transport and signaling.

In this study, we have explored redox reactions within supported lipid bilayers, proof of concept experiments intended to address the response of membrane embedded redox systems. Experimentally, a supported lipid bilayer was formed on top on an indium tin oxide (ITO)-coated glass, mimicking the lateral fluidity of a cell membrane. H4ClPrB-PMHC, a redox sensitive fluorogenic probe analogous to α -tocopherol (Vitamin E) was incorporated within the SLB, and its electrochemical and optical properties were studied using spectro-electrochemical (SEC) total internal reflection (TIRF) microscopy. We will discuss the general methodology, results, and implications of the work in the context of electron transport through relay redox systems.

7. On-substrate deposition of electroactive layers for organic devices

Will Skene, Université de Montréal

The working electrodes in organic electronic devices are typically glass substrates coated with conductive ITO. It will be shown that these electrodes can play an active role in preparing electroactive layers that are deposited on top. It will be shown that post-deposition patterning can be done to design active layers.

8. L'homo-couplage Glaser dans les réactions de polycondensation de semi-conducteurs organique: un couplage compétitif aux propriétés photo-physiques surprenantes

Loïc Tanguy, Université de Sherbrooke (Pierre Harvey)

Plusieurs polymères synthétisés par des couplages de Sonogashira décrits dans la littérature ont été trouvés contaminés par des homo-couplages de type Glaser. Ces impuretés bien que difficilement quantifiables par les méthodes de spectroscopie traditionnelle amènent pourtant des changements drastiques aux propriétés photo-physiques des polymères concernés.

9. Coupling Mechanochemical Syntheses of Advanced Materials with in situ Spectroscopy

Patrick Julien, McGill University (Tomislav Friščić)

Mechanochemical syntheses generally promote fast reaction times, high efficiency, and reduction of solvent cost and waste when contrasted with solution methods. Fortunately, scalable mechanochemical synthesis can be developed for a wide variety of materials including pharmaceutically relevant co-crystals, or functional materials such as luminescent phosphors and metal organic frameworks. A major challenge towards further development of ball milling syntheses is the limited tools available for gaining mechanistic insights into these processes. This presents the development of novel mechanochemical syntheses and application of novel real time spectroscopic approaches using readily accessible bench-top monitoring techniques such as Raman and especially fluorescence spectroscopies. The analysis of in situ data provides fundamental insights into reaction rates and kinetics, and enables the rapid optimization of the synthesis of a wide variety of advanced materials with interesting physical and optical properties. Monitoring of milling reactions enables the discovery of new and potentially isolatable intermediates providing insights into chemical transformations and revealing promising materials. The development of readily accessible in situ techniques for monitoring milling reactions represents a significant advance in the understanding and utility of mechanochemical synthesis.

10. Efficient glass passivation for single molecule fluorescence studies

Yasser Gidi, McGill University (Gonzalo Cosa)

Surface passivation to inhibit unwanted nonspecific interactions is a key requirement for in vitro single molecule fluorescent studies. The standard passivation method involves the covalent attachment of poly(ethylene glycol) (PEG) in two steps. This protocol is time consuming and has a high variability. While improvements have been proposed to the passivation, they all require extensive labour and chemicals leading to costly protocols. Herein, we report an efficient protocol relying on one-step surface grafting of PEG-silane that provides improved passivation performance over the conventional two-step surface PEG passivation method as reported by others, at a minimal time and reagent cost. The protocol described is rooted in a mechanistic understanding of the PEG-silane grafting reaction with the glass surface. Single molecule studies on functionalized surfaces will be presented to validate the performance of the proposed protocol.

11. Simultaneous ultraviolet-spectrophotometric determination of chlorophenol and heavy metal ions by multivariate calibration approaches for organophilic bentonite adsorption study

Jhimi Khoulood, ETS (Claudiane Ouellet-Plamondon)

The purpose of this experiment was to test the effectiveness of organophilic bentonite obtained by ion exchange with Hexadecyltrimethylammonium bromide (HDTMAB) and lecithin on removing pentachlorophenol and the heavy metal pollutants (As, Cr and Cu) from the waters.

This is of attention for the stabilization of mixed wastes in which simultaneous organics and heavy metals contamination occurs.

Therefore, a rapid and inexpensive method for the simultaneous determination of these organic and inorganic pollutants concentrations was researched and developed with the aid of chemometrics methods to study the modified bentonite adsorption capacities. UV-spectra were collected in the 200-400 nm range from a set of aqueous samples at pH=12 containing the above compounds.

This study also showed the significant spectral interference of the UV- spectra of the Pentachlorophenol and Cr showing the need for chemometrics analysis for simultaneous analysis of the mixtures.

Calibration models for the Partial least square(PLS) multivariate method were constructed with the use of spectral data sets. The PLS calibration was utilized to illustrate successfully the application of the proposed method for analysis of the PCP and Cr in adsorption study. It was hypothesized from this study that organobentonite will decrease the heavy metal concentration and adsorb pentachlorophenol to a very high extent due to its organophilic nature.

12. Improving the performance of high-voltage lithium-ion battery cathode using functionalized carbon additive

Hamidreza Saneifar, UQAM (Daniel Bélanger)

In this research, the modification of acetylene black carbon (AB) with an organic molecule via diazonium chemistry has been studied. The modification was carried out with substituted aryl group, C_6H_4-X Where $X = CF_3$. X-ray photoelectron spectroscopy (XPS) confirms the presence of $C_6H_4-CF_3$ group on the carbon surface. The modified and unmodified carbon powders were then used in Li-ion batteries as additives and the high-potential $LiMn_{1.5}Ni_{0.5}O_4$ (LMN) cathode material was selected as the active material for this study. The electrochemical performance of the cathodes with modified and unmodified carbon additives were studied by galvanostatic charging and discharging method between 3.5 and 5.3 V. This high cut off potential was selected to investigate the role of the carbon additive modification on the cathode performance during applying high voltage. The irreversible electrolyte degradation at 5.3 V vs. Li/Li^+ was strongly diminished after modification. The obtained results showed better capacity retention and higher discharge capacity for LMN batteries made with modified carbon additives.

13. Push-pull fluorophores towards NIR emitters

Lei Hu, Université de Montréal (Will Skene)

Conjugated fluorophores have uses in a wide range of applications. Their useful applications can be expanded with emission properties that extended into the NIR. Towards NIR emitting fluorophores, it will be shown that the fluorescence of a common fluorophore can be extended to the cusp of the NIR region when conjugated with electronic donors and acceptors. The solvatochromic effects of electronic push-pull chromophore will be demonstrated.

14. Graphene and MoS₂ Synthesis via Chemical Vapor Deposition

Ehsan Jafarnejad, UQAM (Mohamed Sijaj)

Two-dimensional materials, like graphene and molybdenum disulfide (MoS_2), can be significantly increased the performance of electrochemical energy storage devices due to a combination of high surface area and electrical conductivity. For the present poster, we will show that the graphene MoS_2 atomic layers could be prepared by simple Chemical Vapor Deposition method. The crystallography and morphological studies of resulting 2D materials have been carried out by Raman, Photoluminescence and Scanning Electron Microscopy.

15. Pyroelectric luminescence in barium titanate

Membarka Atantawi, INRS-EMT (Andreas Ruediger)

Pyroelectric luminescence describes two rather different types of light emission from materials with a spontaneous polarisation under changing temperature. In contrast to thermally stimulated luminescence, a well-established technique to determine thermal activation energies from deep traps upon heating, pyroelectric luminescence occurs for both heating and cooling.

A first type of emission, pronounced sparks, visible to the bare eye relate to discharges of the pyroelectric field through the ambient atmosphere. Under high vacuum condition, the sparks become sparse and eventually cease. For previously

illuminated samples (band-band excitation to create meta-stably trapped states), a continuous, however very faint emission is observable. For an intermediate pressure range, both phenomena also coexist.

We present a tentative model to describe the nature of this faint emission that still lacks interpretation more than 30 years after it was first systematically investigated[1]. Our model is based on a field-assisted emission through the Poole-Frenkel effect and possible field emission from deep traps. The model correctly accounts for all qualitative observations, including the dynamics of this luminescence and its sensitivity to phase transitions.

We present results on single crystalline barium titanate in a temperature range from 77 K to 500 K and identify the parameter range in which the continuous emission can persist. It turns out to critically depend on a variety of material parameters including the pyroelectric coefficient, the permittivity, the refractive index, and the conductivity.

1. J.S. Patel and D.M. Hanson, 'Pyroelectric luminescence', *Nature*, 293 (1981) p.445-447

16. Direct Chemical Vapor Deposition Growth of Van Der Waals Heterostructures WSe₂/hBN

Mohammed Alahmadi, UQAM (Mohamed Siaj)

Two-dimensional transition metal dichalcogenides (TMDC) and hexagonal boron nitride (hBN) have attracted increasing attention due to the possibility of stacking or direct growth these materials on top of each other to create heterostructures that offer another promising approach to fabricate novel materials and devices. Among large numbers of substrates, hBN is of particular interest since it possesses an atomically flat surface and free of surface state, which leads to improvements inhomogeneous lattice, structural defects, as well as for electronic and optoelectronic devices. However, Recent success in the synthesis of TMDC: hBN vertical van der Waals heterostructures has required a transfer of hBN. Herein we demonstrate an all-direct chemical vapor deposition (CVD) process for a successful synthesis of a large-area, uniform and high-quality WSe₂: hBN van der Waals heterostructures grown on SiO₂/Si substrate.

17. New Strategy for the Two-Step Growth of Two-Dimensional WSe₂/MoSe₂ Lateral Heterostructures

Mohammed Alahmadi, UQAM (Mohamed Siaj)

Integration transition metal dichalcogenides materials in lateral heterostructures create novel properties different from those of the constituents. Here, we present for the first time a strategy for lateral WSe₂/MoSe₂ heterostructures synthesis via a two-step chemical vapor deposition (CVD) growth. The WSe₂ peripheral domain with a triangular hole was synthesized first followed by MoSe₂ growth inside. The growth MoSe₂ in the inner peripheral WSe₂ domain was occurred due to three inner-edges of WSe₂ function as seed growth. This method consists of W atoms substitution by Mo atoms leading to Mo core lateral structure formation. Our experimental findings reveal that the atoms substitutions occur without changes in the crystal structure of the resulting heterostructures.

18. A Bi-Phasic Scaffold with Bioglass-PLGA composite and Fibrin gel for bone regeneration through endochondral ossification

Dhanalakshmi Jeyachandran, McGill University (Marta Cerruti)

Traditional bone regeneration strategies follow intramembranous ossification by promoting bone growth through direct differentiation of stem cells into osteoblasts. This approach often fails due to poor angiogenesis and hypoxia, leading to apoptosis. Thus, mimicking the process of endochondral ossification, wherein the bone is formed through a cartilage intermediate, would be a more appropriate approach for bone regeneration than direct ossification as it prevents hypoxia-induced cell death. As each tissue and its requirements are much different from other tissues, a bi-phasic scaffold design could be beneficial to support both cartilage and bone.

We propose a bi-phasic scaffold with a layer of fibrin hydrogel, encapsulating and infiltrating a porous Bioglass-PLGA composite layer to support cartilage and bone respectively. The composite layer of the scaffold is prepared by solvent casting/particulate leaching method using paraffin microspheres as a template. Fibrinogen with Mesenchymal stem cells(MSCs) is casted onto the porous composite template and subjected to gelation ensuring even cell distribution.

We prepared a bi-layered scaffold with fibrin hydrogel supporting the cartilage and a composite layer supporting bone formation. Bioglass-PLGA composite layer has evenly distributed and well interconnected spherical pores. Fibrin gel

supported the chondrogenic differentiation of the MSCs and the cells were found to be well distributed throughout the gel layer.

The cells in the gel layer, degrade the gel and reach the composite layer, allowing enough time for the vasculature formation prior to bone growth. As stiffer scaffolds promote hypertrophy, which is the terminal differentiation of chondrocytes before undergoing apoptosis, the stiff BG-PLGA composite layer promotes the hypertrophic differentiation of the chondrocytes. When the hypertrophic chondrocytes die, they will be eventually replaced by osteoblasts brought in by the vasculature, leading to new bone formation.

19. Dormant Singlet Photosensitizer Based on ROS

Wenzhou (Kevin) Zhang, McGill University (Gonzalo Cosa)

Photodynamic therapy for the treatment of cancer and other diseases employs photosensitizers to promote the production of singlet oxygen to eliminate pathological tissue. Due to the cytotoxicity of singlet oxygen, it is imperative to have a high degree of control over its production. Previously, our group has reported a dormant photosensitizer based on a boron-dipyrromethene (BODIPY) chromophore where a chromanol trap moiety serves as a dormant/active control switch via photoinduced electron transfer. Reactive oxygen species (ROS) trigger activation of the sensitizer upon oxidation of the chromanol segment [1]. Building on our previous work we developed a new chromophore with enhanced switching capabilities. Herein we present the results.

1. *Durantini, A.M.; Greene, L.E.; Lincoln, R.; Martinez, S.R.; Cosa, G. J. Am. Soc. Chem. 2016, 138 (4), 1215-1225*

20. Thermo/Light Responsive Microgel Composites for Modulation of Surface Properties: Fabrication and Applications

Charly Ou, Université de Montréal (Suzanne Giasson)

Recent advances in stimuli-responsive materials enable their integration as functional surface elements in nanotechnologies such as microfluidics and Micro Electro-Mechanical Systems (MEMS) where surface forces strongly influence the device performance because of the large surface-to-volume ratio. However, responsive coatings are suffering from major shortcomings such as lack of responsiveness selectivity and reversibility which are critical to design reliable rules for building multifunctional surfaces.

We report the preparation of responsive nanocomposite incorporation of plasmonic gold nanoparticles in thermos-responsive microgels based on poly(N-isopropylacrylamide) (polyNIPAM) microgels. Combined together, these composites show multi-stimuli responsive properties where their sizes can be tuned by direct heat or by light irradiation through photo thermal properties of AuNPs. These composites could be used to prepare a new generation of responsive hierarchical micro/nano-structured coatings whose physical properties (structure and mechanical properties) and surface chemistry can be tuned independently and reversibly using different external stimuli (light, temperature, pH, ionic strength).

21. Synthesis and characterization of nanoparticles Mo₂C by hydrothermal and their electrocatalytic performance for hydrogen evolution reaction

Xuan Thai Tran, UQAM (Mohamed Siaj)

For more energy-efficient and economical hydrogen production, highly active noble metal-free hydrogen evolution catalysts are a priority for all. Herein, we report a one-step facile synthesis of a novel precious-metal-free hydrogen-evolution nanoelectrocatalyst, dubbed Mo₂C that is composed of ultrasmall molybdenum carbide (Mo₂C) nanoparticles. Mo₂C nanoparticles provide an efficient electrocatalysis, leading to their superior HER activity with lower onset overpotential and higher current densities than Mo₂C microparticles. This study opens a new perspective for the development of highly active non-noble electrocatalysts for hydrogen production from water splitting. In addition, the results provide a simple and effective way for the exploration of efficient Mo-based HER catalysts.

22. Studying the corrosion properties of metallic thermal spray coatings using macro and micro electrochemical techniques

Samantha Gateman, McGill University (Janine Mauzeroll)

The success of the renewable/non renewable energy divisions, and other industrial sectors including aerospace and automotive, is significantly owed to the advancement of spray coating technologies as these coatings are essential for maintaining safety, reliability and increasing the lifetime of expensive components and machinery. Such coatings can be composed of metallic materials and unfortunately will undergo corrosion soon after, requiring replacements to protect the system's integrity. Specifically chosen for its impressive stability in aqueous environments, the stabilized ferritic stainless steel, SS 444, with low nickel content has been selected as the material of interest. Unlike bulk steel, thermal spray coatings are known for their complex microstructure and composition. Investigating the mechanism of corrosion the coatings undergo and how their corrosion properties are affected over time can lead to a better understanding about how material degradation can be controlled.

23. Periodic DFT calculations for predicting structure, topology and stability of metal-organic frameworks

Mihails Arhangel'skis, McGill University (Tomislav Frišćić)

Metal-organic frameworks (MOFs) are microporous materials of emergent technological importance for gas storage and separation, catalysis, sensing devices and other advanced applications. The vast variety of possible metal-ligand combinations leads to a wide range of topologies and, consequently, properties. However, prediction of structures and properties of MOF materials is a challenging task which involves exploring a variety of candidates until a suitable structure is found. New, cutting-edge computational methods are expected to bridge this gap, and make MOF design more target-specific. This can be achieved by rationalizing thermodynamic aspects of MOF formation and topological transformations, explaining topological preferences of different systems and predicting the most likely structures for a given metal-ligand system.

This presentation will outline our recent advances in using periodic density functional theory (DFT) calculations[1] to characterize and even predict MOF systems. First, we will show how periodic DFT calculations can be used to explain the thermodynamic pathways observed in mechanochemically-induced topological transformations in MOF systems, demonstrating that such reactions proceed towards thermodynamically most stable structures.[2,3] Specifically, we will present the first evaluation of the accuracy of DFT-calculations in determining energies of MOF structures, by comparing the outcomes of computational modelling to experimentally determined calorimetric values. In addition, we will outline the not yet published results, demonstrating the ability of periodic DFT to correctly predict the topological preferences in a metal azolate system that has not yet been reported.

Finally, this presentation will also outline how the established excellent match between calculated and measured MOF thermodynamic stabilities permitted us to conduct the first full ab initio screening of a previously not reported class of microporous materials, based on the recently isolated pentazolate (pnz-) ligand.[4,5] While demonstrating, for the first time, the ability to use periodic DFT to predict potential structures of not yet synthesized MOFs, this work also reveals a potential route to design MOFs that are inherently thermodynamically stable, while exhibiting low-density structures.

1. Clark, S. J.; Segall, M. D.; Pickard, C. J.; Hasnip, P. J.; Probert, M. I. J.; Refson, K.; Payne, M. C. Z. *Kristallogr.* 2005, 220, 567.
2. Akim'bekov, Z.; Katsenis, A. D.; Nagabhushana, G. P.; Ayoub, G.; Arhangel'skis, M.; Morris, A. J.; Frišćić, T.; Navrotsky, A. J. *Am. Chem. Soc.* 2017, 139, 7952.
3. Calvin, J. J.; Asplund, M.; Akim'bekov, Z.; Ayoub, G.; Katsenis, A. D.; Navrotsky, A.; Frišćić, T.; Woodfield, B. F. J. *Chem. Thermodyn.* 2018, 116, 341.
4. Zhang, C.; Sun, C.; Hu, B.; Yu, C.; Lu, M. *Science* 2017, 355, 374.
5. Arhangel'skis, M.; Katsenis, A. D.; Morris, A. J.; Frišćić, T. *Chem. Sci.* 2018, 9, 3367.

24. Antibacterial and strong dental resin composites containing CNC/ZnO nanohybrids

Yazi Wang, Université de Montréal (Xiaoxia Zhu)

The introduction of antibacterial properties can prolong service life of dental resin composites (DRCs). To this aim, cellulose nanocrystal (CNC)/ZnO nanohybrids were prepared through precipitating Zn^{2+} on the surface of CNC under alkaline condition. Transmission electron microscopy (TEM), X-ray diffraction (XRD), and Fourier transform infrared spectroscopy (FT-IR) measurements confirmed that CNC/ZnO nanohybrids were obtained successfully. The DRCs were prepared through blending CNC/ZnO with organic monomers and silanized SiO_2 and the influence of CNC/ZnO amounts (0-8 wt %) on the antibacterial and mechanical properties of DRCs was investigated. DRCs with CNC/ZnO showed excellent antibacterial properties and the addition of small amount of CNC/ZnO had no adverse effect on the mechanical properties. Instead, there is an improvement in the compressive strength and flexural modulus when 2 wt% CNC/ZnO was added. In conclusion, the introduction of CNC/ZnO can endow DRC antibacterial properties without compromising its mechanical properties.

25. Environmentally friendly synthesis of ultralight, porous boron imidazolate frameworks

Cameron Lennox, McGill University (Tomislav Friščić)

Whereas metal-organic frameworks (MOFs) have been established as the go-to tunable, porous materials, their synthesis still poses significant difficulties from both an environmental standpoint and is a synthetic challenge.[1] A particularly poorly explored class of such materials are boron imidazolate frameworks (BIFs),[2] a rare example of a main group frameworks analogous to zeolitic MOFs based on imidazole linkers. The general design for BIFs is based on replacing the metal nodes of such zeolitic imidazolate frameworks with alternating lithium cations and tetrakis(imidazolato)borate anions. Such a structure, involving lithium and boron nodes, makes these frameworks particularly attractive as ultra-lightweight microporous materials. This presentation will outline our efforts in the development of solvent-free mechanochemical routes[3] for the assembly of a wide range of BIFs, and in particular the use of liquid-assisted grinding (LAG) as a means to control the yield and topological outcome of the reactions.

1. Czaja et al. *Chem. Soc. Rev.* 2009, 38, 1284
2. Zhang et al. *Angew. Chem. Int. Ed.* 2009, 48, 2542
3. Do and Friščić *ACS Centr. Sci.* 2017, 3, 13

26. Elusive Non-Solvated Cocrystals of Aspirin

Shalisa Oburn, University of Iowa (Len MacGillivray)

Here, we report the discovery two non-solvated cocrystals of acetylsalicylic acid (ASA) and 4,4'-bipyridine (4,4'-bipy) in the form of 2(ASA)·(4,4'-bipy). The Form I polymorph was discovered through mechanical dry grinding and Form II was discovered through rapid cooling. Both polymorphs consist of three-component hydrogen-bonded assemblies sustained by O-H...N hydrogen bonds and differ in terms of relative twists of carboxylic acid groups and pyridyl rings. In Form I, the ASA molecules are linked by discrete catemeric methyl C-H...O forces of the acetyl substituents while in Form II the ASA molecules are linked by both infinite methyl C-H...O catemers and centrosymmetric dimers of the acetyl groups. Our results demonstrate importance of neat mechanical grinding in the discovery and design of pharmaceutical cocrystals and polymorphs.

27. Theoretical Study of Azophenine-based NIR Fluorophores

Lei Hu, Université de Montréal (Will Skene)

Near-infrared (NIR) organic fluorophores are an unusual class of materials with potential applications ranging from biological imaging and medical therapy to night-vision devices. However, the luminescence efficiency of NIR emission is lower than achievable in the visible range due to the 'energy gap law'. Exploring molecules with NIR character while possessing high quantum yield is fundamental for the application of NIR fluorophore. Recently, azophenine-based fluorophores were found to be emissive at 780 nm at 77K and can be rendered emissive up to 870 nm (shoulder peak at 930 nm) at 298K after chelating with the BF_2^+ fragments on the HN^+N moiety. Here a serial of azophenine-based fluorophores was designed and theoretical study based on density functional theory (DFT) was performed in order to obtain azophenine-based NIR fluorophores with high NIR emission quantum yield.

28. Enhanced Artificial Photosynthesis Activity for CO₂ reduction into useful fuels using Cu Nanoparticles Decorated BiFeO₃ Nanowires

Peikui Wang, University of Sherbrooke (Jérôme Claverie)

Artificial Photosynthesis conversion of CO₂ to carbon-based products, which can be used directly as fuels or indirectly as fuel precursors, is suggested as one of the promising solutions for sustainability. As a typical multiferroic material, Bismuth Ferrite (BiFeO₃), has been recognized as a potential materials for photovoltaic and visible-light photocatalysis applications, thanks to its suitable band gap (2.2-2.8 eV) and good chemical stability. In this study, Bismuth Ferrite Nanowires decorated with copper nanoparticles (Cu-NPs) have been used to enhance photocatalytic CO₂ reduction under concentrated visible light. The effects of copper nanoparticles in the decorated on BiFeO₃ are shown to significantly enhance the photocatalytic activity of BiFeO₃, primarily through the suppression of electron-hole pair recombination, further modulation bandgap of BiFeO₃.

29. In situ polymer encapsulation-graphitization to synthesize high-performance TiO₂-based photocatalyst

Peipei Liu, University of sherbrooke (Jérôme Claverie)

TiO₂-based photocatalyst (TiO₂-C) are widely popular investigated because they combine the advantages of TiO₂ (low cost, stability, nontoxic and good UV photocatalytic activity) and carbon (inexpensive, good conductor). However, the presence of carbon can also decrease the photocatalytic performance as it can block the passage of light and prevent the reactant from accessing to the TiO₂ surface. Here using a novel interfacial in situ polymer encapsulation-graphitization to synthesize uniform TiO₂@C core-shell photocatalyst and TiO₂-graphite carbon-Au photocatalyst. The resulting TiO₂@C photocatalyst with easily tuned carbon shell possess higher activity. For further study, the plasmonic nanoparticle Au was added to produce three different TiO₂-graphite carbon-Au core@shell structures by simply varying the addition sequence of materials. The photoactivity of TiO₂-graphite carbon-Au photocatalyst was assessed by H₂ generation, degradation of dye and photoelectrochemical cells. The results show the activity is not only highly on the architecture of the catalyst, but also on the type of reaction.

30. In situ Monitoring of Vapour-induced Reactivity of Metal-Organic Frameworks Using a Benchtop Powder X-ray Diffractometer

Igor Huskić, McGill University (Tomislav Friščić)

Zeolitic imidazolate frameworks (ZIFs) are a class of metal-organic frameworks (MOFs), topologically analogous to zeolites, with tetrahedrally coordinated metal ions and imidazolate ligands. Like most MOFs, ZIFs are often highly porous with large guest-accessible surface areas. Recent research results suggest that ZIFs have exceptional thermal and chemical stability, being able to withstand temperatures >500 °C, and remaining porous in boiling aqueous bases. Because of the ease of preparation and low toxicity of most ZIFs, they have been hailed as some of main candidates for gas separation, capture and storage, particularly for CO₂ scrubbing from flue gas.

We have developed a simple benchtop powder x-ray diffractometer (PXRD) setup. Using this, we investigated the stability of several zinc-based ZIFs in non-ambient atmospheres similar to flue gas environment. In the presence of water most ZIFs appear stable over a period of days or months, but in the presence of CO₂ they rapidly convert to non-porous carbonate phases. Such degradation is greatly exacerbated in the presence of ammonia, with full decomposition taking place in a matter of hours.

31. Development of bile acid-based nanoparticles for biomedical applications

Alexander Cunningham, Université de Montréal (Julian Zhu)

Physico-chemical properties frequently limit the use of recently discovered therapeutic molecules. To circumvent these issues, drug delivery nanocarriers have the potential for safe and efficient spatiotemporal delivery of therapeutic molecules. To develop successful therapeutic delivery systems, we need to improve the biocompatibility and the efficiency of drug encapsulation/release. Bile acid-based amphiphilic block copolymers offer a promising solution. Bile acids are excellent candidates for biomaterials due to their non-toxicity, amphiphilic properties, their relative abundance in nature, and the convenience of chemical modifications. We have grafted chains of poly(ethylene glycol) and poly(allyl glycidyl ether) of various lengths onto the hydroxyl groups of cholic acid via anionic ring-opening polymerization. The design of this structure aimed at improving the flexibility and stability of the micelles for dual drug and gene delivery directed towards anti-cancer treatment. Doxorubicin and siRNA were both successfully encapsulated into the nanoparticles with high amounts of loading. The formulations are stable and versatile and show great potential towards effective treatment of breast cancer.

32. Films Langmuir-Blodgett composés de polymères et de nanoparticules d'or : auto-assemblage et caractérisation

Marie-Pier Côté, Université Laval (Anna Ritcey)

Un grand intérêt est porté sur les nanoparticules d'or grâce à leurs propriétés physico-chimiques et leurs propriétés plasmoniques intéressantes pour la création d'une plateforme de détection nanostructurée. Cependant, la conception de nanostructures métalliques à faible coût avec un arrangement ordonné à grande échelle demeure un défi important. Dans ce contexte, les approches ascendantes basées sur l'auto-assemblage sont particulièrement intéressantes, malgré leur tendance à présenter une plus grande hétérogénéité que les techniques descendantes. Utilisant l'approche ascendante, la technique Langmuir-Blodgett est une avenue intéressante pour la fabrication de films monomoléculaires formés de nanosphères d'or et de polymères. Étant donné l'hétérogénéité des nanostructures, les mesures d'ensemble donnent lieu à de larges bandes plasmoniques dans les spectres d'extinction. Ainsi, l'objectif principal de ce projet est de corrélérer la structure de plusieurs nanostructures uniques avec leurs propriétés plasmoniques. Pour ce faire, la méthode d'auto-assemblage est optimisée afin de distancer suffisamment ces arrangements pour ne pas être limité par la résolution optique. Par la suite, les propriétés optiques sont sondées avec la microscopie en champ sombre, tandis que la structure est imagée par microscopie électronique de balayage. Finalement, d'autres caractérisations supplémentaires ont été effectuées afin de comprendre les propriétés d'auto-assemblage. L'intérêt de cette étude est d'identifier la structure donnant lieu à la meilleure sensibilité de détection en vue d'élaborer un dispositif bon marché.

33. Coupling of a bioreactor to a portable SPR for the synthesis and analysis of antibodies

Philippe Blain, Université de Montréal (Jean-François Masson)

When an antibody is modified, the interaction antigen-antibody may be affected. To observe the kinetic of those kinds of reactions one of the favored method is the SPR. But between synthesis of the antibody and its test in a SPR apparatus a substantial time may have passed, thus increasing the test time. This is why, the coupling of a miniature SPR and a bioreactor may be interesting. This could permit to monitor the synthesis of the antibody and its affinity to the target antigen in 'real' time.

The presentation will focus around the development of a program to find kinetic constant (K_d, K_{on}, K_{off}) and the results of the tests to minimize unspecific adsorption of antibody on multiple SAM.

34. Antimicrobial Graphene-Oxide Sponges for Water Treatment

Applications

Anya Filina, McGill University (Nathalie Tufenkji)

Access to clean, safe drinking water is critical to protecting public health worldwide. Our research group recently developed a robust, graphene-oxide based sponge with high adsorption capacity for various organic, pharmaceutical and heavy metal contaminants. The graphene-oxide sponge can be used as a filter material in both batch and continuous flow systems. In this work, the antimicrobial properties of the sponge were improved by functionalizing with natural, food-grade antimicrobial agents; namely, nisin, lysozyme and ϵ -poly-L-Lysine. Immobilization of the antimicrobial agents on the sponge surface was confirmed and the antimicrobial efficacy of the functionalized sponge was evaluated against two model organisms *E. coli* K12 and *B. subtilis* 6633. Material performance in continuous flow systems will be evaluated in the second phase of this work. Potential applications of the novel material in a water treatment context include bacterial removal and improvement of filter longevity.

35. Elucidating the effect of membrane packing on the behaviour of antimicrobial peptide GL13K

Hala Youssef, Concordia University (Christine DeWolf)

While the contribution of electrostatic interactions to the insertion of antimicrobial peptides into model membranes has been discussed extensively in the literature, there are fewer studies that elucidate the effect of membrane rigidity and packing on the interaction. GL13K is a thirteen residue, cationic antimicrobial peptide that is highly selective for both Gram-positive and Gram-negative bacteria. We probe the impact of membrane packing on the behaviour of GL13K by incorporating cholesterol (Ch) or branched diphytanoylphosphatidylglycerol (DPhPG) in negatively-charged dioleoylphosphatidylglycerol (DOPG) model membranes.

Our focus thus far has been monolayer studies coupled with spectroscopic techniques to elucidate the nature of the interaction between the peptide and the outer leaflet of lipid bilayers. We studied the interaction of GL13K with various DOPG:Ch and DOPG:DPhPG mixed lipid systems and observed a significant effect of the membrane composition on the depth of peptide insertion as well as the size of the inter-peptide β -sheet structures.

36. Electrodeposition of $\text{CH}_3\text{NH}_3\text{PbI}_3$ perovskite solar cell

Tao Liu, UQAM (Joshua Byers)

Perovskite solar cells (PSCs) have emerged as a promising renewable energy source due to their high power conversion efficiency and low-cost fabrication via solution process. However, the commonly used spin coating process induces surface defects on the deposited perovskite film by uncontrolled precipitation and inter-diffusion reaction, therefore limits their large-scale manufacturing for commercialization. Here, an electrodeposition technique is introduced to yield high-quality $\text{CH}_3\text{NH}_3\text{PbI}_3$ perovskite film. PbO_2 film is electrodeposited on TiO_2 /FTO scaffold first and then subjected to chemical bath conversion to sequentially generate PbI_2 and $\text{CH}_3\text{NH}_3\text{PbI}_3$. This process allows the easy control of film thickness and crystal grain size of $\text{CH}_3\text{NH}_3\text{PbI}_3$ to optimize morphology and electro-optical properties of $\text{CH}_3\text{NH}_3\text{PbI}_3$ film, which offers a simple, inexpensive and scalable method to improve power conversion efficiency and fabrication reproducibility of $\text{CH}_3\text{NH}_3\text{PbI}_3$ PSCs.

37. The role of cholesterol in lung surfactants in the presence of nanoparticles

Jennifer Coulombe, Concordia University (Christine DeWolf)

The role of cholesterol in lung surfactants has been puzzling researchers for a number of years as it can vary between species and with certain diseased states. The composition of lung surfactant is known to modulate its interaction with airborne pollutants such as nanoparticles. These airborne particles can enter the lungs, potentially altering lung function. This work focuses on the role of cholesterol in the interaction of nanoparticles with lung surfactant. The model system of lipids investigated was a 70:30 ratio of 1,2-dipalmitoyl-sn-glycero-3-phosphocholine (DPPC) and 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphoglycerol (POPG) to which was added 5 wt% cholesterol. Changes in function were observed using grazing incidence x-ray diffraction (GIXD), Brewster angle microscopy (BAM) and surface pressure-area isotherms. Results currently show that cholesterol affects the extent to which even small quantities of nanoparticles in the subphase (0.001 wt%) can alter lung surfactant physicochemical properties.

38. Effect of DHBA Binding Modes on the Oxidation of Iron Oxide Nanoparticle

Sinan Abi Farraj, McGill University (Amy Blum)

The potential use of functionalized super-paramagnetic iron oxide nanoparticles (IONPS) in industry and medical applications requires a thorough understanding of the ligand effect on the nanoparticles' reactivity and magnetic properties. Previous studies in this field have reported the various binding modes of dihydroxybenzoic acid (DHBA) isomers to IONP and other research has determined the effect of oxidation on the magnetic behaviour of the IONP. This study aims to determine the relationship between the DHBA ligand binding mode and the consequent degree of oxidation observed in the IONP. Using UV-vis and Fourier Transform Infrared Spectroscopy, the various binding modes of the DHBA ligand to the IONP was validated and an in-depth analysis of the rate of oxidation of the IONP was conducted using X-ray Photoelectron Spectroscopy and Powder X-ray Diffraction. Overall, This study will help further the understanding of the effect of ligand-design on the final properties of the IONP for targeted industrial applications

39. Gelation study of bile acid-based molecular hydrogel system

Puzhen Li, University of Montreal (Xiaoxia Zhu)

Gelation can take place in aqueous or organic media by the self-assembly of small molecules or polymers, producing gels with fibrillar networks. Such gels have numerous potential applications. However, conditions for gelation and the property of gels formed are not well understood. Our group studied the gelation process of a series of bile acids and their derivatives as gelators in water and proposed the "marginal solubility" theory as the pre-requisite for the formation of molecular gels. We studied the structures and mechanical properties of the molecular gels by various techniques including rheometry, transmission electron microscopy (TEM), Fourier transform infrared spectroscopy (FT-IR) and, more recently, by Nuclear Magnetic Resonance (NMR).

40. Matériaux de Haute Performance à Base de Polynorbornène

Régis Imbeault, Université de Sherbrooke (Jérôme Claverie)

Nous avons mis au point des polynorbornènes (PNBE) fonctionnalisés de haute performance à partir de procédures de synthèse simples, peu coûteuses et respectueuses de l'environnement. Ces polymères permettent la préparation d'un large éventail de matériaux fonctionnels aux propriétés thermiques, optiques et mécaniques exceptionnelles, qui surpassent la plupart des polymères commerciaux courants. Nous avons par exemple développé des thermodurcissables robustes, sans bisphénols, avec des températures de transition vitreuse (T_g) élevées ($>300^\circ\text{C}$). Ces thermodurcissables peuvent être générés sous forme de pièces épaisses, de films minces, et également sous forme de fibres via électrofilage. Les PNBE sont également d'excellents candidats pour stabiliser les nanotubes de carbone (CNTs) en solution (aqueuse ou organique) sans nécessiter l'usage de tensioactifs. Ainsi, nous avons réussi à produire par électrofilage des fibres composites formées d'une matrice à base de PNBE fonctionnalisé et d'un renfort constitué de CNTs dispersés uniformément dans les fibres. Du fait de leurs très hautes propriétés physico-chimiques et de leur faible coût anticipé, ces nouveaux matériaux peuvent d'une part rivaliser avec de nombreux produits commerciaux, tout en proposant un alternatif plus vert, et d'autre part apporter de nouvelles solutions pour des applications de pointe.

41. Doping of Mesoporous Titania Films with Silver Nanoparticles for Enhanced Photocatalytic Efficiency

Diane Rawach, Université de Sherbrooke (Jérôme Claverie)

Doping photocatalysts with metallic nanoparticles is essential for the enhancement of their photocatalytic efficiency under visible light. As suggested in the literature, the localized surface plasmon resonance of metallic nanoparticles induces a high absorption in the visible light spectral range, which can improve the photocatalytic efficiency. Photocatalysis is a promising technology that could be used to depollute water/air, to produce fuel through water-splitting and CO₂ reduction and for photovoltaic cells. Titanium dioxide is the most commonly used photocatalyst for these applications. However, its range of activity is limited to the UV spectrum, which is a major limitation to its use. Therefore, it is important to develop and improve the photocatalytic efficiency of TiO₂. To achieve this goal, we have coated TiO₂ nanoparticles on a conductive glass substrate (such as FTO) and doped it with silver nanoparticles. Electrochemical analyses and H₂ production measurements under solar simulation are performed on mesoporous TiO₂ films doped with silver nanoparticles to study their photocatalytic efficiency.

42. Hierarchical Biomimetic Lubricants for Restoring Lubrication of Cartilage: Synthesis, Surface Assembly and Lubrication Performance

Sa Liu, Université de Montréal (Julian Zhu)

Synovial joint is one of the most effectively lubricated systems in nature consisting of articular cartilage and lubrication complex with hierarchical structure formed by synergistic interaction among synovial fluid components. Osteoarthritis is a typical joint disease caused by dysfunction of cartilage lubrication, which affects mostly men and women above the age of 60. A pair of hierarchical biomimetic lubricants with the unique assembly ability with fibronectin and type II collagen in cartilage have been designed and synthesized. They are hyaluronic acid-grafted-(poly-2-acrylamide-2-methylpropanesulfonic acid sodium) (HPA) and hyaluronic acid-grafted-(poly-2-methacryloyloxyethyl phosphoryl choline) (HPM), respectively. In both cases, hyaluronic acid was used as the backbone and anionic and zwitterionic polymers were respectively grafted as side chains. Their assembly behavior were characterized by use of quartz crystal microbalance (QCM) and fluorescence confocal microscopy. HPA and HPM exhibited priority to bind with fibronectin and collagen. To determine the lubrication properties of HPA/HPM as biolubricants, native porcine hyaline cartilage was applied as the friction pairs and showed promising results. Surface force apparatus (SFA) is used to study the lubrication mechanism. Therefore, these newly developed HPA/HPM biolubricants show great potential to alleviate the conditions of osteoarthritis.

43. Growth characteristics of silica-carbonate microstructures under the influence of Chicago Sky Blue Dye

Alicia McTaggart, Concordia University (Louis Cuccia)

Spurred by lessons learnt from the ability of nature to 'design' biominerals with a high degree of control over their shape, size, mineral phase and hierarchical assemble over multiple length scales, a multitude of bottom-up research strategies have been geared towards developing self-assembled inorganic materials having superior functionality and complexity. Of particular interest are 3D nano-crystalline composite materials, characterized by long-range orientational order and highly curved surfaces, which can be synthesized from the coupled reaction of the carbonates of barium, strontium and aragonite-type calcium carbonate with silica in alkaline (pH ~10-11.9) environments under the influence of atmospheric CO₂. These silica-carbonate microstructures include cardioid sheets, helicoids, 'worms', flower-like and globular structures. In this work, we aim to show how the size and predominant morphologies of silica-carbonate microstructures can be tuned as a function of sulphonated azo dye concentration in addition to its method of incorporation in the crystallization solution. Indeed, this research also provides indirect evidence for accelerated growth rates of the microstructures from solutions containing dye as implied by an increase in size relative to control experiments without dye during a growth period of 1.5-2 hours. Directed strategies to control both shape and size are of fundamental importance since it is well-known that the chemical composition and physical properties of a material are intimately connected to its function. Light and scanning electron microscopy (SEM) are the principle tools used for the characterization of the as-formed microstructures.

44. Nanocomposites polymère/nanoparticules pour le développement de matériaux à actuation magnétique

Renaud Lussier, Université Laval (Anna Ritcey)

Les nanoparticules magnétiques font l'objet de recherche scientifique extensive due à leurs applications potentielles variées, allant de la catalyse à des applications médicales ou alors dans le traitement des eaux pour n'en citer que quelques exemples. L'échelle de taille nanométrique représente un atout essentiel à chacune de ces applications. Les nanoparticules d'oxyde de fer sont les nanoparticules magnétiques les plus utilisées grâce à leur facilité de synthèse, fonctionnalisation et dispersion dans divers médiums. Un contrôle de la taille et morphologie des nanoparticules est également possible. L'incorporation de nanoparticules magnétiques dans un polymère peut, d'une part, en permettre de contrôler ses performances mécaniques et, d'autre part, provoquer de déformation du matériau en présence d'un champ magnétique externe.

L'utilisation de polymères souple à actuation magnétique est présente dans les domaines de la microfluidique et de la biomimétique. L'objet du présent projet de recherche est le développement de membranes polymères à actuation magnétique pour utiliser comme miroirs déformables pour l'optique adaptative. Des miroirs ferrofluidiques ont précédemment été développés au sein de notre laboratoire avec de bonnes performances, mais le remplacement du ferrofluide par une membrane élastomère permettra de faciliter l'implantation dans des systèmes optiques variés. Le matériau proposé est une membrane d'élastomère de polydiméthylsiloxane dans laquelle ont été incorporée des nanoparticules d'oxyde de fer. Une seconde couche de PDMS sert de couche optique. Finalement, une couche d'aluminium nanométrique peut être déposée pour augmenter la réflectivité de la membrane. Une étude sur les stratégies de modulation des propriétés mécaniques du matériau composite par l'incorporation de nanoparticules à faibles concentrations, de la chimie de surface et de l'organisation de celles-ci est entreprise. L'ajout de nanoparticules réticulant avec les chaînes de polymères est une technique couramment utilisée pour renforcer les élastomères avec pour conséquence d'en augmenter substantiellement le module d'élasticité. Ici, nous tentons de préserver un faible module tout en augmentant la résistance aux bris du polymère.

Finalement, le développement de surfaces sensibles à l'application de champs magnétiques externes est en cours. Le principe est de faire croître une chaîne polymère sur une surface et d'y greffer une ou quelques nanoparticules magnétiques en bout de chaîne. Une application possible est de contrôler la mouillabilité de la surface avec l'application d'un champ magnétique externe. Pour ce faire, on emploie un polymère et des nanoparticules ayant une polarité différentes et on utilise le champ magnétique pour modifier la conformation des chaînes de polymères. Dans notre cas, un dérivé hydrophile de polynorbornène est synthétisé sur une surface d'or avec des nanoparticules d'oxyde de fer fonctionnalisées avec de l'acide oléique en bouts de chaînes.

45. Single phase (Co,Ni)O oxide as protective coating of Cu-Ni-Fe inert anodes for Al production

Saeed Mohammadkhani, INRS-EMT (Daniel Guay, Lionel Roue)

Canadian aluminum production is an important source of greenhouse gases (GHGs) with 6 Mt of CO₂ emitted in 2014, which is equivalent to the amount of GHG generated annually by 2 million cars. This is due to the fact that current technology uses carbon anodes that consume during the electrolysis of aluminum to form CO₂ according to the overall reaction: $\text{Al}_2\text{O}_3 + 3/2 \text{C} = 2 \text{Al} + 3/2 \text{CO}_2$. A significant reduction in GHG emissions from Canadian aluminum smelters can only be based on the emergence of new technologies. As such, the most effective solution would be to replace the consumable carbon anodes with so-called inert anodes that emit O₂ rather than CO₂ and that are based on the following overall reaction: $\text{Al}_2\text{O}_3 = 2 \text{Al} + 3/2 \text{O}_2$. This would reduce GHGs by 75 to 100% depending on the type of emissions (CO₂, CF_x, NO_x, SO_x, etc.). However, the design of inert anodes is a major challenge because of the severe conditions during aluminum electrolysis that require materials with excellent corrosion and thermal shock resistance while having the same adequate electrochemical properties.

Among inert anodes studied so far, Ni-Fe-Cu-based alloys appear to be the most promising owing to their ability to form a layer of nickel ferrite (NiFe₂O₄) on the surface of the anode upon Al electrolysis. This nickel ferrite has low solubility in a cryolithic medium. However, the formation of the nickel ferrite protective layer is slow and, depending on the experimental conditions, might not be formed fast enough to provide effective protection of the underlying substrate Cu-

Ni-Fe alloy. One strategy to help in the formation of this layer is to coat the Cu-Ni-Fe alloy with a sacrificial layer that would be stable for a period long enough to allow the formation of NiFe_2O_4 on the surface of the anode.

In this present study, $\text{Co}_x\text{Ni}_{1-x}\text{O}$ solid solutions with $x = 0.15, 0.25, 0.375, 0.5$ mol. % were prepared. Solid solutions were synthesized by either extensive (20 h) high energy ball milling of CoO and NiO powders or milling for a short period of time (15 min) of Co_3O_4 and NiO powder followed by heat treatment in air at 1000°C . The composition and crystalline structure of the compounds were determined by, energy dispersive X-ray spectroscopy and X-ray diffraction measurements. In both cases, $\text{Co}_x\text{Ni}_{1-x}\text{O}$ solid solutions were formed over the whole composition range. However, the HEBM method leads to significant contamination of the produced solid solutions due to the erosion of the WC milling tools. Thermo-gravimetric analyses (TGA) were performed to analyse the thermal stability. It was shown that $\text{Co}_{0.5}\text{Ni}_{0.5}\text{O}$ is stable at high temperature, while solid solutions with $x = 0.15, 0.25, 0.375$ decompose to Co_3O_4 and $\text{Co}_{0.5}\text{Ni}_{0.5}\text{O}$ after heating at 800°C . The use of these solid solutions as protective coatings in a cryolithic medium will be discussed.

46. Tobacco Mosaic Virus-Templated Self-Assembly of Aqueous-Stable Superparaagnetic Iron Oxide Nanoparticles into Ring Structures Using Click Chemistry

Shoronia Cross, McGill University (Amy Blum)

The development of ultradense magnetic data storage technologies requires the production of ever-smaller bits. The challenge is to build nanoscale magnetic bits, capable of being individually switched, and which can be assembled in a close-packed array with minimum bit-bit coupling. It has been shown that magnetic coupling can occur between neighboring magnetic nanoparticles (MNPs) in self-assembled nanoring structures, generating chiral, bistable domains, known as flux closure (FC) states. The magnetostatic fields within these FC states are confined within the ring structure, thus minimizing stray fields, and making MNP nanoring structures appealing as magnetic bits. Reported self-assembled MNP ring structures, however, are produced by evaporative techniques, and produce low yields of oblong, polydisperse rings with relatively large diameters, which cannot be assembled into organized arrays or layers. Constructing nanoscale assemblies with positional control at the nanometer level requires a templating method with high specificity and monodispersity, such as that offered by tobacco mosaic virus (TMV) coat protein, which, as a biomolecule, is inherently monodisperse in size, shape and surface chemistry. As a scaffold for nanoparticle self-assembly, TMV disks not only produce well-defined nanostructures, but close-packed structures wherein coupling between neighboring nanoparticles, which is essential to forming FC states, can occur. The EDC coupling reaction is utilized to conjugate propargylamine to the surface of iron oxide nanoparticles (IONP) coated in 3,4-dihydroxyphenylacetic acid (DOPAC), to yield solution exposed alkyne groups on the IONP surface (IONP-alkyne). The solution exposed N-terminal amines of the TMV disks are similarly used to conjugate 5-azidopentanoic acid to the outer surface of the TMV disk, yielding solution exposed azide groups (TMV-azide), through EDC coupling. The copper-catalyzed azide-alkyne cycloaddition (CuAAC) reaction is then applied to covalently bind the IONP-alkyne to the TMV-azide disks, in order to form templated self-assembled ring structures for further characterization and FC studies. These structures not only open novel potential avenues for the assembly of ultradense data storage devices through the self-assembly of virus-templated superparamagnetic IONPs, but also provide an assembly, upon which, the fundamentals of FC states can be studied.

47. Viedma Ripening of Conglomerate Crystals that Exhibit Racemic Twinning

Daliah Farajat, Concordia University (Louis Cuccia)

The origin of chirality and its role in biology are of great intrigue within many disciplines of science. In medicine, chirality is crucial for the binding specificity of drugs[1]. Characterizing and developing methods for chiral amplification therefore have both practical industrial applications as well as fundamental interests. The aim of this study is to explore attrition enhanced deracemization[2], also known as Viedma ripening, of conglomerate crystal systems as a means of chiral amplification. Specifically, the experiments aim to explore Viedma ripening as a means of obtaining homochiral crystals from conglomerate systems that exhibit racemic twins. Racemic twinning is clearly an obstacle for resolution methods that rely on crystallization. The conglomerates studied herein are 1-(p-toluenesulfonyl)uracil, which has been reported to form racemic twins, and 1-(1-naphthylsulfonyl)uracil, which forms homochiral crystals[3]. Our results show that homochiral crystals of both compounds can be obtained by Viedma ripening.

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48. Covalent PEDOT coating on Pt/Ir electrodes via Diazonium Chemistry

Danny Chhin, UQAM (Steen Schougaard)

Poly (3,4-ethylenedioxythiophene) (PEDOT), have recently been coated onto Pt/Ir electrodes intended for neural applications, such as deep brain stimulation (DBS). This modification reduces impedance, increases biocompatibility, and increases electrochemically active surface area. However, direct electropolymerization of PEDOT onto a metallic surface results in physically adsorbed films that suffer from poor adhesion, precluding their use in applications requiring in vivo functionality

We propose a new attachment strategy, whereby PEDOT is covalently attached to a surface through an intermediate phenylthiophene layer, previously deposited by electrochemical reduction of a diazonium salt. The two-step process was investigated on platinum disk macroelectrodes and expanded to platinum/iridium microelectrodes intended for neural implantation. The covalently attached PEDOT film maintained strong adhesion even after 10 minutes of ultrasonication (vs. 10 s for physically adsorbed PEDOT films).

49. Études des interactions physicochimiques entre nanoparticules multi-fonctionnelles et substrats biologiques

Huu Trong Phan, Université de Montréal (Suzanne Giasson)

Au cours de ces dernières décennies, des nanoparticules dites « intelligentes » à base de brosse mixte de polymères stimulables ont attiré une grande attention. Ces recouvrements permettent à aux nanoparticules (vecteurs) utilisées dans le domaine biomédical d'être sensibles à différents stimuli dans le but de contrôler indépendamment différentes propriétés (camouflage et ciblage), ce qui permet délivrer une cargaison thérapeutique au site d'intérêt de manière contrôlée et programmée. Le but de ce projet est d'étudier et d'optimiser les paramètres impliqués dans l'interaction nanovecteur-cellules, à savoir l'affinité nanoparticules-cellules, la densité surfacique des polymères, le ratio entre agents de ciblage/furtivité, le pH, la température. Pour le moment, nous avons réussi à synthétiser et caractériser une couche mixte des polymères thermosensibles sur la surface de nanoparticules d'or. En perspective, nous étudierons les interactions et la spécificité entre les nanovecteurs multifonctionnels avec des modèles de surfaces biologiques dans des conditions différentes (pH, température).

50. Synthèse et application d'une nouvelle résine fonctionnalisée pour complexer les métaux nobles

Barbara Martin, Université de Sherbrooke (Jérôme Claverie)

Une nouvelle résine fonctionnalisée avec une phosphine de Verkade[1] a été développée pour complexer et retirer les métaux, tel que le palladium, l'argent, l'antimoine et le cuivre, des polymères ainsi que des molécules organiques. Cette résine, grâce à la phosphine de Verkade, permet une forte complexation des métaux et est très peu coûteuse, facile à produire même à grande échelle et recyclable.

La catalyse au palladium est très utilisée pour la synthèse de produit organique et la création de lien carbone-carbone, grâce aux réactions de couplage de Heck, Suzuki ou encore Stille. Ce type de catalyse peut aussi être utilisé pour faire des polymérisations comme pour le P3HT, qui est l'un des polymères conjugués les plus utilisés pour les cellules photovoltaïques organiques, ou encore pour le polynorbornène[2] qui est un polymère développé dans notre laboratoire et qui possède de très bonne propriété mécanique, thermique et de dispersion.

Le problème majeur de ces catalyses homogènes au palladium est que le catalyseur reste piégé dans le produit final, le catalyseur, très coûteux, n'est donc pas réutilisable. De plus il peut provoquer des problèmes de santé (réactions allergiques, irritation de la peau, dommage au foie, rein et système nerveux central) et des baisses de performance dans les cellules photovoltaïques, ce qui pose un problème pour de nombreuses applications.

La résine que nous avons développé permet donc de facilement retirer les métaux à la fin de la réaction de couplage ou de polymérisation et de récupérer le palladium qui pourra ensuite être recyclé et réutilisé.

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51. Zinc oxide nanowires as antibacterial coatings

Nicholas Lin, McGill University (Nathalie Tufenkji, Christopher Moraes)

Hydrothermal growth of zinc oxide (ZnO) nanowires provides scalable antibacterial coatings with low toxicity towards mammalian cells. In this work, we annealed ZnO nanoparticles onto glass at several seeding densities to achieve a range of ZnO nanowire thicknesses and surface coverages. Hydrophobicity, or water repellency, of the ZnO nanowire coatings increased with increasing surface coverage. Moreover, using the Gram-positive bacterium *Bacillus subtilis* as a model organism, we found that a low surface coverage was more bactericidal, killing surface-attached cells in 20 mins, but a high surface coverage was more preventative of *B. subtilis* attachment. This suggests that ZnO nanowire coatings can be prepared for various antibacterial specifications by simply adjusting the initial seeding density before hydrothermal growth.

52. pH- and photo switching studies of poly(acrylic acid-co-coumarin) as well as its brushes grafted to silica surfaces

Hu Zhang, University of Montreal (Will Skene, Suzanne Giasson)

We report the preparation of a responsive poly(acrylic acid-co-7-(2-methacryloyloxyethoxy)-4-methylcoumarin) (P(AA-co-CMA)) copolymer by reversible addition-fragmentation chain-transfer (RAFT) and its brushes grafted from silica substrates. For the P(AA-co-CMA) copolymer, it can be prepared either by hydrolyzing the tert-butyl group postpolymerization or by polymerizing directly from acrylic acid and coumarin monomers. The photo-responsive behaviors of the hydrophilic and hydrophobic were investigated by UV-Vis absorption spectroscopy in tetrahydrofuran (THF) and water. In solution, the copolymers could be reversibly cross-linked and de-cross-linked using two different wavelengths of light. The results demonstrate that the cross-linking density can be adjusted with irradiation time (or the intensity). Although the photocleavage of coumarin photodimers appeared incomplete, a reversible photocontrol of the crosslinking density could be achieved to a certain degree. With the polymer solution repeatedly exposed to alternating UV light at $\lambda > 310$ nm and λ 260 nm for 10 cycles, the reversible change in the dimerization degree (cross-linking density) was observed.

53. Nanoscale characterization and interfacial crystallization of natural hollow milkweed fibers reinforced PCL/PVC

Phuong Nguyen Tri, ETS (Claudiane Ouellet-Plamondon)

This work reports the nanoscale characterization of the structure of milkweed fibers, which have special properties due to their superlight weight, natural superhydrophobic and hollow properties. AFM-IR in combination with high resolution SEM are used to analyse the morphology and chemical composition at the nanoscale of milkweed fibers in order to provide a better understanding their structure, especially on the fiber surface. The extraction of wax by chloroform will be done and then quantitatively analyzed by GS-MS to achieve chemical composition and provide a model for the molecular assembly of these compounds. The effect of fiber morphology on the interfacial crystallization and segregation at the interface of the PCL/PVC blend will be highlighted.

54. Fabrication de capteurs imprimés de H₂S à base de PEDOT:PSS et d'acétate de cuivre sur substrats flexibles

Najet Belkhamssa, ETS (Ricardo Izquierdo)

Au cours des dernières années, l'électronique imprimée a gagné beaucoup d'intérêt en raison des avantages que son utilisation pourrait entraîner. Parmi ceux-ci, il y a la réduction de la complexité ainsi que du coût de fabrication et une polyvalence dans les dispositifs conçus. Parmi les matériaux organiques conducteurs existants, le PEDOT:PSS s'est avéré prometteur pour la fabrication de dispositifs imprimés flexibles et même transparents. Le travail présenté ici est axé sur l'élaboration d'un capteur imprimé flexible de H₂S et la caractérisation de sa couche sensible à base de PEDOT:PSS et d'acétate de cuivre. La caractérisation complète du composé organique (PEDOT:PSS et acétate de cuivre) est présentée, telle que la spectroscopie UV-visible, infrarouge à transformée de Fourier (FTIR), tout comme les propriétés conductrices du mélange. Une optimisation de cette couche a été faite en fonction des ratios d'acétate de cuivre et de PEDOT:PSS. L'optimisation de la concentration en cuivre entre 0.083 mM et 1 mM permet une augmentation de la conductivité passant de $4 \times 10^{\text{TEXT}}-6 \text{ S cm}^{-1}$ jusqu'à 0.001 S cm^{-1} . Ce mélange a ensuite été déposé sur un substrat flexible de PET sur lequel des électrodes d'aluminium avaient préalablement été imprimées par la méthode de transfert thermique. Les résultats des changements de propriétés électriques après une exposition au H₂S de la couche sensible du composite PEDOT:PSS et acétate de cuivre sont présentés. Une fois optimisé, ce type de capteur imprimé pourrait facilement être intégré à un système à utilisation unique, telle une couche, permettant la détection de gaz libéré par de la matière fécale.

55. Epitaxial (100) (Ir,Ni)O₂ thin films prepared by pulsed laser deposition for the oxygen evolution reaction

Gaetan Buvat, INRS-EMT (Daniel Guay)

Considered as a promising way to store renewable energy, water electrolysis is limited by the slow kinetics of the Oxygen Evolution Reaction (OER). Materials which are able to decrease the overpotential are then required, and in this regard iridium and ruthenium oxides are the most active electrocatalyst. However, their high cost and low abundance make these materials unsuitable for large scale applications. One alternative is then to limit the amount of the precious metals by substituting them with another electroactive compound/element.

To design new materials, invaluable information can be obtained through the use of single crystals and well oriented thin films. Several studies have shown how the surface structure determine the reaction mechanisms and performance of a material. For example, Stoerzinger et al. have reported that the (100) surface of IrO₂ and RuO₂ is more active in alkaline environments than the most thermodynamically stable (110) surface[1].

Based on these considerations, we decided to explore the Ir-Ni-O system and to take advantage of the Pulsed Laser Deposition technique (PLD) to synthesise single crystalline thin films of Ir_{1-x}Ni_xO_{2-δ}. Fifteen atomic percent of Ni in IrO₂ oriented along the (100) surface allows to increase by almost two decades the current density of the parent compound. These results will be presented in this communication and a correlation will be established between the structural and physico-chemical properties on one side, and the electrochemical characterization and OER performances on the other side.

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56. Using polymeric encapsulation for the design of a stimulus-responsive cement

Kevin Daoust, Université de Sherbrooke (Jérôme Claverie)

Precise control over cement hydration kinetics is essential for the fabrication of any concrete structure. Too slow or too rapid settling times can result in catastrophic deterioration of mechanical properties and significant cost increase. In this communication, we present a polymeric nanoencapsulation strategy for the fabrication of a cement with a built-in heat or pH-triggered hydration mechanism. Conceptually, the cement will not settle in the presence of water until it is triggered by the stimulus. Once the trigger is applied, it will settle at virtually the same rate as the non-encapsulated cement.

To achieve this goal, we have encapsulated the cement particles with a nanoencapsulation technique based on RAFT (Reversible Addition Fragmentation chain Transfer) polymerization, resulting in cement particles which are uniformly covered by a layer of polymer of tunable thickness. We have first explored the fabrication of a cement encapsulated by a

copolymer of styrene and maleic anhydride which is insoluble in water at neutral pH, but water soluble at basic pH. The polymeric capsule prevents the cement hydration and settling unless base is added the medium. In another approach, we have tuned the T_g of the polymeric capsule slightly above room temperature so that moderate heating becomes necessary to trigger settling.

57. Nanodisk arrays for environmental Raman sensing

Benjamin Charron, Université de Montréal (Jean-François Masson)

Our research is based on a plasmonic nanostructured surface. The nanostructure is an array of silver nanodisks coated with a bilayer film of silver and gold. It benefits from coupling of the gold film's propagative surface plasmon (PSP) with the array's Bragg vector. The resonance between the PSP and the Bragg vector gives rise to Bragg mode which amplifies local plasmonic field on the edges of the disks.

Arrays with different composition were fabricated with photolithography to evaluate both if the composition affected the plasmonic band's wavelength and which composition enhanced Raman scattering the most. Promising result were obtained, demonstrating a constant plasmonic band position and a great enhancement for some of the sensors.

58. Detection of Nanoscale Phase Separation in Nanoparticles with Mixed Ligand Shells

Brenda Guzman, McGill University (Linda Reven)

Spontaneous phase separation has been detected in mixed ligand shells of nanoparticles for both low molecular weight and polymeric ligands. Although there is growing interest in such 'patchy nanoparticles', the majority of the studies have been theoretical rather than experimental due to difficulties in preparing significant quantities of nanoparticles with controlled ligand compositions. Experimental validation has also lagged to due to the lack of appropriate tools to detect nanoscale phase separation. Here we apply NMR methods developed for characterizing heterogeneities in complex materials on different length scales to nanoparticles with polymer and low molecular weight mixed ligand shells. The mixed ligand shells consisted of different ratios of aromatic (polystyrene or phenyl) and aliphatic (polyethylene oxide or dodecyl) phosphonic acids on 4 nm ZrO_2 nanoparticles. The results for 1H NOESY, $1H$ double quantum MAS, 1H spin diffusion and 1H - ^{13}C HETCOR NMR experiments on the nanoparticles with polymer versus small molecule ligand shells were compared. In the case of the low molecular weight mixed ligand shells, model systems consisting of Janus particles or physical mixtures of nanoparticles functionalized with only one ligand were studied to calibrate the $1H$ spin diffusion experiments originally developed for polymeric materials.

59. From Oxidative Mechanochemistry to Accelerated Ageing: Solid-State Assembly of Al-Based Molecular and Supramolecular Materials

Jean-Louis Do, Concordia University, McGill University (Louis Cuccia, Tomislav Friščić)

Due to its low molecular weight, abundance, and well-studied chemistry,[1] the inclusion of aluminium (Al^{3+}) in and its use as a model metal for functional materials is desirable.[2,3] Aluminum chemistry, however, has largely been confined to the solution phase and the use of soluble salt precursors. In contrast, aluminum metal, despite its value and availability as a resource for academic and industrial applications, has not been widely considered as a source of reactive aluminium due to the non-trivial nature of its activation. Such processes have traditionally required harsh conditions including, but not limited to, the use of high temperatures as well as strongly acidic or alkaline conditions.[4]

Mechanochemistry and accelerated ageing have previously been shown to enable the chemical activation and transformation of extremely inert starting materials[5] without the need of bulk liquids and has gained attention in recent years as means to reach unique, cleaner, and more efficient reactivity.[6,7] Herein, we present our results in the development of a solvent-free, solid-state approach to the activation of aluminum metal. Utilizing widely available and non-specialized reagents, we are able to conduct rapid and mild transformations of aluminium metal into a variety of molecular and supramolecular materials.

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60. Electrochemically modulated fluorescence turn-on of TEMPO pre-fluorescent derivatives

Thibault Amiaud, University of Montreal (Will Skene)

Electroactive compounds are materials that undergo reversible electrochemistry. When electroactive compounds are highly conjugated, they undergo color changes that can be visually tracked by the common user when either electrochemically oxidized or reduced. The fluorescence of convention fluorophores can also be switched off electrochemically. However, there is still a challenge to turn on the fluorescence electrochemically of otherwise quenched fluorophores. The synthesis of an electroactive pre-fluorophore coupled with radical TEMPO will be presented. Its electrochemically mediated fluorescence will be shown.

61. Synthesis and characterization of n-type CuGaS_2 nanoparticles for water splitting application using visible light

Kassoum Sangare, UQAM (Benoît Marsan)

In this work, Ga-doped CuGaS_2 nanoparticles were successfully synthesized via a colloidal technique using GaCl_3 , Li_2S and CuCl as Ga^{3+} , S^{2-} and Cu^+ precursors, respectively, in N-methylimidazole solvent. After filtration and annealing under argon at 600 °C for 2 h, XPS, EDX and ICP-AES analyses revealed an excess of gallium with bulk Ga:Cu ratio of 1.02 and surface ratio even greater. The as-synthesized CuGaS_2 X-ray diffraction studies confirmed a pure chalcopyrite crystalline phase with crystallite size of ca. 17.2 nm. UV-visible measurements showed that Ga-doped CuGaS_2 has a direct bandgap energy of 2.41 eV. Capacitance measurements carried out on as-synthesized CuGaS_2 films in aqueous 0.5 M KOH electrolyte, using electrochemical impedance spectroscopy, confirmed the n-type conductivity. The material Fermi level was found to be -0.78 V vs Ag/Ag^+ , while the corresponding majority charge carrier density was calculated to be $8.6 \times 10^{17} \text{ cm}^{-3}$. The valence band maximum energy and the conduction band minimum energy were determined to be -6.31 eV and -3.90 eV, respectively. The photoresponse of Ga-doped CuGaS_2 films deposited onto FTO conducting glass substrates was studied in aqueous 1 M Na_2SO_3 electrolyte using a solar simulator.

62. New cobalt sulfide catalyst material for hydrogen production

Hayet Cherfouh, UQAM (Benoît Marsan)

The electrolysis of water uses electricity to split the water molecules into hydrogen (H_2) and oxygen (O_2) gases. This process corresponds to the reverse reaction used in H_2/O_2 fuel cells. Water splitting by the photoelectrochemical process uses a semiconducting electrode material (usually the photoanode) and a conductive catalytic material (cathode) immersed into an aqueous electrolyte. The semiconductor acts as a catalyst on which the photogenerated electrons and holes participate, respectively, in reduction and oxidation reactions[1]. This work aims at studying cobalt sulfide (CoS) as a (photo)catalyst material for the production of hydrogen from an aqueous medium[2]. CoS possesses remarkable electrocatalytic properties and this material is much less expensive than platinum which has a limited earth abundance[3]. CoS films were prepared by electrodeposition onto a conductive glass substrate (FTO: fluorine-doped tin oxide/glass), combining several experimental conditions (pH of solution, time of deposition, etc). Scanning electron microscopy (SEM) images show that the morphology of CoS films is uniform and that the catalyst particles are adhering well to the FTO/glass substrate. The energy dispersive X-ray (EDX) spectroscopy analysis confirms the presence of the expected elements, composed of cobalt and sulphur for CoS, with signature of tin and oxygen for the substrate, and traces of carbon. The estimated Co/S atomic ratio is about 2, which suggests an excess of Co over S. The transmittance and electrical measurements of CoS films, determined respectively by UV-Visible spectroscopy and electrochemical impedance spectroscopy, show quasi-transparent (~80 %) and low resistive (~11 μ) films. Potentiodynamic measurements (from -0.5 V to -2.5 V vs Ag/AgCl) carried out in aqueous 0.5 M K_2SO_4 electrolyte show an increase in the current when the potential becomes more negative with significant production of H_2 . Photocurrent-potential measurements, obtained using a solar simulator and a potentiostat, show a small increase in the cathodic photocurrent (~0.6 mA) recorded for CoS films at -1.6 V vs Ag, suggesting that CoS material has more catalytic than photocatalytic properties.

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63. Removal of Copper(II) from aqueous solutions by chitosan electrospun nanofibers in a fixed-bed adsorption column

Malak Didouh, UQTR (Bruno Chabot, Éric Loranger)

Water is fundamental to life but also essential to wealth of countries contributing to all aspects of personal welfare and economic life. Industries are among the largest water user in Canada. However, they are also producing large volumes of wastewaters containing various types of contaminants and particularly toxic substances such as heavy metals. To ensure sustainability of the resource, removal of heavy metals from wastewater is mandatory. Activated carbon adsorption is one of the most effective processes to remove them from aqueous solutions. However, the high cost of activated carbons can limit their applications. Therefore, there is a growing need to find cheap and effective alternative sorbents to activated carbon. This study is focusing on the development of a porous chitosan electrospun nanofiber mat for adsorption of Copper(II) in aqueous solution using a fixed bed adsorption column. Chitosan is well known for its improved affinity for heavy metals. However, electrospun chitosan nanofiber membranes are too weak to withstand flow conditions in a fixed-bed column. We have thus developed a composite material combining a thin porous electrospun mats with a rigid support to improve strength properties. Subsequently, a dynamic adsorption study was carried out on an experimental setup to determine the effect of the initial concentration and the flow rate on the breakthrough curves. Empirical and mathematical simulations were conducted in order to predict the breakthrough behavior for other process conditions. Results are promising and demonstrate the ability of the chitosan electrospun nanofiber composite material to adsorb heavy metals under dynamic conditions.

64. Investigating Catalytical Behavior of Ag-Nanorings on Hydrogen Evolution Reaction

Yani Pan, McGill University (Janine Mauzeroll)

The growing energy crisis and current state of pollution have made searching for clean energy extremely important for modern industry. Hydrogen energy is a clean energy and has attracted great attention to potentially solve the environmental problems. Since Fujishima's groundbreaking work on utilizing TiO_2 electrode to catalyze water-splitting

reaction in 1972, a series of semiconductors were developed as photocatalysts to produce hydrogen, which represents an excellent strategy to transform solar energy into chemical energy.

However, catalysts solely based on semiconductors suffer from low efficiency due to inherent limitations. One strategy to enhance the efficiency of solar energy utilization is to incorporate the plasmonic noble metallic nanostructure into the semiconductor. By varying the size and shape, these plasmonic nanomaterials have the potential to shift light absorbance to visible region and they have been used in photocatalysis due to their well-known surface catalytic properties like the localized surface plasmon resonance (LSPR) effect.

As one of the most abundantly used noble metals, silver nanoparticles are generally supported on semiconductor substrates for plasmonic catalysis. In this work, we aimed at exploring the possibility of using isolated silver nanostructures for photocatalysis. The tobacco mosaic virus (TMV) coat protein was used as a command surface to grow and assemble silver nanorings into sub-30 nm rings. These are the smallest silver nanorings to date. In the ring structure, the neighboring particles have in-plane coupling properties, which made them have the potential to show better performance in photocatalysis. They were tested for water splitting reaction. In addition, comparisons were made with pure free silver nanoparticles for the same reaction.

65. A Thermodynamic Map for the Rational Design of Thermoresponsive Polymers in Aqueous Solution

Chuanzhuang Zhao, Ningbo University (Julian Zhu)

Thermoresponsive polymers have drawn much attention of researchers due to their potential applications in many different areas. To tailor properties of such materials to meet the practical requirements, the rational design of the polymers is necessary and important. In this presentation, we propose a thermodynamic map to guide the rational design of thermoresponsive polymers. The map is a plot with the mixing enthalpy (ΔH_m) and mixing entropy (ΔS_m) as its two axis, and is divided into four regions: UCST, insoluble, LCST and soluble. We are going to summarize how ΔH_m and ΔS_m are affected by those supramolecular interactions in polymer aqueous solutions, such as: hydrophobic interactions, hydrogen bonding and ionic interaction. Accordingly, the location of a designed polymer on the map and its responsive temperature ($T_c = \Delta H_m / \Delta S_m$) can be determined. Validity of this thermodynamic map is exemplified by our recent results on the designing of UCST polymers from non-responsive monomers, such as acryl acid, acryl amide, and acryl nitrile.

66. Residual Chirality in Carbon Dots from Enantiomers of Amino Acids

Florence Victoria, Concordia University (Rafik Naccache)

Carbon Dots (CDs) are one of the new members in the carbon nanoparticle family. They are primarily composed of amorphous sp^2 carbons with sizes ranging within 10 nm. These nanoparticles have demonstrated excellent tunable fluorescence, low toxicity, chemical inertness and biocompatibility. These versatile properties of CDs are determined by the starting materials and they can be synthesized from various carbon sources and passivating agent. As such, we are interested in exploring residual chirality in these carbon nanomaterials by starting with chiral amino acid precursors. This is due to the fact that chirality has been very important in pharmaceutical research for drug development and design, as well as in applications of organocatalysis, enantioselective recognition and chiral sensing. We report a facile, one-step microwave-assisted synthesis of chiral CDs from both enantiomers of cysteine, serine, and alanine.

67. Biocompatible Ratiometric Temperature Sensing in Dual-Emitting Carbon Dots

Jun-Ray Macairan, Concordia University (Rafik Naccache)

Temperature sensing in an organism is crucial in the development of diagnostic and therapeutic tools. Thermometry can be used for early detection of cancers, inflammations and diseases which include localized temperature irregularities. The recent advancements in field of nanomaterials have propelled research groups into making nanoparticles for various

applications such as drug delivery, biosensors and bioimaging. Herein, focus is put on nanothermometry using carbon dots. These carbon-based nanoparticles possess attractive properties for biological applications (high biocompatibility, low cytotoxicity, versatile optical properties, water soluble, etc.). In this project, dual-emitting carbon dots are synthesized using a one-step microwave-assisted reaction. With its unique dual-emitting character, monitoring for temperature can be accomplished via ratiometric measurements of the two emissions.

68. Metal-Induced Fluorescence Quenching in Carbon Dots for Sensing Applications

Farah Noun, Concordia University (Rafik Naccache)

Heavy metal contamination from anthropogenic sources is a great environmental concern. This research focuses on the development of a novel, cheap and green method for heavy metal capture using carbon dots, fluorescent nano-spheres composed primarily of carbon and oxygen. The photoluminescent properties of both functionalized and un-passivated carbon dots will be exploited to develop quenching assays as both qualitative and quantitative indicators for successful heavy metal capture. The quenching mechanism in both selective and non-selective metal binding will then be determined through ultra-fast spectroscopy techniques.

69. Solid-state NMR and Electrochemical Dilatometry Study of Charge Storage in Supercapacitor with Redox Ionic Liquid Electrolyte

Yanyu Wang, Université de Montréal (Dominic Rochefort)

Redox ionic liquids are emerging as promising new electrolytes for supercapacitors, which provide higher capacitance and energy density than organic or ionic liquid electrolytes. The fundamental studies of charge storage mechanism in supercapacitors are of critical importance for the development and applications of devices. Solid-state NMR (SS-NMR) methodology that has the ability to give atomic information on local environments within electrodes has been recently developed to study the mechanism of charge storage in supercapacitors at molecular level. The charge storage in supercapacitors with organic or ionic liquid electrolytes has been studied by SS-NMR. However, there is until now no research on charge storage mechanism in supercapacitors with redox-active electrolyte published. The studies of charge storage mechanism in supercapacitors with redox ionic liquids electrolyte are therefore highly required. In this context, we employ SS-NMR techniques combined with electrochemical dilatometry measurements that are associated with charge induced strain of electrode to investigate in depth the charge storage in supercapacitors during charging process. It is revealed that the charging process of supercapacitors with redox ionic liquid electrolyte EMIM FcNTf/ACN is driven by different charge regimes for different voltages, that is, charge storage on positive electrode occurs via co-ion desorption at low voltage range and subsequently counter-ion adsorption at higher voltage range, whereas charging on negative electrode occurs exclusively by counter-ion adsorption over the studied voltage range. The electrochemical dilatometry measurements show macroscopic dimensional change of the electrodes during charging and further confirm the proposed mechanism obtained from SS-NMR. The results give a detailed picture of the charging mechanism of supercapacitors with redox ionic liquid electrolyte, providing new insights on the charge storage of supercapacitors.

70. Kinetic Isotope Effects Provide Experimental Evidence for Proton Tunneling in Methylammonium Lead Triiodide Perovskites

Yan-Fang Chen, INRS-EMT (Emanuele Orgiu)

The occurrence of proton tunneling in MAPbI₃ hybrid organic inorganic perovskites is demonstrated through the effect of isotopic labeling of the methylammonium (MA) component on the dielectric permittivity response. Deuteration of the ammonium group results in the acceleration of proton migration (inverse primary isotope effect), whereas deuteration of the methyl group induces a normal secondary isotope effect. The activation energies for proton migration are calculated to be 50 and 27 meV for the tetragonal and orthorhombic phases, respectively, which decrease upon deuteration of the ammonium group. The low activation barrier and the deviation from unity of the ratio of the pre-exponential factors ($A_H/A_D = 0.3-0.4$) are consistent with a tunneling mechanism for proton migration. Deuteration of the PEDOT:PSS hole transport layer results in a behavior that is intermediate between that of the deuterated and undeuterated perovskite, due to extrinsic ion migration between the two materials.

71. Self-organization of polymer nanostructures and their transition from continuous fibers to aligned dots over large areas

Ilknur Eryilmaz, INRS-EMT, UQAM (Emanuele Orgiu)

This presentation will describe the controlled characterization of PMMA nanofibers and nanodots with a novel wet-processing method able to deliver in minutes over the large areas, effective on both polymers and carbon nanotubes, termed ASB-SANS (Auxiliary Solvent-Based-Sublimation Aided NanoStructuring)[1]. This technique serves as a versatile nanofabrication tool in order to achieve nanopatterns in desired morphology on the substrate at room temperature and standard atmosphere. In particular, we show how it is possible to control the topologic transition from continuous fibers to aligned dots via simply tuning the ternary solution composition which consists of a target material, an auxiliary solvent, and a sublimating substance. Here the focused points will be the preparation method, characterization and application of achieved patterns as lithographic masks[2]. Moreover, the fibers/dots width and inter-pattern distance variations have been analyzed qualitatively with respect to the composition and relation between the morphology and the composition displayed in the ternary diagram. The sizes and relative distances of the formed patterns appear to be an exponential decay function of the relative concentration of the auxiliary solvent in the composition show consistency with the well-known polymer chains diffusion laws. In the sequel, some of the produced patterns have been used as masks for a substrate (Si/native SiO_x) and submitted to Inductively Coupled Plasma-Reactive Ion Etching (ICP-RIE) lithographic process. This process evidenced that the patterns transfer their features to underlying substrate with remarkable aspect ratios over areas as large as several millimeters square which shows an interesting potential of ASB-SANS in practical applications in photovoltaic (as light trapping surfaces)[3], surface-enhanced sensors[4,5] and plasmonics[6].

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72. Templated Synthesis of μm -long Ni nanowires for O₂ evolution

Minghui Hao, INRS-EMT (Daniel Guay)

Electrochemical water splitting is recognized as a promising technology for sustainable energy conversion. To promote the apparent catalytic oxygen evolution reaction (OER), various types of nanostructures were developed based on non-noble transition metals[1]. In this work, arrays of Ni nanowires (Ni NWs) were synthesized using template electrodeposition through a porous Aluminium anodic oxide (AAO) membrane. Following AAO dissolution, arrays of Ni NWs are observed, with uniform diameter (ca. 300 nm) and lengths varying from 2 to 20 μm according to the electrodeposition duration. Extensive electrochemical characterization of these 1D-Ni nanostructures revealed enhanced electrochemically active Ni surface area, as assessed by the coulombic charge involved during the potentiodynamic formation of $\alpha\text{-Ni(OH)}_2$ [2]. Both OER activity and OER stability in 1M KOH electrolyte are also found to be enhanced due to the 1D nanostructure. Following extensive oxygen evolution, nanoscale surface roughness was observed along the whole length of NWs, demonstrating that O₂ gas evolution is not restricted to the utmost external surface of NWs. This is confirmed by electrochemical impedance spectroscopy measurements. The OER performances of these Ni NWs will be presented.

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2. M. Alsabet, M. Grden, et G. Jerkiewicz, *Electrochemical Growth of Surface Oxides on Nickel. Part 1: Formation of $\alpha\text{-Ni(OH)}_2$ in Relation to the Polarization Potential, Polarization Time, and Temperature*, *Electrocatalysis*, vol. 2, no 4, p. 317-330, déc. 2011.

73. Studying the Diffusion Properties of Li^+ in Li-ion Battery Cathodes

Jeremy Dawkins, McGill University (Janine Mauzeroll)

With the consequences of climate change being at an unprecedented high, many attempts are being made to reduce the carbon footprint of nations worldwide, as exemplified by the Paris Climate Agreement of 2015. At the heart of most of these discussions is the goal to replace fossil fuel based energy sources with renewable energy sources such as wind and solar. The problem with these energy sources are their inconsistent energy outputs throughout the day, which often do not coincide with peak-hours of energy consumption. In order to solve this fundamental problem, energy storage solutions such as batteries are required. Lithium ion batteries (LiB) are currently one of the best contenders in this field because of their high reliability and energetic capacity. There is, however, room for improvement in LiB, considering a substantial amount of energy is wasted on charge and discharge cycles because of sources of overpotential. One of these overpotential sources is the slow diffusion of Li^+ ions within the battery, a value described by the Li^+ apparent diffusion coefficient D_{Li^+} . The intent of this project is to develop a reliable and robust method to determine D_{Li^+} . This would allow for the characterization of the Li^+ diffusion coefficient in current and new battery cathode materials.

74. Bactericidal Mechanisms of MoS_2 Nanosheets - Langmuir Schaefer Films

Jack Minchom, McGill University (Nathalie Tufenkji)

Molybdenum disulfide (MoS_2) nanosheets demonstrate potential for the development of novel antimicrobial materials; yet, no studies have explored the formation of thin films or coatings using these nanosheets. Three antimicrobial mechanisms for MoS_2 nanosheets have been proposed, including physical piercing, reactive oxygen species (ROS) dependent oxidative stress, and ROS independent oxidative stress. The motivation for this work was to develop antimicrobial films consisting of flat MoS_2 nanosheets to isolate the oxidative stress mechanisms. The Langmuir-Schaefer technique was used to create thin films of MoS_2 nanosheets on a polystyrene substrate. The aggregation of the MoS_2 nanosheets in NaCl enabled the high surface pressure formation of the films above the water subphase. The antibacterial performance of the films was evaluated against model bacterial species in the absence of nanosheet edge effects. Future work will investigate the bactericidal mechanisms of the film including ROS-independent and dependent oxidative stresses measured by fluorescent probes.

75. Étude de la contribution des métaux de transition dans la structure locale du $\text{LiMn}_x\text{Fe}_{1-x}\text{PO}_4$

Laurence Savignac, UQAM (Steen Schougaard)

Le développement de batteries à haute performance contribue à l'amélioration de l'efficacité du stockage d'énergie dans le domaine de l'énergie durable. Dans l'élaboration de matériaux de cathode à haute densité énergétique, un enjeu majeur est la conséquence de l'incorporation de métaux de transition sur la structure. Ce facteur est d'autant plus important considérant le processus de transition de phase auquel la structure olivine est assujettie lors de la désintercalation/intercalation des ions lithium. Dans l'objectif de distinguer la contribution respective du Mn et du Fe dans l'environnement local du groupement phosphate, ces travaux font l'étude des modes de vibrations du PO_4 dans le $\text{LiMn}_x\text{Fe}_{1-x}\text{PO}_4$ pour différentes compositions en manganèse. Plus spécifiquement, la spectroscopie infrarouge à réflectance totale atténuée (ATR-IR) a été utilisée en considérant la symétrie du tétraèdre PO_4 pour sonder des elongations symétriques ('1), asymétriques ('3) ainsi que les déformations dans le plan symétriques et asymétriques ('4). Un élément clef de cette étude est la synthèse à l'état solide et l'utilisation de matériaux avec un ratio contrôlé de métaux de transition. La structure cristalline de chaque produit a été analysée par diffraction des rayons X (DRX) puis la relation linéaire entre les paramètres de maille et la composition en Mn a permis de confirmer l'incorporation homogène du manganèse dans la structure par la loi de Vegard.

76. Detection of Manganese Ion Dissolution from Battery Materials in an Air-Free Environment using Anodic Stripping Voltammetry

Mojgan Hatami, UQAM (Steen Schougaard)

In recent years, the use of manganese in positive electrode materials in lithium ion batteries (LIBs) has seen increased interest. LiMn_2O_4 is an excellent candidate, displaying excellent electrochemical performance, while also being lower cost and less toxic than LiCoO_2 . However, this material also has several disadvantages, including poor capacity retention during charge-discharge cycling or storage, particularly at elevated temperatures. One possible explanation for this poor capacity retention is the dissolution of manganese into the electrolyte solution, thereby compromising the structure of the positive electrode material. Confirmation of this hypothesis requires the detection of manganese ions in the electrolyte solution of LIBs.

Anodic stripping voltammetry (ASV) is a well-established electrochemical technique capable of detecting heavy metals in solution at low concentrations. By combining this technique with scanning electrochemical microscopy (SECM), it should be possible to measure the concentration of Mn^{2+} ions in solution, while also providing spatial resolution. Furthermore, in order to be relevant to LIB systems, these ASV-SECM measurements should be performed in an inert atmosphere (i.e. glovebox), rather than in aqueous solutions.

Using 25 μm Pt disk microelectrodes as a backbone, we electrochemically deposited a mercury drop onto the tip, forming Pt/Hg microelectrodes in a glovebox. These Pt/Hg microelectrodes were characterized using optical microscopy, as well as electrochemically using methyl viologen as a redox mediator. In 5 mM $\text{Mn}(\text{Cl})_2$ solution, we demonstrate that these SECM tips can successfully detect Mn^{2+} ions in propylene carbonate (PC), including both amalgamation and stripping peaks. Ongoing research efforts include performing calibration curves with standard solutions of manganese and measuring the dissolution of manganese from a LiMn_2O_4 positive battery electrode.

77. Using Resonance Raman to study measure exciton-ligand vibronic coupling in colloidal CdSe nanocrystals

Timothy Mack, McGill University (Mark Andrews, Pat Kambhampati)

Resonance Raman (RR) spectroscopy is an effective tool for probing the extent the exciton-phonon coupling in colloidal semiconductor nanocrystals (NCs); however, there are conflicting reports in the literature of whether exciton coupling to covalently bound surface ligand vibrational modes can be observed. Recent theoretical and computational studies have posited that such couplings can occur through resonance with ligand-nanoparticle charge-transfer states, particularly in the case of asymmetric vibrational modes of ligands with states that lie within the semiconductor bandgap. Such couplings are predicted to lead to large enhancements of the Raman scattering of certain ligand modes.

Here we show Raman spectra of ligands covalently bound to the surface of 2-5 nm colloidal CdSe NCs through resonant excitation of the NC. The strong observed Raman scattering of the ligand modes appears to be consistent with theoretical prediction. To conduct these measurements, we use the cheap and commercially available capping ligand thiophenol (PhS), which is a widely employed surface-enhanced Raman scattering molecular tag. PhS conveniently mitigates the strong background photoluminescence which generally impedes RR measurements of semiconductor nanocrystals. It is also effective at displacing commonly used native phosphonic acid or amine ligands at room temperature, thus avoiding the use of higher temperatures which may lead to unwanted CdS shell growth. The approach is simple and can be employed on CdSe nanocrystals synthesized within our group, as well as commercially available samples. Furthermore, this strategy may be made generally applicable to study exciton-ligand interactions in a variety of semiconductor NC materials.

78. Towards perpetual Dynamic Component Exchange Using A Surface immobilized Anchor for Azomethine Substitution

Michael Lerond, Université de Montréal (William Skene)

An aryl aldehyde was grafted onto an ITO coated glass substrate and it served as an anchor for preparing electroactive azomethines. The reversibility of the covalent $\text{N}=\text{H}$ bond was exploited for dynamic component exchanges. The immobilized azomethines underwent multiple step-wise component exchanges with different arylamines. We first studied the capacity of the azomethines to be reversibly hydrolyzed several times. Then, multiple component exchange cycles

were done by immersing the ITO substrate in an arylamine solution followed by rinsing. In presence of a large excess of arylamine, the azomethines component exchange was spontaneous. Each erase-write sequence was electrochemically confirmed. Both the reversibly hydrolysis and component exchange cycles served as a proof of concept for perpetual dynamic component exchange.

79. One-pot reaction to synthesize Au-decorated ferrite/mesoporous silica core-shell nanoparticles

Fanny Casteignau, Université de Sherbrooke (Nadi Braidy)

In the framework of producing 'nano reactors' using complex structures, we present a pathway to produce a multifunctional structure made of ferrite core with a mesoporous shell decorated by Au nanoparticles. We first produce the Fe_3O_4 core by reduction of Fe nitrate using an autoclave at 200°C for 8h. Using known techniques, we then show the possibility of controlling the SiO_2 thickness over Fe_3O_4 nanoparticles (NPs) with the $\text{Si}/\text{Fe}_3\text{O}_4$ ratio and the amount of TEOS added in the reaction. We then coat the ferrite core with Au NPs-decorated mesoporous silica using a one-pot reaction (Zhu & al, 2003) that consists of mixing gold precursors, silica stabilizers and silica precursor (TEOS) on the same flask under mechanical agitation. Compared to the existing 10-days long method to produce similar structures (Zhao & al, 2016) our pathway requires less steps, takes a tenth of the time and is more efficient for achieving the desired structure. These structures are intended for nano-reactors in which the Au catalysts can be locally and remotely heated by the ferrite core using magnetic induction.

80. Deposition of thiol ω -functionalized phenolic surfactant from the air-water interface

Renaud Miclette Lamarche, Concordia University (Christine DeWolf)

Surfactants ω -functionalized with thiols chemisorb from solution onto gold surfaces to form a self-assembled monolayer (SAM) by immersion. An alternative is to pre-assemble the monolayer at the air-water interface (the so-called Langmuir monolayer) followed by deposition onto a gold substrate. This approach should permit variation of the organization that is not attainable using solution self-assembly. The behavior of the bola surfactant Langmuir monolayer is first assessed using Langmuir film balance, Brewster angle microscopy and AFM. From this information the location of the thiol at the interface, whether pointing toward the air or submerged in the subphase, is inferred. This permits an appropriate deposition geometry to be determined, where the gold substrate is either pushed into the subphase or pulled out of it in a Langmuir Blodgett deposition. The resulting thicknesses of the deposited films are measured using ellipsometry and used to determine the impact of the deposition conditions on the resulting film.

81. Nouveaux copolymères à base de pyromellitique diimide et leur application en tant que matériau actif au sein de cathode de batterie Li-ion

Nicolas Zindy, Université Laval (Mario Leclerc)

Le domaine du stockage de l'énergie demande l'utilisation de matériaux rares qui sont par le fait même assez dispendieux à extraire. C'est par exemple le cas du cobalt présent en tant que matériau actif à la cathode sous forme d'oxyde de cobalt dans les batteries lithium-ion. L'une des alternatives qui pourraient permettre de remplacer ce matériau est l'utilisation d'un matériau organique afin de diminuer le coût de production et l'impact environnemental des matériaux utilisés. Cependant, les matériaux organiques se trouvent contraints d'incorporer des stratégies qui limitent leur solubilité vis-à-vis de l'électrolyte pour prévenir une perte de performance au fil des cycles de charge et de décharge. Le pyromellitique diimide est une unité qui a démontré pouvoir être utilisée comme matériau de cathode en batterie Li-ion, via la réduction de ses cétones, lorsqu'incorporée dans un macrocycle, un polyimide ou sous forme de sel, comme stratégie stabilisante. Par ailleurs, une technique de polymérisation émergente dans le domaine de l'électronique organique permettant le couplage d'un lien C-Br et C-H aromatique référant à la poly (hétéro)arylation directe (PHAD) est utilisée pour des dérivés de thiophène. Certains exemples d'arène possédant des atomes de fluor à proximité des liens C-H activables afin d'augmenter leur réactivité ont permis d'obtenir des polymères conjugués de haute masse molaire. Les fonctions imides du pyromellitique peuvent d'une manière similaire activer les liens C-H aromatiques et permettre d'obtenir des matériaux inédits. Dans ce cas, la stratégie stabilisante est l'incorporation de l'unité électroactive dans un polymère conjugué comme

l'ont démontré certains copolymère performant dans le domaine. Le premier objectif du projet était de synthétiser par la technique de la polymérisation par (hétéro)arylation direct (PHAD) de nouveaux polymères à base de pyromellitique diimide dans le but de remplacer l'oxyde de cobalt en tant que cathode dans les batteries Li-ion. Des conditions réactionnelles ont pu être optimisées pour copolymériser le pyromellitique diimide et le 1,4-dibromobenzène à des masses molaires allant jusqu'à 31 kg/mol. Les matériaux ont pu être efficacement utilisés en tant que cathode en batterie Li-ion afin d'obtenir des capacités allant jusqu'à 73 mAh/g. Un second objectif était de faire varier la nature de la chaîne latérale des polymères pour vérifier leur impact sur les performances. Trois aspects ont été abordés, soit : la longueur de la chaîne latérale, la possibilité de cliver la chaîne latérale après la polymérisation, et la réticulation de polymère via la chaîne latérale. Les résultats démontrent une plus grande stabilité pour les polymères ayant une chaîne latérale plus longue, ainsi qu'un degré de réticulation supérieure. L'utilisation d'une chaîne latérale clivable démontre de moins bons résultats. Finalement, le troisième objectif était de vérifier la possibilité d'utiliser une anode de sodium, au lieu du lithium qui est performant mais couteux. Il a été possible de démontrer que ces copolymères de pyromellitique diimide se réduisent à un plus haut potentiel corrigé avec le sodium qu'avec le lithium. Des calculs selon la théorie de la fonctionnelle de la densité (DFT) ont été appliqués pour expliquer l'avantage structurel du polymère lors de la réduction avec le sodium.

82. Effect of cold rolling and ball milling on first hydrogenation of $\text{Ti}_{0.5}\text{Zr}_{0.5}(\text{Mn}_{1-x}\text{Fe}_x)\text{Cr}_1$, $X=0, 0.2, 0.4$

Sakine Khajavi, UQTR (Jacques Huot)

Despite their relatively low capacity, metal hydrides of AB₂ types are interesting alloys for hydrogen storage. One of the problems faced by all types of metal hydrides is the detrimental effect of air exposure on the hydrogen storage capacity. Usually, when a metal hydride is exposed to the air, the hydrogen capacity is drastically reduced. In this investigation, we show that cold rolling is very effective in restoring the hydrogen capacity of an air exposed alloy. The alloys studied had the composition $\text{Ti}_{0.5}\text{Zr}_{0.5}(\text{Mn}_{1-x}\text{Fe}_x)\text{Cr}_1$. The alloys were synthesized by arc melting where $X = 0, 0.2$, and 0.4 . Microstructure and crystal structure of all alloys were investigated respectively by SEM and X-ray powder diffraction. The hydrogenation kinetics and capacity was measured a Sievert's type volumetric apparatus. We found that, after air exposition, none of the alloys absorbed hydrogen. However, mechanical deformation by ball milling or cold rolling restored the full capacity with fast hydrogenation kinetics. In the case of ball milling, short milling time (5 minutes) produced a beneficial effect but longer milling time reduced the hydrogen capacity. On the other hand, cold rolling just once made the hydrogenation fast with maximum capacity. Therefore, we could conclude that cold rolling is the best way to reactivate an air exposed metal hydride.

83. Functionalizing the surface of lithium metal in order to use the electrolyte 1 M LiPF_6 in acetonitrile

David Lepage, Université de Montréal (Dominic Rochefort)

In lithium battery technology, the use of lithium metal (Li) in liquid electrolyte remains challenging because of its reactivity towards the electrolyte and the formation of dendrites during its cycling. We propose to benefit from the high reactivity of Li by immersing it in fluoroethylene carbonate, to spontaneously decompose into a passivation film.¹ This new functionalised lithium (Li-FEC) is characterized by X-ray Photoelectron Spectroscopy, Electrochemical Atomic Force Microscopy and Scanning Electron Microscopy to determine its composition and morphology. Analysis shows that a hybrid material is formed on the Li metal surface from the decomposition of FEC and LiF. This passivation layer prevents Li to react with the organic solvent while remaining permeable to lithium ions. These properties allow the plating/stripping of the lithium into a symmetric cell with the electrolyte 1 M LiPF_6 in acetonitrile (1M LiPF_6 -ACN) with high stability, whereas acetonitrile decomposes readily on unprotected Li metal. A full cell with LiFePO_4 as cathode, 1M LiPF_6 -ACN as electrolyte and Li-FEC as anode is assembled to show the potential application of this approach.

84. Influence of the Molecular Weight and Bonding Type on Photo-Orientation of Hydrogen-Bonded and Ionically Bonded Azopolymer Complexes

Mahnaz Kamaliardakani, University of Montreal (C. Geraldin Bazuin, Christian Pellerin)

Supramolecular chemistry is an efficient and convenient way to bond a commonly-used photopassive homopolymer to a photoactive azo compound. We investigated the influence of the supramolecular bonding type, hydrogen bonding vs. ionic bonding, and of the molecular weight of the polymer host on the photoresponsive properties of azopolymer complexes, in particular their photoinduced molecular orientation (θ) and surface-relief grating (SRG) diffraction efficiency (DE). To that end, poly(4-vinylpyridine) (P4VP) of three molecular weights (MWs) (5k, 50k, and 200k) was hydrogen-bonded (H-bonded) at equimolar ratio with 4-hydroxy-4-dimethylaminoazobenzene (azoOH), and the quaternized derivatives of the three P4VPs (P4VPMes) were ionically bonded via ion exchange to methyl orange (MO), where the OH functionality of the azo is replaced by a sulfonate group, and their photoinduced properties were studied. The findings clarify that photoresponse of spin-coated films of the ionically bonded complexes both in terms of θ and DE values, is much greater than that of the analogous H-bonded complexes. Furthermore, although there is no significant dependence of θ on molecular weight for either series, there is a clear relationship between DE and the polymer MW, with the low MW complex showing a higher DE than the two higher MW complexes. This suggests that chain entanglement plays a more important role than the glass transition temperature for the phototransport in these systems. These results contribute to practical guides for the design of supramolecular photosensitive polymers for SRG applications.

85. A Step toward designing electrodes for higher energy density lithium-ion batteries

Steeve Rousselot, Université de Montréal (Mickaël Dollé)

Conventional composite electrodes consisting of a mixture of active material, carbon black and polymeric binder spread on a metallic current collector could impede the development of high energy density batteries as a large part of its composition only act as dead weight in addition to manufacturing cost (solvent evaporation, safety issue).

To overcome this issue, binder-free, self-standing and flexible electrode only made of active material (AM) and single wall carbon nanotubes (SWNT) were previously investigated[2]. In an AM/SWNT configuration, electrodes with up to 95 wt.% of active material could be prepared, the balance being only 5% of SWNT that promoted a high specific capacity and stable cycling.

Thanks to its abundance and low environmental impact, it is expected that LiFePO_4 (LFP) should represent 25% of the cathode market in 2025 compare to 10% currently[1]. However, LFP lacks of electronic conductivity and its moderate potential mitigates its specific energy.

The remarkably high electronic conductivity obtained thanks to the CNT network in the self-supported electrodes allowed the cycling of uncoated LFP particles. Still, some performance loss evidences that the SWNT network not fully incorporate some AM particles.

In order to reach a multiscale conductivity, polymerisation of the 3,4-ethylene-dioxythiophene (EDOT) by reinsertion of lithium into $\text{Li}_{(1-x)}\text{FePO}_4$ was attempted. EDOT polymerization on uncoated LFP is well known to create a conductive coating on the particles[3]. With help of SWNT and PEDOT, an conductive network between the particles is targeted.

Macroscopic and microscopic scale of the electrode can be reached thanks to the SWNT and the PEDOT leading to an uncoated LiFePO_4 PEDOT self-standing electrode. After the details of the electrode preparation and their physico-chemical properties, the electrochemical performance will be discussed and compared to that of a conventional electrode.

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86. SPR Sensing of Aminoglycoside Antibiotics with Gold Nanoparticles

Marie-Pier Dinel, Université de Montréal (Jean-François Masson)

Our research aims to develop a SPR technique able to detect aminoglycosides. Aminoglycoside antibiotics are small polycationic molecules used to treat infections of gram-negative bacteria. They inhibit a ribosomal subunit that interferes with synthesis of essential proteins to the cell membrane. Aminoglycosides at a too high concentrations in human fluids are toxic and lead to nephrotoxicity or ototoxicity. Surface Plasmon Resonance (SPR) sensing is a simple, fast and real-time technology, which is often promoted for clinical diagnostics due to the possibility of label-free monitoring biological interactions using a compact and portable instrument. However, SPR sensing is often not sensitive enough to detect small molecules like drugs.

We are thus investigating methods for signal enhancement using nanoparticles. This biosensor is composed of a gold film where Enhanced intracellular survival enzyme (EIS) have been fixed. A competition between aminoglycosides and gold nanoparticles functionalized with a derivate antibiotics is created for the active site of the EIS. In this presentation, we will discuss the various methods and parameters investigated to increase the sensitivity of the SPR, decrease the background signal, and detect the aminoglycosides.

87. Biophysical effects of interaction between hydrophilic nanoparticles and pulmonary lung surfactants: influence of nanoparticles concentration and charge

Olga Borozenko, Concordia University (Christine DeWolf, Antonella Badia)

Human exposure to nanomaterials is inevitable given the increasing presence in the environment of nanoparticulates generated by industrial activities. Colloidal silica is the most abundant air pollutant in industrial regions. Due to their exceptional chemical reactivity, silica nanoparticles (NPs) can potentially inhibit lung surfactant and cause difficulties in breathing. The present study investigates the biophysical effects of NP charge and concentration on the phase behavior of model lipid mixtures and clinical pulmonary surfactant. A surfactant monolayer was formed at the air-water interface over a NPs-containing subphase. The Langmuir film balance was used to examine the lipid surface activity, while Brewster angle microscopy and Atomic Force Microscopy allowed the study of the overall morphological changes to the film. We obtained clear evidence that silica NPs influence the lipid monolayer at concentrations as low as 0.001%. The revealed biophysical mechanism of NP interaction with pulmonary surfactant brings new insight in understanding how inhaled NPs impact pulmonary function.

88. Controllable Design of Polycrystalline Synergies: Hybrid FeO_x Nanoparticles Applicable to Electrochemical Sensing antineoplastic Drug in Mammalian Cells

Haifeng Zhou, Université de Montréal (Jean-François Masson)

Investigations on interplay between sensing platform performance and crystal phase of material are the new beginning of designing advanced bioanalytical systems. Herein, FeO_x nanoparticles

(NPs, ~100 nm), including superfine magnetic (Fe₃O₄) and hematite (α -Fe₂O₃) nanocrystals in single particles, have been employed to verify the synergistic effect between the electrocatalytic property and the polycrystalline structure of the materials. Moreover, this strategy overcomes that single crystal phases generally suffer from serious agglomeration and poor electrical conductivity. More importantly, hybrid metal oxides (e.g., α -Fe₂O₃/Fe₃O₄) with variable oxidation states remarkably facilitate the efficient redox charge transfer.

Taking the detection of Flutamide (FLT) in prostate cancer cells (VCaP cells) as example, the dynamic ranges of the oxidation states from the different crystal phases were integrated into a single electrochemical sensor interface. Furthermore, good selectivity, accuracy, satisfactory sensitivity (769.1 μ A mM⁻¹ cm⁻²) and low detection limits (64 nM) were achieved. Going beyond the conventional singlecrystal phase-driven electrochemical biosensing, the elaborate of polycrystalline structure in a single particle may open a new approach for the design of outstanding electrode materials,

which not only can significantly improve the performance of sensing platforms, but also can be used to rationally design the material properties according to the applications.

89. Effect of different heat treatments on physical and mechanical properties of flax fibers reinforced PLA composites

Marie Bayart, Sherbrooke University (Mathieu Robert, Saïd Elkoun)

This research aims at studying the influence of heat treatments (HT) on polylactic acid (PLA) composites reinforced with flax fibers. A TiO₂ coating was applied on the fibers prior to composites processing. In other words, this study intends to enhance the interfacial and mechanical properties of composites by controlling crystallization of the PLA matrix.

In this study, flax fabrics were coated with a titanium dioxide film in its anatase form to enhance the interfacial adhesion between flax fibers and PLA. Composites were processed by thermo-compression. As-received fibers/PLA composites and pure PLA were used as references. Dynamic Mechanical Analysis (DMA) in tensile mode was performed at different temperatures of 80, 110 and 130°C. This was to investigate the influence of temperature on PLA crystallization behavior and thus, on the mechanical and thermal properties of the three materials. An optimal duration of heat treatment was found for each temperature thanks to this method, where a peak of storage modulus was observed.

Differential Scanning Calorimetry (DSC) was also carried out on the three materials crystallized in quiescent conditions at each temperature and optimal duration respectively. Short Beam Shear (SBS) and impact tests (Notched Izod) were performed on HT specimens to correlate DMA/DSC results with the differences of interfacial and mechanical properties obtained between the different materials. Scanning Electron Microscopy (SEM) observations were carried out to support the conclusions drawn from this research.

Results showed significant differences in the mechanical behavior of both composites investigated by DMA. It has been concluded that the differences in the storage modulus of the DMA traces can be explained by the fact that the interface between the fibers and the matrix of as-received fibers/PLA composites was weak and partially destroyed by crystal growth. Conversely, the interface was protected in the case of TiO₂-coated composites. This hypothesis was confirmed by SBS and impact tests. The interfacial adhesion drastically decreased after a longer HT for as-received composites whereas it remained the same or was even enhanced for coated composites. The fracture behavior of the different PLA composites was also different. On the one hand, coated fibers/PLA composites revealed a fragile behavior because of the strong adhesion between the fibers and the matrix and their high crystallinity levels. On the other hand, cracks propagated around the fibers in the as-received fibers/PLA composites. Fibers easily debonded from the matrix, revealing a poor interface coming from a weak adhesion between the fibers and the matrix.

90. Complementary hydrogen bonding induces dramatic electronic perturbation giving rise to electrical conductivity in weak aromatic donor/acceptor molecules

Chenghao Liu, McGill University (Dmitrii Perepichka)

π -Conjugated organic compounds possess a range of useful optoelectronic properties that are dictated by their molecular structure and their supramolecular arrangement. While much efforts in the past decades have been put into tuning the molecular structure to achieve desired properties, rational supramolecular control remains a challenge. Here we present a series of controllable supramolecular co-assemblies of poly(hetero)cyclic aromatic hydrocarbons via two-point hydrogen bonding. The hydrogen bonding interaction results in significant modulation of the HOMO/LUMO levels of the molecular components leading to a very strong charge transfer interaction in the weak donor-acceptor pairs. The resulting co-crystals displayed a low bandgap (Eg 1 eV) with intense charge transfer absorption extending to the IR region. Beyond this, we were able to detect significant temperature-dependent EPR signals and electrical conductivity for some co-crystals. We will report details of DFT calculations, X-ray crystallographic analysis, absorption / EPR spectroscopy, and electrical measurements, uncovering structure-properties relationships in this new class of organic conducting materials. We will also describe new opportunities created by these materials for bulk heterojunction organic photovoltaics and bioelectronic applications.

91. Developping the next generation of indoor wood products: Chemistry for the benefit of wood

Stéphanie Vanslambrouck, Université Laval (Véronique Landry)

NSERC/Canlak Industrial Research Chair in interior wood-product finishes (CRIF) aims to develop densification and finishing solutions to increase the use of wood in both residential and non-residential applications. Increasing the use of wood is closely related to enhanced surface mechanical performance and, incidentally, reduced wear and maintenance challenges. Improving fire performance is another major challenge, which is expected to become increasingly important in the coming years. CRIF's mission is to improve the performance (mechanics, fire and appearance) of wood products so that they appear as obvious choices for building decision makers. CRIF's research program will focus on the densification of wood products (DENSIFY axis), on the development of high-performance mechanical and fire-resistant finishes (PROTECT axis) and, to a lesser extent, on the modification of the appearance of wood surfaces (DECORATE axis). As part of CRIF's research program, strategies based on the use of low volatile organic compound (VOC) compounds, photochemistry, cure-on-command polymerization and stimuli-sensitive materials will be employed.

92. An Investigation of REE Dissolution from Carbonate Mineral into Deep Eutectic Solvents

Ali Entezari-Zarandi, Université Laval (Faical Larachi)

Solubility of rare earth metals from their carbonate mineral, bastnäsite was mimicked through dissolution of individual carbonates of Y, La, Ce, Nd and Sm employing different ionic liquids based on choline chloride (deep eutectic solvents). Urea, malonic acid and citric acid were used in different proportions regarding choline chloride in order to form the deep eutectic solvents (DES) of desired viscosity and functionality. The results obtained shows promising leads on selective dissolution of rare earth metals with the use of solvato-metallurgical processes, thus starting the separation of different REE members from the very first steps.

93. Développement de nouveaux copolymères de dicétopyrrolopyrrole fluoré pour applications en cellules solaires

Eliane Soligo, Université Laval (Mario Leclerc)

L'industrie de l'énergie solaire est actuellement dominée par les matériaux de silicium. Bien que cette technologie permet d'atteindre des rendements de conversion énergétique élevée en cellules solaires, les ressources mondiales de silicium sont limitées, et ces matériaux sont dispendieux à fabriquer, et difficiles à purifier et à mettre en oeuvre.[1] Une alternative à l'utilisation de silicium est la fabrication de cellules solaires à hétérojonction donneur-accepteur à partir de matériaux organiques, tel des polymères. L'utilisation de polymères permet la fabrication de cellules solaires en solution, ce qui facilite la mise en oeuvre.[2] Les unités accepteurs couramment utilisées sont des dérivés du fullerène. Des copolymères de type riche-pauvre sont utilisés comme unité donneur dans l'hétérojonction. En effet, la combinaison d'une unité riche et d'une unité pauvre des copolymères permet de moduler la largeur de bande interdite avec la HOMO du polymère dominée par l'unité riche et la LUMO par l'unité pauvre.[3]

En tant qu'unité pauvre, le dicétopyrrolopyrrole (DPP) a déjà prouvé sa grande efficacité dans différents copolymères pour les piles solaires à haut rendement de conversion énergétique. Il s'agit d'un monomère de choix en raison de son bon coefficient d'absorption, des fortes interactions π - π de sa structure conjuguée et de sa faible bande interdite.[4] Le DPP est formé de trois parties : l'unité centrale bilactame, un substituant aromatique de chaque côté, et des chaînes alkyles sur les unités lactames pour augmenter la solubilité du DPP dans différents solvants organiques. Les cellules solaires comportant le DPP comme monomère dans leur unité donneur ont obtenu des rendements de conversion énergétique allant au-delà de 9%.[5]

Le projet porte sur la synthèse de copolymères de type riche-pauvre comportant une unité thiényl-dicétopyrrolopyrrole fluoré. L'effet recherché par l'ajout du fluor sur les polymères étudiés est, entre autres, d'augmenter la stabilité de la molécule et de baisser les niveaux énergétiques du polymère obtenu.[6] Des polymères fluorés sont comparés à leur analogue non fluoré avec pour objectif d'augmenter le rendement de conversion énergétique des dispositifs fabriqués avec ces matériaux.

1. Jung et al. *Org. Electron.* 2016, 31, 149-170.

2. Pei et al. *Chem. Mater.* 2014, 26, 594-603.
3. Chandran, D. et al. *Macromol. Res.* 2013, 21, 272-283.
4. Janssen et al. *Chem. Commun.* 2014, 50, 679-681.
5. Choi et al. *Adv. Mater.* 2015, 27, 3318-3324.
6. Bura et al. *Macromol.* 2017, 50, 7080-7090.

94. Developing antimicrobial nanocellulose using natural antibacterial agents

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Hairy nanocellulose (HNC) was functionalized with aldehyde groups to facilitate the attachment of antibacterial agents, lysozyme and nisin. The immobilization process does not require any linker or activator, which makes it more straightforward. XPS and FTIR analyses showed successful attachment of both nisin and lysozyme onto the HNC. The efficacy of the conjugated nanocellulose against the model bacteria *B. subtilis* and *S. aureus* was tested in terms of bacterial growth, cell viability, and biofilm formation/removal. The results show that the minimum inhibitory concentration of the conjugated nanocellulose is higher than that of lysozyme and nisin in free form, which was expected given that immobilization reduces the possible spatial orientations of these proteins. We observed that *S. aureus* developed resistance to free nisin following 24 h of exposure. Interestingly, we did not observe this phenomenon when the bacteria were exposed to the conjugated nanocellulose, demonstrating that immobilization effectively retains the activity of antibacterial agents over long time periods. These characteristics make the developed conjugated nanocellulose a potential candidate to be used in wound dressings.

95. Functionalized Cellulose Fibres for Textile Applications

Martin Sickinga, McGill University (Theo van de Ven)

Global industrial textile is produced from non-renewable petroleum sources (polyester) and from cotton which requires the use of pesticides and large volumes of water. Canada's vast forest reserves provide a means to produce carbon-neutral textile. Currently, cellulose based fibres are produced by the rayon process using carbon disulfide, which is highly toxic. In addition, textile dyeing is also one of the most polluting processes in this industry. Therefore, an environmentally sensitive and economically viable innovation is necessary to transform renewable carbon in textile manufacturing. Functionalizing cellulose via periodate oxidation and/or chlorite reactions enables the production of filaments that can be converted into yarn. This research also explores means of adding color to the filaments directly while spinning online.

96. Copper-Reduced Graphene Oxide Core-Shell Nanowire Films Using as Transparent Conductive Electrodes in High-Performance Suspended Particle Devices

Shengyun Huang, INRS-EMT (Dongling Ma)

The energy crisis is a major challenge of the 21st century. Managing buildings' environment in a smart way has attracted a great deal of interest to address the current energy issue because the construction sector uses as much as 30 to 40% of the primary energy in the world. Smart windows, such as those based on suspended particle devices (SPDs), provide dynamic control of photon flow that minimizes the energy loss, as well as improves human comfort. These windows are fabricated by sandwiching an electro-optically active layer between two transparent electrodes. Although significant progress has been made in identifying the optimal materials for such windows, there is still a great need to improve their key elements, especially the performance of electrodes.

Herein, we report a novel SPD, which was built upon copper-reduced graphene oxide (Cu-rGO) core-shell nanowire (NW) films as transparent conductive electrodes (TCEs) for the first time. The Cu NWs were firstly wrapped with GO and then deposited on glass by vacuum filtration followed by thermal annealing, leading to the TCE with both high transparency and conductivity. The sandwich-structured SPD fabricated using these new TCEs shows excellent transmittance change of 42 %, fast switching time (20 s and 40 s for color bleaching and recovery respectively) and superior stability, which are comparable to those of SPDs based on indium tin oxide electrodes. These impressive results strongly suggest the bright prospect of these novel TCEs in SPDs in particular, and further, in a wide variety of optoelectronic devices in general.

97. Plasma synthesis, characterization and catalytic activity of mixed oxide ferrites

Nicolas Dumaresq, University of Sherbrooke (Nadi Braid)

Transition metal ferrites are being considered as a green alternative to noble metal catalysts for an array of chemical reactions. In addition, their magnetic properties make them recoverable from the reaction media. Solution spray induction plasma is a novel method to synthesize large quantities (>30 g/h) of highly pure mixed metal ferrite nanoparticles. This one-step method offers an excellent control on the stoichiometry with the added advantage that the particles are individual faceted and have a narrow size distribution, ~30-60 nm. We present a study on the structure/catalytic properties relationship of Cu-ferrite nanoparticles produced by solution spray thermal plasma. Samples were produced using metal nitrates precursor solutions with various Cu to Fe ratio (Cu:Fe = 1:5, 3:7, 1:2, 1:1, 4:1). Samples with Cu:Fe > 3:7 favoured the formation of up to 30% mass of tetragonal spinel alongside the cubic $\text{Cu}_{0.25}\text{Fe}_{2.75}\text{O}_4$ allotrope. The tetragonal fraction can be easily increased with annealing at T350°C. Furthermore, with increasing Cu content in the feed, excess Cu tend to form a CuO layer decorating $\text{Cu}_{0.25}\text{Fe}_{2.75}\text{O}_4$ nanoparticles that can be reduced to metallic copper with a 2 hours H_2 treatment at 300°C. We will investigate the catalytic performance of these particles on the alcohol amination reaction and the Huisgen 1,3-dipolar cycloaddition reaction.

98. Plasma Synthesis of Spinel Oxide Nanoparticles and their Electrocatalytic Activity for the Oxygen Reduction Reaction

Ji Yun Chen, INRS-EMT (Ana Tavares)

The oxygen reduction reaction (ORR) is at the heart of rechargeable metal-air batteries and fuel cells. However, the development of both technologies is hindered by the slow kinetic of the ORR, and by the use of expensive noble catalysts necessary to achieve high electrical currents at lower overvoltage. Here we will present our recent studies on CoFe_2O_4 and $\text{Co}_{0.5}\text{Mn}_{0.5}\text{Fe}_2\text{O}_4$ electrocatalysts for ORR, as potential low cost and alternative catalysts to Platinum. The catalysts were synthesized by thermal plasma, a scalable process capable of producing the desired type of nanomaterial with high quality. Electrochemical characterization of spinel / carbon thin films in O_2 -saturated 0.1 M KOH revealed that the half-wave potential for the $\text{Co}_{0.5}\text{Mn}_{0.5}\text{Fe}_2\text{O}_4$ -based electrode is only 140 mV more negative than that of 20 wt% Pt/C electrode, and among the best reported in the literature for this type of oxide catalyst.

99. Spectroscopic description of the odd-even effect in Self-Assembled Monolayers (SAMs)

Fadwa Ben Amara, Université de Montreal (Antonella Badia)

In this work, a spectroscopic evidence of the odd-even effect in SAMs is presented.

Infrared Reflection Absorption Spectroscopy (IRRAS) allows for a structural study of the SAMs on gold substrate.

First, odd-even manifestations in methyl and ferrocene terminated SAMs are observed and explained. Then, the spectroscopic proof of the odd-even effect is correlated with surface potential measurements.

100. A Non-toxic aqueous Process for the Production of Textile from Kraft Pulp

Theo van de Ven, McGill University

The biggest issue facing our planet is climate change, caused mainly by emissions generated by combustion of fossil fuels by industry, automobiles and heating of buildings. To mitigate climate change, we should make extensive efforts to find economically sustainable solutions for the use of wood, while at the same time planting more trees than that we cut. At present the large scale uses of wood are: building materials, paper and textile. This study deals with a new way of making functional cellulose fibers, which can be made into filaments, smart textiles, high value cellulose biomaterials, such as superhydrophobic fibers and fibers of high tenacity, as well as high value dyed fibers. In the novel process, kraft fibers are chemically modified in water and made into a dope by dissolving it in an alkaline solution. The dissolved cellulose is regenerated in the acid bath of a spinneret, producing cellulose filaments, which can be further functionalized if desired. Trials on a demonstration spinneret show that such fibers can be spun at industrially speeds and drawing rates. Properties of the novel fibers, such as tenacity, elongation and water take-up are compared to those of rayon and cotton.