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**Université de Sherbrooke**

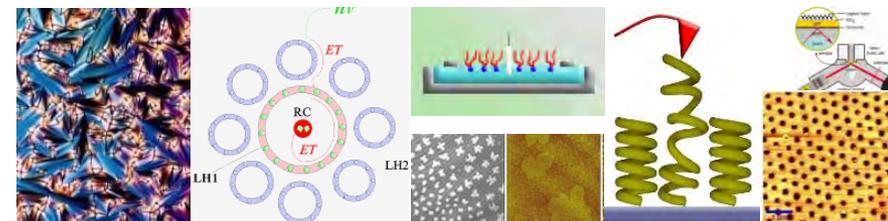


**18 Sept. 2012**

**Centre Culturel**



Student symposium  
 Colloque étudiant  
 2012





***Special thanks to/Remerciements:***

**CSACS Coordinator:** Petr Fiurasek

**CSACS Student Committee:**

Andrea Greschner (McGill) – Chair

Amir Sheikhi (McGill)

Alireza Shams (McGill)

André Bessette (McGill)

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Karina Carneiro (McGill)

Katherine Bujold (McGill)

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Olga Borozenko (U. de M.)

Rolf Schmidt (Concordia)

If anyone is interested in being a part of the student committee or helping to organize this event next year, please email Petr at [csacs.chemistry@mcgill.ca](mailto:csacs.chemistry@mcgill.ca) or talk to one of the people thanked above.

Les personnes intéressées à participer au comité étudiant ou à l'organisation de cet événement l'an prochain sont invitées à communiquer par courriel au [csacs.chemistry@mcgill.ca](mailto:csacs.chemistry@mcgill.ca) ou à parler avec une des personnes remerciées ci-dessus.

<b>Schedule / Horaire</b>	
10:00	Registration, refreshments, and poster setup Inscription, rafraîchissements, et installation des affiches
10:45	Welcoming remarks/Discours d'ouverture
10:50	<b>Amir Sheikhi</b> (McGill University)
11:10	<b>Feng Qi</b> (McGill University)
11:30	<b>Alireza Shams</b> (McGill University)
11:50	<b>Olivier Boissière</b> (Université de Sherbrooke)
12:10	Lunch
12:45	<b>Poster session Group A: Posters 1-13</b>
14:00	<b>Hang Hu</b> (McGill University)
14:20	<b>Fei Li</b> (McGill University)
14:40	<b>Graham Hamblin</b> (McGill University)
15:00	Coffee break/pause café
15:30	<b>Bin Yan</b> (Université de Sherbrooke)
15:50	<b>Zhongkai Cui</b> (Université de Montréal)
16:10	<b>Carolyn Madwar</b> (McGill University)
16:40	Wine and cheese / vins et fromages
17:00	<b>Poster session Group B: Posters 14-26</b>
18:15	Reception/Vote for best talk and poster Réception et vote pour la meilleure présentation et affiche
18:30	Announcement of Winners/ annonce des gagnants
19:00	Adjourn-Bus leaves/ ajourner-retour à Montréal

21)<sup>B</sup> Mauricio Franco (University of Montreal)  
Studies on the interaction of plasmid DNA  
pUC19 with a mixed-valence vanadium oxide,  
 $V^{10}O_{24} \cdot 12H_2O$ , in buffered medium

22)<sup>B</sup> Thomas Edvardson (McGill University)  
Towards integration of DNA nanostructures  
with lipid bilayers

23)<sup>B</sup> Amlan Kumar Pal (University of Montreal)  
Low-Energy, Red Emission from a  
Ruthenium(II)-to-2,2'-Bipyridine 3MLCT State  
in a new class of Ruthenium(II)-polypyridyl  
complexes

24)<sup>B</sup> Chih-Ying Wang (McGill University)  
Diffusion in hydrogel-supported phospholipid  
bilayer membranes

25)<sup>B</sup> André Bessette (University of Montreal)  
Exploring the Scope of Aza-Dipyrromethene  
based MII Homoleptic Complexes for Light-  
Harvesting Applications

26)<sup>B</sup> Fiora Rosati (McGill University):  
Assembly of Metallated Structures from DNA-  
based Building Blocks

15)<sup>B</sup> Chris McLaughlin (McGill University)  
**One-Step Synthesis of DNA Cages from Unmodified Strands: Geometric Diversity, Nuclease Stability, Cellular Uptake and Inhibition of Gene Expression.**

16)<sup>B</sup> Audrey Laventure (Université de Montréal):  
**UV Cross-Linking of Films and Electrospun Nanofibers Prepared from Byssal Proteins**

17)<sup>B</sup> Sreenivasulu Bandi (University of Montreal):  
**The coordination-driven self-assembly approach for the synthesis of an M1L2, M2L4 and M3L4 type complexes from Pd (II) and flexible pyridine ligands**

18)<sup>B</sup> Kai Lin Lau (McGill University)  
**DNA nanotube guided assembly of GNPs**

19)<sup>B</sup> Patricia Robert (Université de Montréal )  
**Ultrafast deformation and relaxation of polystyrene blends by time-resolved infrared spectroscopy**

20)<sup>B</sup> Justin Conway (McGill University)  
**3D DNA Prisms: Synthesis, Structure and Resistance To Nuclease Degradation**

***Olivier Boissière (University of Sherbrooke)***  
**Effect of reversible cyclisation of a telechelic PNIPAM with coumarin moieties**

An  $\alpha, \omega$  poly (*N,N* isopropylacrylamide) (PNIPAM) with coumarin moieties has been synthesized in order to test, first, if an intrachain photocyclisation was reachable and then to test the effect of this reversible photocyclisation on the lower critical temperature (LCST) of the PNIPAM. It rose that, as long as the concentration of this polymer was above about 0.3mg/mL the cloud point of the solutions was not related to PNIPAM but to coumarin instead.

***Bin Yan (University of Sherbrooke)***  
**Near-Infrared Light Triggered Dissociation of Block Copolymer Micelles Using Upconverting Nanoparticles**

We demonstrate a novel strategy enabling the use of a continuous-wave diode near infrared (NIR) laser to disrupt block copolymer (BCP) micelles and trigger the release of their 'payloads'. By encapsulating NaF<sub>4</sub>Tm<sub>2</sub>Yb<sub>3</sub> upconverting nanoparticles (UCNPs) inside micelles of poly(ethylene oxide)-*block*-poly(4, 5-dimethoxy-2-nitrobenzyl methacrylate) and exposing the micellar solution to 980 nm light, photons in the UV region are emitted by the UCNPs, which in turn are absorbed by *o*-nitrobenzyl groups on the micelle core-forming block, activating the photocleavage reaction and leading to the dissociation of BCP micelles and release of co-loaded hydrophobic species. Our strategy of using UCNPs as an internal UV or visible light source upon NIR light excitation represents a general and efficient method to circumvent the need for UV or visible light excitation that is a common drawback for light-responsive polymeric systems developed for potential biomedical applications.

8)<sup>A</sup> Wei Chung Chen (McGill University)  
Pickering Emulsions Stabilized by Nanocrystalline Cellulose

9)<sup>A</sup> Amir Sheikhi (McGill University)  
Electroacoustic investigation on the colloid-hydrogel nano-composites aging process

10)<sup>A</sup> Katherine Bujold (McGill University)  
Sequence Responsive Unzipping DNA Nanocubes as Potential Drug Delivery Vehicles

11)<sup>A</sup> Timothy Gonzalez (McGill University)  
Polarized Confocal Raman Observations of Photoinduced Anisotropy in Thin Films

12)<sup>A</sup> Tim Morse (McGill University)  
UV Curable Polymer Films Reinforced with Nanocrystalline Cellulose

13)<sup>A</sup> Nicole Avakyan (McGill University)  
Poly(adenine) self-assembly mediated by a small molecule

14)<sup>B</sup> Patrick Julien (McGill University)  
The Solid State Synthesis of MOF-74 for use in Friedel-Crafts Alkylations

- 1)<sup>A</sup> Y uneng Lu (McGill University)  
**Accelerated aging: low-energy, solvent-free reactions for the formation of ZIFs**
- 2)<sup>A</sup> Andrew O'Connor (University of Montreal)  
**Using Re(I) Aza-Dipyrromethene Complexes for the Self-Assembly of High-Energy Light-Harvesting Antennas**
- 3)<sup>A</sup> Kevin Conley (McGill University)  
**Self-Assembly of A Cellulose Derivative**
- 4)<sup>A</sup> Félix Lussier (University of Montreal)  
**Synthesis of novel triazine ligands**
- 5)<sup>A</sup> Cristina Mottillo (McGill University)  
**"Accelerated aging": A novel, energy-effecient technique for the quantitative synthesis of zeolitic imidazolate frameworks**
- 6)<sup>A</sup> Surjith Kumaran (University of Sherbrooke)  
**Stimuli-Responsive Polymer Brushes: From Controlled Release to Switchable Protein Binding**
- 7)<sup>A</sup> Hongji Zhang (University of Sherbrooke)  
**Optically Triggered Shape-Memory Polymer-Gold Nanocluster Composite Materials**

***Amir Sheikhi (McGill University)***  
**Colloidal spheres-hydrogel interfacial friction**

To achieve longer circulation time and higher stability, drugs are usually loaded into tiny spheres known as micro- and nano-drug agents. Upon the introduction of these colloidal spheres into the body, they interact with various tissues, which are soft, porous materials. To shed light on the colloidal behavior at soft interfaces, we developed a novel optical tweezers interfacial microrheology experiment. Active and passive microrheology of silica spheres at hydrogel-electrolyte interfaces were performed in a microfluidic cell. For the first time, the effect of lipid bilayer and polymer-tethered lipid bilayers on the colloidal interfacial behavior on a hydrogel was studied. A Nyquist analysis on more than 30 sets of laser power-drive frequency combination experiments furnished dynamical friction phase diagrams.

*Zhongkai Cui (University of Montreal)*

**Formation of pH-sensitive cationic liposomes from a binary mixture of monoalkylated primary amine**

**and cholesterol**

Some systems composed of a monoalkylated amphiphile and a sterol can unexpectedly form a stable liquid-ordered lamellar phase. These include negatively charged mixtures of unprotonated palmitic acid (PA)/sterols, protonated PA/cholesterol sulphate (Schol), and mixtures of positively charged cetylpyridinium chloride/cholesterol (Chol) and Schol. These bilayers can be extruded using conventional methods to obtain large unilamellar vesicles (LUVs). The passive permeability of these LUVs was drastically limited, a phenomenon associated with the high sterol content. By selecting the suitable monoalkylated amphiphile, it is possible to craft a specific response to a given stimulus. For example, pH variations can trigger the release from LUVs formed with palmitic acid and sterols. These sterol-rich non phospholipid liposomes constitute an interesting family of nanovectors. In the present work, the possibility to form non phospholipid liposomes with mixtures of stearylamine (SA) and cholesterol was investigated. The phase behavior of SA/Chol binary mixtures in various proportions was characterized by differential scanning calorimetry, infrared and <sup>2</sup>H NMR spectroscopy. It is found that an equimolar SA/Chol mixture can form a liquid-ordered lamellar phase. Moreover this phase is pH-sensitive as it undergoes a transition from a liquid-ordered phase to a solid state when the pH is increased from 5.5 to 12. LUVs have been successfully extruded from these SA/Chol mixtures at pH 7.5. Release experiments indicate the relatively low permeability of the liposomes as well as the possibility to trigger the release by a pH increase. These LUVs are, to our knowledge, the first positively charged liposomes showing pH-triggered release.

*Fei Li (McGill University)*

**Nanoparticle gel electrophoresis: bare charged spheres in polyelectrolyte hydrogels**

Nanoparticle gel electrophoresis has recently emerged as an attractive means of separating and characterizing nanoparticles. Consequently, a theory that accounts for electroosmotic flow in the gel, and coupling of the nanoparticle and hydrogel electrostatics and hydrodynamics, is required, particularly for gels in which the mesh size is comparable to or smaller than the particle radius. Here, we present an electrokinetic model for charged spherical colloidal particles undergoing electrophoresis in charged (polyelectrolyte) hydrogels: the gel-electrophoresis analogue of Henry's theory for electrophoresis in Newtonian electrolytes. We compare numerically exact solutions of the model with several independent asymptotic approximations, identifying regions in the parameter space where these approximations are accurate or break down. As previously assumed in the literature, Henry's formula, modified by the addition of a constant electroosmotic flow mobility, is accurate only for nanoparticles that are small compared to the hydrogel mesh size. We derived an exact analytical solution of the full model by judiciously modifying the theory of Allison et al. (2007) for uncharged gels, drawing on the superposition methodology of Doane et al. (2010) to account for hydrogel charge. This furnishes accurate and economical mobility predictions for the entire parameter space.

***Hang Hu (McGill University)***

## **Density functional theory study of self-assembled monolayers on multi-faceted gold nanorod**

Over the past decades, ab initio density functional theory (DFT) simulation have contributed significantly to the understanding of self-assembled monolayers on gold surfaces. However, despite years of intensive research and real life applications, the exact formation mechanism and configuration of self-assembled monolayers (SAMs) on gold nanoparticles and nanorods are still under debate. The major issue here is the size and surface defects, as most of the simulations have failed to adequately represent real life systems. This conference proceeding reports a novel ab initio density functional theory simulation approach to study alkanethiol and gold nanocomposite. Density functional theory (DFT) calculations on SAM of hexanethiol on a multifaceted one dimensional octagonal gold nanorod have been performed. Electron density mapping on the nanocomposites have found that only the top two layers of gold atoms contributed to the charge transfer to sulfur atom. This suggest that smaller basis can be used to simulate inner gold atoms as they do not contribute to the structure of SAM. The structure optimization of gold nanorod was performed with a mixed basis, the outermost layer of gold atoms used double-zeta plus polarization (DZP), the layer below used double-zeta (DZ) and the inner layers used single zeta (SZ). The result are compared with simulations using DZP for all atoms, or mixed DZP and DZ. The results for all other 3 setup is very similar. The bond length is between the gold atom is  $3.09\text{\AA}$  for DZP/DZ/SZ mixed,  $3.04\text{\AA}$  for DZP/DZ mixed and  $3.02\text{\AA}$  for DZP only. This means that to save computational resources, a mixed basis system can be adopted for future nanorod simulations. Phonon dispersion calculations and ab initio molecular dynamics (AIMD) was used to study the stability of the system. From the phonon dispersion simulation it found that the nanorod system is dynamically stable. In addition, AIMD simulation also prove that the system is finite temperature stable at 300K. Finally, alkanethiol ligands with various lengths were added to the surface. This is to study the corner and edge effects on the ligand packing for a multifaceted nanorod system. The ligands will arrange themselves to reduce total system energy by bending towards free space. This leads to significant surface reconstruction with each facet of the nanorod forming a positive or negative concavity. These results contribute to the evolving atomic-level characterization of self-assembled monolayers on gold surfaces by shedding light on conformation and stability.

***Alireza Shams (McGill University)***

## **Modeling of Disclination Loops in Bent-core Liquid Crystals**

The relaxation of disclination loops serves as a useful tool to characterize material properties as well as to reveal texture stability and pattern formation mechanisms in anisotropic soft matter. Bent-core liquid crystals are topic of interest because of their interesting properties such as ferroelectricity and their texture which is affected by the polarity and biaxiality. In most of previous models, disclination loops have been considered as perfect circles which rarely occur in real experiments for bent-core LCs. In this study, using the balance between the elastic and the viscous forces, we drive a general model to predict the shape of loops. Solving a set of time-dependent partial differential equations, in which curvature (K) and velocity (V) are defined as a function of time (t) and arc-length (s), and validating results with experimental data lead to finding important viscoelastic properties. This new model is also useful to predict other novel structures.

**Carolyn Madwar (McGill University)**  
**Tracking Membrane-Specific Cytoskeletal**  
**Organization in Living Cells using Model Lipid**  
**Microdomains**

Lateral asymmetry exhibited through the heterogeneous distribution of lipids, proteins and other components in biological membranes is thought to be fundamental to various cellular events, including signaling, protein/receptor trafficking, and membrane fusion. The occurrence and maintenance of such heterogeneity within the plane of the biological membrane is not yet understood. The approach introduced here allows exploration of how co-existing lipid microdomains of a well characterized model system interface with biological membranes. Co-existing lipid microdomains are formed on a spherical solid substrate [1] and co-cultured with living cells [2] in order to study the relationship between the presence of lipid microdomains and the respective ordering of cellular cytoskeletal networks in response to membrane heterogeneity. Both actin filaments and microtubules, two major cytoskeletal components, are found to preferentially extend and assemble around the fluid lipid domains. Due to its experimental versatility, this system can be extended to experiments involving cell culture in other important biological procedures without losing the structural integrity of the membrane domains formed on the solid supports.

[1] G. Gopalakrishnan, I. Rouiller, D. R. Colman, R. B. Lennox Langmuir 2009, 25, 5455.  
[2] G. Gopalakrishnan, P. Thostrup, I. Rouiller, A. L. Lucido, W. Belkaid, D. R. Colman, R. B. Lennox ACS Chem. Neurosci. 2010, 1, 86.

**Graham Hamblin (McGill University)**  
**Rolling Circle Amplification-Templated DNA**  
**Nanotubes Show Increased Stability and Cell**  
**Penetration Ability**

DNA nanotubes hold promise as scaffolds for protein organization, as templates of nanowires and photonic systems, and as drug delivery vehicles. We present a new DNA-economic strategy for the construction of DNA nanotubes with a backbone produced by rolling circle amplification (RCA), which results in increased stability and templated length. These nanotubes are more resistant to nuclease degradation, capable of entering human cervical cancer (HeLa) cells with significantly increased uptake over double-stranded DNA, and are amenable to encapsulation and release behavior. As such, they represent a potentially unique platform for the development of cell probes, drug delivery, and imaging tools.

***Feng Qi (McGill University)***

## **Accelerated aging: nature's green strategy for metal-organic material synthesis**

Inspired by “mineral weathering” processes,[1] we now describe a solvent-free and low energy synthetic approach, termed "accelerated aging",[2] which starts from solid metal oxides and produces 1-D, 2-D and 3-D close-packed or open metal organic coordination frameworks under mild conditions. Such frameworks are traditionally obtained through high temperature and pH-controlled hydrothermal processes.[3] In contrast, accelerated aging is conducted under mild thermal energy input (temperatures up to 45 °C) or can be even accomplished at room temperature if a brief mechanical activation process is applied. Accelerated aging implements the principles of green chemistry and atom economy by using each starting material only in the amount specified by the composition of the final product, avoiding high temperatures and organic solvents, and by generating water as the only side product. This mild solid-state methodology is readily scaled up to at least 10 gram amounts, suggesting applicability at large scales.