Joint Workshop 2018

Le Centre National de la Recherche Scientifique (CNRS) and McMaster University

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<td>8:00 – 9:00</td>
<td>Breakfast Faculty Club - Participants registration</td>
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<td>9:00 – 10:00</td>
<td>Welcome - Rob Baker (Vice-President, Research, McMaster University), Peter Mascher (Vice-Provost, International Affairs, McMaster University), Antoine Rauzy (French Embassy in Canada), Xavier Morise (Director, CNRS Bureau Washington), Yves Bréchet (High Commissioner to Atomic Energy, France)</td>
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<td>10:00 – 10:40</td>
<td>The tools available for Canada-France academic cooperation involving CNRS Xavier Morise (Director, CNRS Bureau Washington), Antoine Rauzy (Science and Higher Education Attaché, French Embassy in Canada)</td>
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<td>BREAK</td>
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<td>11:00 – 12:00</td>
<td>Group Panel 1: Key-features of the collaboration between McMaster and CNRS groups in Materials Science; Presentations by: Gianluigi Botton (McMaster), Hatem Zurob (McMaster), Matthieu Bugnet (Lyon), Muriel Veron (Grenoble)</td>
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<td>12:00 – 14:00</td>
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<td>14:00 – 15:00</td>
<td>Group Panel 2: Key-features of the collaboration between McMaster and CNRS groups in Pure &amp; Applied Mathematic; Presentations by: Patrick Speissegger (McMaster), Nicholas Kevlahan (McMaster), Lia Bronsard (McMaster)</td>
<td>McMaster University - The University Club</td>
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<td>15:00 – 16:00</td>
<td>Group Panel 3: Key-features of the collaboration between McMaster and CNRS groups in Theoretical Chemistry; Presentations by: Paul Ayers (McMaster), Julia Contreras-Garcia (Paris), Christophe Morell (Lyon)</td>
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<td>16:00 – 16:20</td>
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<td>16:20 – 16:40</td>
<td>Highlights of current activities in Dept. of Mathematics and Statistics, Hans Boden, Chair, Department of Mathematics and Statistics (McMaster)</td>
<td>McMaster University - The University Club</td>
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<td>16:40 – 17:10</td>
<td>Overview of McMaster University’s international positioning and strategy, Peter Mascher (Vice-Provost, International Affairs, McMaster University)</td>
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<td>17:00 – 19:00</td>
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<td>19:00</td>
<td>DINNER</td>
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<td><strong>Tuesday, February 6</strong></td>
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<td>8:30 – 10:10</td>
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<td>10:10 – 10:30</td>
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<td>19:00</td>
<td>DINNER (FACULTY CLUB)</td>
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<td><strong>Wednesday, February 7</strong></td>
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<td>7:30 – 8:30</td>
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<td>8:30 – 10:30</td>
<td>Wrap up of breakout session</td>
<td>Reflections</td>
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<td>10:30 – 11:00</td>
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<td>11:00 – 12:00</td>
<td>General conclusions of the workshop</td>
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<td>8:30</td>
<td>Yvon Maday</td>
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<td>8:55</td>
<td>Mounir Mesbah</td>
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<td>9:20</td>
<td>Miha Zaloznik</td>
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<td>9:45</td>
<td>André Phillion</td>
<td>Department of Materials Science and Engineering</td>
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<td>Olivier Isnard</td>
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<td>10:55</td>
<td>Yurij Mozharivskiy</td>
<td>Department of Chemistry and Chemical Biology</td>
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<td>11:20</td>
<td>Muriel Braccini</td>
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<td>11:45</td>
<td>Hugo Van Landeghem</td>
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<td>12:10</td>
<td>LUNCH BREAK</td>
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| 13:30  | Jean-Christophe Sangleboeuf  
UMR 6251  
Rennes | Shock in metallic glasses | Thomas Dubos  
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Palaiseau | Structure-preserving numerical methods for atmospheric flows | Walter Craig  
Department of Mathematics and Statistics  
McMaster | The mathematics of ocean waves and tsunami prediction |
| 13:55  | Frédéric Pailloux  
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Poitiers | Investigations of ceramics and composite materials by TEM: overview of recent studies in Poitiers | Nicholas Kevlahan  
Department of Mathematics and Statistics  
McMaster | Dynamically adaptive computational methods for climate modelling | Lia Bonsard  
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McMaster | Droplet phase in a nonlocal isoperimetric problem under confinement |
| 14:20  | Peter Mascher  
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McMaster | The Role of Rare Earth Doping in Silicon Photonics | Georges-Henri Cottet  
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Grenoble | Eulerian models and level set methods for fluid-structure interaction problems | Edwin Kermarrec  
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| 14:45  | Jean-Pierre Landesman  
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Rennes | Technology-related thermomechanics on III-V semiconductor compounds and applications | Bartek Protas  
Department of Mathematics and Statistics  
McMaster | Extreme Vortex States and the Hydrodynamic Blow-Up Problem | Bruce Gaulin  
Department of Astronomy  
McMaster | New Quantum Materials in the Brockhouse Institute for Materials Research |
| 15:10  | COFFEE BREAK      | COFFEE BREAK      | COFFEE BREAK      |
| 15:30  | Patrick Cassam-Chenaï  
UMR 7351  
Nice | New ideas to reduce the computational complexity of non-orthogonal geminal methods for strongly-correlated electronic systems | Jean-Christophe Harmand  
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Orsay/Saclay | III-V nanowire growth: from ex situ to in situ experimental investigations | Stan Alama  
Department of Mathematics and Statistics  
McMaster | On Saturn-ring defects in a nematic liquid crystal |
| 15:55  | Hans Boden  
Department of Mathematics and Statistics  
McMaster | Cobordism and concordance of virtual knots | Ray LaPierre  
Department of Engineering Physics  
McMaster | Nanowire Optoelectronics | Patrick Speissegger  
Department of Mathematics and Statistics  
McMaster | A generic instance of Roussarie’s conjecture |
| 16:20  |                    |                    |                    |
| 16:30  | Tour CanmetMATERIALS |                    |                    |
Nonlinear eigenvalue problems occur in many mathematical models used in science and engineering such as the calculation of the vibration modes of a mechanical structure in the framework of nonlinear elasticity, the ground state of the Gross-Pitaevskii equation describing the steady states of Bose-Einstein condensates, or for the Hartree-Fock and Kohn-Sham equations used to calculate ground state electronic structures of molecular systems in quantum chemistry and materials science.

The approximation of the solutions to these problems is of major importance and different methods are proposed depending on the various applications these solutions aim at. These approximation are based on different ingredients. First comes the notion of degrees of freedom, associated with the basis sets that are used to approximate the solutions of these problems. This leads to a discrete problem that can be solved, hopefully, on a computer. The discrete problem is, per force, nonlinear and performant algorithms must be designed to solve efficiently this discrete problem. These two ingredients (and there may be more of them) that allow to solve the original problem must be well tuned so that the approximation of the solution is good enough.

The exact solution being unknown, arguments to estimate the error committed by the approximation need to be proposed and, these last years, a large number of contributions about the numerical analysis of these eigenvalue problems have been published dealing with the “a priori” and the “a posteriori” analysis.

We shall present, in a unified manner, some approaches that have been proposed in the literature that go from perturbation theory (well known in the computational community) to residual based errors (that are typically use in other communities).

Bone mineral is composed of carbonated hydroxyapatite crystals which a key play a role on the biomechanical properties and calcium homeostasis, two of the main functions of bone. Hence, any alteration of the structure and composition of the mineral could affect either or both those functions. It is, now, well know that the mineral nanocrystals in bone have unusually small dimensions (platelet shaped with ~ 5 nm in thickness) with respect to geological crystals of similar structure and composition. However, their characterization remains a daunting challenge since electron microscopy methods generally provide a limited view of the structure that may not be representative of the whole tissue/organ, while X-ray scattering “only” provides an average information. This presentation will describe how the use of quantitative scanning small-angle X-ray scattering (qsSAXSI) can be used to overcome those limitations. A selected set of results will be presented illustrating possible nanoscale pathological modifications of the mineral phase and highlighting the importance of a multiscale approach to account for the histological (microstructural) heterogeneity [1,2].


**8:30 | BREAKOUT SESSION 3**

The steel bridges between Canada and France: from classical metallurgy to architectured materials  
D. Fabrègue, A. Weck, E. Maire, H. Zurob, J. Adrien  
UMR 5510 Lyon

Long term collaboration on the thematic of steel has been set up between CNRS and McMaster. The initial study aims at looking at the deformation and fracture process in steels and in model materials. The elaboration was made in Canada whereas the characterization was realized at the synchrotron in France. There are still a lot of work to be done and an ANR has been proposed a few years ago to better understand the fracture of multiphased steels. We want to go further on modeling of the damage in these materials. Moreover, we also propose here to work on architecture materials together by studying for example the corrugated materials in terms of microstructure and of mechanical properties.

**8:55 | BREAKOUT SESSION 1**

The Backward Reliability Curve and its use in validation of measurement properties of a Health Related Quality of Life instrument  
Mounir Mesbah  
LPSM, Sorbonne Université, Paris

Quality of life is an important variable in health sciences. It measurement remains an important issue. Statistical validation of quality of life measures is mainly done through the validation of specific measurement models linking responses to several questions to a theoretical unobserved latent variable representing quality of life. In this work, we show how to use the Backward Reliability Curve to validate certain properties underlying these measurement models, the unidimensionality and the local independence of the questions. We present simulation results and show applications to real Health Related Quality of Life data.

**8:55 | BREAKOUT SESSION 2**

Correlative Microscopy Approaches for Investigating Biominerals  
Kathryn Grandfield  
Dept. of Materials Science & Engineering / School of Biomed. Eng., McMaster University

Biominerals make up some our most important tissues, such as our bones and teeth. Uncovering the mechanisms of biomineralization or biomaterial-tissue interactions is complicated by the complex and 3D hierarchical structure and chemical heterogeneities of many natural biominerals. Elucidating the multi-length-scale spatial and chemical structure of tissues such as bone or cementum has the potential to shed light on their mineralization mechanisms and lead to improvements in the design of biomaterials for joint replacement and dental applications. In our work we explore the structure, formation and attachment of human bone to biomaterials such as titanium with advanced correlative microscopy approaches. This talk will introduce a range of correlative 3D to 4D approaches to investigate mineralized tissues and the bone-implant interface, including X-ray computed tomography, on-axis electron tomography, electron energy loss spectroscopy tomography, and atom probe tomography.

**8:55 | BREAKOUT SESSION 3**

Exploring the gas-surface interaction of nanocatalysts in the environmental transmission electron microscope  
Matthieu Bugnet  
UMR 5510 Lyon

Transmission electron microscopy (TEM) is a well-established characterization technique to combine bulk as well as surface analysis in a wide range of materials at the nanoscale. Since the large majority of materials are not utilized in moderate or high vacuum, investigating them in situ in the TEM in more realistic environmental conditions appears necessary to understand fundamental structural and chemical aspects at surfaces in several fields of research such as catalysis, corrosion, or crystal growth. In this respect, control of the nature and the pressure of the atmosphere surrounding the specimen while allowing nanoscale down to atomic resolution in a transmission electron microscope is of great importance. Surface phenomena observed on individual nanoparticles, and induced by the partial pressure and temperature within a dedicated Cs-corrected environmental TEM (ETEM), will be presented, with a particular focus on heterogeneous catalysis applications. For example, controlling the atomic mobility at surfaces of ceria (CeO2) nanocubes under reducing and oxidizing conditions sheds light on the surface structure and chemistry, and opens a field of study for direct visualization of atomic scale phenomena such as carbonate adsorption [1]. The microscopy group in Lyon also works on the development of fast electron tomography for beam sensitizes materials and dynamic studies under environmental conditions [2]. Recent examples will be presented, such as the combustion of soot by zirconia, allowing the activation energy of the soot combusion to be evaluated [3].

During solidification different physical phenomena are in strong dynamic interaction. They involve a large range of spatial scales, from the nanoscale to the macroscale of an industrially cast piece. All these phenomena are the origin of defects and structural heterogeneities in products made by solidification processing (casting, welding, additive manufacturing) and are thus of prime industrial importance. In process-scale (macroscale) modeling, the smaller scales are approximated by models based on averaging methods. This requires careful simplification and averaging of the microscale phenomena and interactions. We present the most recent applications of state-of-the-art models to industrial solidification processes (casting of steel ingots, DC casting of Al alloys). We then discuss the path towards improved predictive and quantitative capabilities based on hierarchical multiscale modeling.

Structural quality and stability of nano- / micro crystals are fundamental problems that bear important consequences for the performances of small-scale devices. Stability and mechanical behavior is clearly modified as compared to bulk materials (size effect) and functional properties are largely influenced by elastic strain and depend critically on the presence of crystal defects. It is thus of prime importance to be able to measure and monitor quantitatively, if possible by noninvasive means, the stability of structures against external mechanical stimuli. Instrumented indentation combined with emerging Bragg coherent diffraction 3D imaging techniques (synchrotron radiation) have the potential to address such fundamental problematics.

Transmission electron microscopy is an invaluable technique to study the detailed structure and the chemical state of materials at unprecedented spatial resolution. In today’s modern electron microscopes, it is possible to tackle problems requiring the highest energy resolution to detect losses down to 70meV, and highest spatial resolution, down to the angstrom level, so that atomic resolved spectroscopy with high spectroscopic sensitivity and resolution can be obtained. This leads to the potential of covering excitation phenomena from the mid-infrared, soft-X-rays and even hard-X-ray regime.

In this presentation, various examples of applications of electron microscopy will be given to highlight how microscopy and spectroscopy are essential to understand the properties of a broad range of materials such as nanocatalysts, metallic alloys, plasmonic materials and functional oxides.

Meso-scale multi-physics models based on granular materials are finding use in gaining understanding of defect formation mechanisms during metallic-alloy solidification processes. In this talk, research is presented on the use of meso-scale models for predicting hot tearing/solidification cracking in aluminum alloy casting and welding processes. These models couple solidification modules, mechanical deformation modules, fluid-flow modules, and defect modules in order to first construct the microstructure of the semi-solid, second to simulate deformation and intergranular flow, and finally to comprehensively predict crack formation. Examples will be given for wrought and foundry aluminum alloys.
Study of phase transformations in Steel and New titanium alloys

Muriel Veron
UMR 5266 Grenoble

An Automated Crystal Orientation and phase Mapping technique (ACOM) was developed for TEM’s in our laboratory, which proved to have a good reliability and a reasonable acquisition time (ASTAR). This technique has many applications such as studying deformation mechanisms in structural materials e.g., steels or magnesium alloys, but also to address new challenges, for instance in-situ deformation of nano-crystalline films. Here the technique is used to investigate materials that have a TRIP behavior, i.e., that during plastic deformation, due to dislocation activity, new martensitic phases are produced. As a first example, austenitic TRIP steels are studied after deformation, to characterize at a fine scale deformation mechanisms and orientations of new phases induced by plasticity. Other materials, such as new titanium alloys are also inducing phase transformation with plastic deformation, and detailed analysis will be shown.

High Manganese Austenitic Twinning Induced Plasticity Steels: A Review of the Microstructure Properties Relationships

Olivier Bouaziz
UMR 7239 Metz-Nancy

A significant increase in the research activity dedicated to high manganese TWIP steels has occurred during the past five years, motivated by the breakthrough combination of strength and ductility possessed by these alloys. Thus a review of the relations between microstructure and mechanical properties is presented focusing on plasticity mechanisms, strain-hardening, yield stress, texture, fracture and fatigue. This summarized knowledge explains why TWIP steel metallurgy is currently a topic of great practical interest and fundamental importance. Finally, this publication indicates some of the main avenues for future investigations required in order to sustain the quality and the dynamism in this field of interest.

Magnetic properties of rare-earth-transition metal intermetallic compounds

Olivier Isnard
UPR 2940 Grenoble

Intermetallic compounds based on rare-earth (R) and transition metals (T) form an important class of materials for energy conversion or storage with various applications such as permanent magnets, magnetostrictive sensors, magneto-optical devices, hydrogen storage materials, others are foreseen in near future such as magnetocaloric refrigeration... These materials are also challenging our fundamental understanding of magnetism and basic research is needed to improve their functional properties. Indeed, they are combining two different kinds of magnetism, the itinerant electron magnetism of T elements with the localized magnetism of the 4f electronic shells of the R elements. In order to illustrate some of the studies performed at the Néel Institute, several examples of recent results on the intrinsic magnetic properties of R-T intermetallic compounds will be shown on T=Fe or Co rich compounds. The effect of applied pressure, atomic substitution and or interstitial element insertion are some of the means used to probe the magnetic phase diagram and the structural behavior of these compounds investigated by neutron diffraction, synchrotron radiation as well as high magnetic field.
Three current directions of research will be shortly presented.

1. Model Hamiltonians.
   A form of the electronic Hamiltonian is considered in which the interaction between electrons is modified such as to allow an easier access to approximate solutions to the Schrödinger equation. [1]

   Instead of relying on experience, databases are nowadays produced, and statistical tools are used on them to provide recommendations for the methods to use. However, these tools are not necessarily as reliable as it seems. [2, 3]

3. Quantum mechanical tools for visualizing the chemical bond.
   A simple model shows that for a time-dependent process existing tools (localized orbitals, laplacian of the density, electron localization function, maximum probability domains) are not equivalent. [4]


This presentation will highlight applications of the density functional theory (DFT) to prediction of structure and functional properties of optoelectronic materials, 2D materials, and organic-inorganic interfaces. It will be shown how the effective band structure of semiconductor alloys can be used to assess optical and charge transport characteristics of materials used in solar cells, telecommunication lasers, and thermoelectric applications. Studies of isoelectronic substitutional defects enable predictions about formability of semiconductor alloys, the band gap evolution, and changes in the band alignment. By combining DFT capabilities of simulating charged structures and 2D materials, it becomes possible to capture a reversible structural transition between insulating and metallic phases in transition metal dichalcogenide monolayers due to the presence of excess charge carriers. Finally, the adsorption of organic molecules at the surface of nanomaterials allowed the development of novel strategies for the surface modification, dispersion, and advanced synthesis of nanoparticles. Ab initio simulations are used to identify most stable surfaces, their reconstructions, and probe the adsorption strength of molecules in the presence of a solvent.

Magnetic refrigeration has a potential for large-scale industrial applications. The discovery of the giant magnetocaloric effect in Gd5Si2Ge2 around room temperature¹ can make this possibility a reality.

The related RE5X4 phases prove to have rich structural chemistry and interesting physical properties. Modification of the electron concentration is a powerful tool to tune the structure and magnetism of RE5X4 and can be implemented via chemical substitution on the RE or X sites. Detailed analysis of the resulting transitions and bonding in these phases provides insights into the structure-property relationship and allows formulating some guiding principles for the design of new magnetocaloric materials.

References:
A flexible ansatze for N-electron wavefunctions that subsumes the wavefunctions used in traditional configuration interaction approaches, coupled cluster methods, geminal-product wavefunctions, electron-group-function approaches, matrix-product states, and tensor-network states is presented. In this approach, desirable properties of wavefunctions (e.g., quasiparticle interpretations; size-consistency) are expressed as properties of a function that determines the coefficients of Slater determinants as (generally nonlinear) functions of the input parameters. Some of these key properties will be presented, allowing us to generate entirely new wavefunction forms that have desirable formal properties and yet, in some cases, are fully applicable to strongly correlated systems. A perturbative form of this approach will also be presented; the perturbative expression is especially useful for generating initial guesses for the wavefunction optimization.

Modelling the evolution of microstructure during thermomechanical processing is an essential step for optimizing the processing conditions and achieving the desired material properties. In this presentation, we review progress in three areas in which researchers from McMaster and CNRS collaborated to advance the state-of-the-art in the field. The first area is that of ferrite growth during austenite decomposition. The second area concerns the interaction between recovery, recrystallization and precipitation during the hot-rolling of microalloyed steels. The third example to be discussed will focus on the development of architectured and functionally graded materials. The impact of these developments on the field of physical metallurgy will be highlighted along with the need to strengthen collaborations between McMaster and CNRS.

In SIMaP laboratory, SIR group, focusing on Surfaces, Interfaces and Reactivity in materials, works on three main themes: high temperature oxidation of metals, physico-chemical properties of surfaces and mechanics of interfaces. The common objective is the durability of materials under environmental or and mechanical solicitations. Metal/oxide interfaces is then a system widely studied in the group. Indeed, metal/oxide interface is found in various applications, from hot processing to energy, from microelectronics to medicine. Nevertheless, it is often a weak spot in terms of mechanical resistance which is still an issue for system reliability and durability. Some of the group activities focusing on the interaction of chemistry and mechanics on metal/oxide system durability will be presented: first, at high temperature, the influence of metal alloy chemistry on the mechanical resistance of oxide scale (toughness and adhesion); at lower temperature, the slow crack growth at metal/oxide interface under environment and/or cyclic solicitations.
The Dual Descriptor [1] is one of the local reactivity indicators defined in the density functional theory of chemical reactivity [2,3]. It is mathematically defined as the second derivative of the electron density with respect to the number of electrons:

\[ f^{(2)}(\mathbf{r}) = \left( \frac{\partial^{2} \rho(\mathbf{r})}{\partial N^{2}} \right)_{N} = \left( \frac{\partial^{2} \eta}{\partial \mathbf{r}^{2}} \right)_{N} \]

It has been shown that its sign is an indicator of the electrophilicity/nucleophilicity of a reactive site within a molecule [4,5]. This feature has been extensively applied in organic chemistry [6,7]. Recently, new physical bases have been given to the DD [8] by expanding the electron density of a perturbed ground state through excited densities [9]. This expansion had led to the proposal of state specific dual descriptors. Part of the talk focuses on the application of these descriptors, especially how they help describing chemistry in cases where indexes based upon frontier orbitals fail. A third descriptor depicting the polarization of the electron density due to an electrostatic potential is presented. Examples of application of this toy model will be exposed. Besides, an efficient algorithm has been proposed to partition real space descriptors into domains of univocal reactivity and to accurately characterize their properties [10]. The main goal of this talk is to present these new tools as well as their applications [11].

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Quantum Chemical Topology (QCT) provides insight into the electronic organization in Cartesian space by means of the analysis of 3D functions with chemical meaning such as the electron density. We will review several aspects of this approach and dwell on their relationship with both mathematics and material science.

One of the main flaws of QCT is that it is barely predictive. This is so due to the lack of a direct (known) link between electron density topology and energetics (and hence properties). We have explored using a potential energy surface that includes chemical quantities explicitly, so that properties provided are directly related to the inherent organization of electrons within the regions provided by topological analysis.

One way to approach this gap is to build energy models relying on topology. This can be done by comparing with energy partitions from topological partitions. However, the integrations schemes not centered in atoms need to be adapted. Hence, this area could be enriched by new sampling techniques.

Another way is to resort to potential or energy models. One such example is the Bond Charge Model by Parr (BCM) [1], to describe the energetics of electron pairs. Coupling this to conceptual DFT, the band gap of solids can be univocally defined [2]. Applied to zinc-blende solids as a model case, trends in band gap can be predicted in terms of bond properties (length, charge, crystalline structure- Figure 1).

Potential models also provide insight into the distribution of electrons, and enable to explain their redistribution upon changes in the external conditions (e.g. pressure).

Hence, with these model systems, properties of material science can be understood and predicted from their chemical bonding pattern.

References:
Shock in metallic glasses

J-C. Sangleboeuf1, B. Jodar1, D. Loison1, M. Nivard1, H. Orain1, Y. Yokoyama2, E. Lescoute3, L. Berthe4

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2) Institute for Material Research, Tohoku University, Sendai, Japan
3) CEA/DAM/DIF, Arpajon, France
4) PIMM, UMR CNRS 8006, Paris, France

High Velocity debris shielding is of concern since the amount of orbiting space objects is continuously increasing. Thus, the space industry is always searching for innovative and effective materials combining high mechanical properties and lightweight. The Bulk Metallic Glasses family appears to be suitable for such applications. Therefore, the suitability of a ternary ZrxCu90-xAl10 Bulk Metallic Glass (with x = 45, 50, 55, 60) is investigated by characterizing its dynamic behavior at high pressure and high strain rate (107-108 s-1). Laser irradiation of various pulse durations (350 fs, 600 ps and 5 ns) were used to generate different shock waves profiles to study the strain rate dependency on the spalling process. Ejecta velocities were measured for several sample thicknesses and pulse durations by Photonic Doppler Velocimetry and transverse shadowgraphy. Spall velocity diagram for 350 fs shots emphasize two distinct velocity domains that may be attributed to a rheological/material behavior change. Scanning Electron Microscopy observations performed on the recovered fracture surfaces highlight the presence of a peculiar feature known as “Cup and Cone”. The presence of cups and cones and their morphologies are revealed to be strongly strain rate and compositional dependent. This last dependency can be correlated to specimens Poisson’s ratios that are known to have a role on the fracture behavior of Bulk Metallic Glasses. Furthermore, cups are found on sample while cones are observed on spall. By investigating the cups and cones morphologies, two distinct regions are observed: a smooth viscous-like in the center and a flat peripheral one with a large vein-pattern. Energy Dispersive Spectroscopy measurements conducted on these features bring an atomic segregation out taking place during spallation. A mechanism for the initiation and the growth of these cups and cones but also a process for atomic segregation during spallation will be presented.
**Dynamically adaptive computational methods for climate modelling**

Nicholas Kevlahan  
Dept. of Mathematics & Statistics, McMaster University

This talk reviews adaptive methods for partial differential equations and outlines a dynamically adaptive wavelet method for a hydrostatic climate model on the sphere. The adaptive grid hierarchy is a dyadic subdivision of the icosahedron, which is optimized to ensure good geometric properties.

Distinct biorthogonal second generation wavelet transforms are developed for the pressure and the velocity, together with compatible restriction operators to ensure discrete mass conservation and no numerical generation of vorticity.

This project is an initial step towards developing a full dynamically adaptive climate model. I will also discuss some outstanding issues in sub-grid parameterization of multiphysics processes (e.g. unresolved turbulence, cloud formation, precipitation, effect of topography).

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**Droplet phase in a nonlocal isoperimetric problem under confinement**

Lia Bronsard  
Dept. of Mathematics & Statistics, McMaster University

We begin with a variational model for the self-assembly of diblock copolymers under confinement, which takes the form of an isoperimetric problem which is both nonlocal and nonhomogeneous. That is, we seek minimizers in the form of characteristic functions of fixed volume. The energy consists of three competing terms, and minimizers should reduce their perimeter (as in the classical isoperimetric problem,) but also prefer spatial separation into disjoint components, which are confined by an attractive potential. We consider periodic configurations in the small volume fraction limit, in which one phase forms vanishingly small droplets in a sea of the complementary phase. Introducing a small parameter, which represents the radii of the droplets, we show that the minority phase splits into several droplets which converge to the maximum value of the confining potential, at an intermediate scale $1/3$. Isolating the droplets at the scale $1/3$ requires a fine analysis of the blown-up problem, using concentration-compactness and the regularity properties of minimizers of the nonlocal isoperimetric problem on $\mathbb{R}^3$. This is joint work with Stan Alama, Rustum Choksi and Ihsan Topaloglu.

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**The Role of Rare Earth Doping in Silicon Photonics**

Peter Mascher  
Department of Engineering Physics, McMaster University

In order for Si-based materials to be used in solid-state lighting (SSL) schemes it is necessary to have precise control of the optical emission from these materials. This can be accomplished through the use of rare earth dopants such as Ce, Tb, and Eu to obtain blue, green, and red emissions, respectively. After a brief review of the latest developments in the field, this talk will focus on the luminescence of rare earth (Ce, Tb, Eu) doped silicon oxides, nitrides, and carbides. We have demonstrated very high, optically active concentrations of the rare earths by using in-situ doping processes, using electron cyclotron resonance chemical vapour deposition (ECR-CVD) or inductively coupled plasma (ICP) CVD as low thermal budget processes for film deposition. We will describe the salient features of the deposition systems and correlate important process parameters with the observed luminescence. Finally, we will discuss some of the challenges in developing electrically driven lighting cells suitable for SSL and in particular, for the development of widely tuneable Si-based light sources.

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**Eulerian models and level set methods for fluid-structure interaction problems**

Georges-Henri Cottet  
UMR 5224 Grenoble

After reviewing the activities of my lab and of my research group in applied mathematics, I will discuss research led in this group in the 10 last years concerning models and algorithms for fluid-structure interaction problems. Fluid-structure interaction problems are in general dealt with by methods where specific models for fluids and structures (typically eulerian for fluids and lagrangian for structures) are used and coupled at the interface with appropriate boundary conditions. These methods require to discretize the domains with meshes that fit the fluid-solid interfaces. The alternative we develop is to see both media as a single fluid, with space and time varying rheology, in an Eulerian approach. The interface between the media is captured by a level set function which is advected by the fluid velocity. The computational mesh does not need to fit the interfaces.

I will describe these methods, discuss advantages and drawbacks compared to more classical methods, and illustrate them with applications in biophysics for the simulation of biological vesicles and cells.
A Quest for Classical and Quantum Spin Liquid phases in Kagome Materials

Edwin Kermarrec
UMR 8502 Orsay

The kagome geometry, a two dimensional lattice made of corner sharing tetrahedra, has fascinated artists and architects who used it to decorate historical monuments and many objects of our everyday lives. More recently, it has also been of high interest to solid-state physicists as it questions our fundamental understanding of quantum states of matter, a very topical subject in modern condensed matter physics, as highlighted by the 2016 Nobel Prize in physics.

I will first present our research group at the Laboratoire de Physique des Solides (LPS), which focuses on the study of novel electronic states of matter using spectroscopic techniques (NMR, μSR, ARPES and inelastic neutron scattering) at low temperatures. Then, I will present selected examples of current research on kagome materials developed both at the LPS and at McMaster University. This area of research clearly requires an interdisciplinary approach, at the crossroads of physics, mathematics and chemistry of materials.

Technology-related thermomechanics on III-V semiconductor compounds and applications

Jean-Pierre Landesman
UMR 6251 Rennes

Mechanical stress can be a concern for semiconductor devices, both in microelectronics and photonics, especially for “nanodevices”. Mechanical stress can be a cause of performance reduction or reliability limitation, but it can also be used to tune some of the local properties of the semiconductor materials “on demand”. There are examples where controlled crystal deformation is used in that way in Si devices fabrication for some years already.

Mechanical stress can be due for example to the presence of thin dielectrics at the surface, but it can also be induced / modified by some of the fabrication processes. Plasma etching is of these processes that can strongly impact the semiconductor crystal. Using different techniques to probe and map crystal deformation, namely the degree of polarization of photo-luminescence and the spectral imaging in cathodo-luminescence, we have been able to revisit classical models for the thermomechanics of crystal deformation below thin dielectric films and also demonstrate the importance of monitoring the crystal deformation at every step in the fabrication of some modern photonic or opto-electronics devices based on GaAs and InP.

Extreme Vortex States and the Hydrodynamic Blow-Up Problem

Bartek Protas
Dept. of Mathematics & Statistics, McMaster University

In the presentation we will discuss our research program concerning the study of extreme vortex events in viscous incompressible flows. These vortex states arise as the flows saturating certain fundamental mathematical estimates, such as the bounds on the maximum enstrophy growth in 3D. They are therefore intimately related to the question of singularity formation in the 3D Navier-Stokes system, known as the hydrodynamic blow-up problem. We demonstrate how new insights concerning such questions can be obtained by formulating them as variational PDE optimization problems which can be solved computationally using suitable discrete gradient flows. In offering a systematic approach to finding flow solutions which may saturate known estimates, the proposed paradigm provides a bridge between mathematical analysis and scientific computation. [Joint work with Diego Ayala and Dongfang Yun]

New Quantum Materials in the Brockhouse Institute for Materials Research

Bruce Gaulin
Department of Astronomy, McMaster University

The Brockhouse Institute for Materials Research (BIMR) is home to Canada’s most extensive infrastructure for the synthesis and growth of new inorganic materials. A particular specialty of the BIMR are quantum materials, whose low temperature properties are determined by the quantum nature of single electrons, or $S=1/2$ effective particles. These are often transition metal oxides that can be grown by floating zone image furnace techniques. I will discuss recent work on new quantum and geometrically-frustrated pyrochlore magnets, and also high temperature superconductors, whose basic properties defy our intuitions, and could underly transformative future applications.
15:30 | BREAKOUT SESSION 1

New ideas to reduce the computational complexity of nonorthogonal geminal methods for strongly correlated electronic systems

Patrick Cassam-Chenaï
UMR 7351 Nice

The Lewis electron-pair picture pervades all of chemistry and a substantial domain of materials science. "Geminals" are electron-pair quantum states which are used to express approximate solutions of the Schrödinger equation of polyelectronic systems. In quantum chemistry, geminal-based methods are potentially more effective than the traditional ones based on the orbital picture: electrons occupy orbitals and experience only the average effect of each other. This is especially true for strongly correlated-systems. However, the computational cost of using arbitrary geminal wave functions is non-polynomial in the system size.

It is therefore an important challenge to find additional constraints on geminal models which preserve the accuracy of the wavefunction description while reducing the calculations to polynomial cost. The Ayers' group at McMaster has developed one such successful geminal model called AP1roG because the wavefunction is an antisymmetric product of geminals with one distinct reference orbital occupied in each geminal [1]. This ansatz relaxes the so-called "strong-orthogonality" constraint between geminals. The latter makes wavefunction matrix element computations very easy but appears too drastic from the physical point of view, since the geminal electron pairs are then distinguishable.

We have followed a different path to relax the strong-orthogonality constraint. We have defined the geometrical concept of n-orthogonality [2] which can be viewed as a graded indistinguishability measure for electronic states: 1-orthogonality coincides with strong orthogonality, the larger n the less distinguishable the n-orthogonal electronic states will be. We have studied geminal models constrained by n-orthogonality relations for different values of n, imposed to different combinations of geminal product states [3]. However, in this work the scaling of matrix element computations was still unsatisfactory. We will present new ideas developed since then to remedy this problem.

References

15:30 | BREAKOUT SESSION 2

III-V nanowire growth: from ex situ to in situ experimental investigations

Jean-Christophe Harmand
Centre de Nanosciences et de Nanotechnologies, CNRS, Univ. Paris-Sud, Univ. Paris-Saclay

The fabrication of devices based on III-V nanowires requires a good understanding and a good control of the growth mechanisms which govern their properties. Growth kinetics, crystalline structure, morphology, chemical composition, formation of hetero-interfaces, doping efficiency are the important characteristics to master. Our laboratory has been investigating this field for several years and I will illustrate some of our recent results.

The insertion of chemical markers at regular time intervals during growth of GaP nanowires allows us to retrieve the time evolution of their length and diameter. Combined with modeling, these experimental data are analyzed to infer the pathway of Ga adatoms before their incorporation in the solid phase [1]. Regarding doping, cathodoluminescence is used to determine the carrier concentration in single Si-doped aAs nanowires [2]. Beyond these post-growth investigations, we implemented in situ nanowire growth by molecular beam epitaxy in a transmission electron microscope. With this unique instrument, we explore the mechanisms involved in the crystal phase selection of Au-catalyzed GaAs nanowires.

References:
**15:30 | BREAKOUT SESSION 3**

On Saturn-ring defects in a nematic liquid crystal  
Stan Alama  
Dept. of Mathematics & Statistics, McMaster University  

We consider energy minimizing configurations of a nematic liquid crystal, as described by the Landau-de Gennes model. We focus on an important model problem concerns a nematic surrounding a spherical colloid particle, with normal anchoring at the surface. For topological reasons, the nematic director must exhibit a defect (singularity), which may take the form of a point or line defect. We consider two physical regimes in which “Saturn-ring” configurations will be energetically favorable: the case of colloids of small radius, and the case of strong applied magnetic fields. This represents work in collaboration with L. Bronsard and X. Lamy.

**15:35 | BREAKOUT SESSION 2**

Nanowire Optoelectronics  
Ray LaPierre  
Dept. of Engineering Physics, McMaster University  

Semiconductor nanowires are being developed for the next generation of optoelectronic devices. The free lateral surfaces of nanowires allow elastic relaxation of lattice misfit strain without the generation of dislocations, permitting the integration of III-V materials on silicon substrates. Furthermore, nanowires permit high optical absorption due to an optical antenna effect. The self-assisted vapor-liquid-solid method is now a well-established technique for the growth of III-V nanowires on silicon substrates. In this method, an array of holes in a SiO2 film is used for metal droplet collection, which seeds the growth of nanowires. We will present the growth, materials characterization, and device fabrication of some nanowire optoelectronic devices including photovoltaics, infrared photodetectors, and betavoltaics.

**15:35 | BREAKOUT SESSION 3**

A generic instance of Roussarie’s conjecture  
Patrick Speissegger  
Dept. of Mathematics & Statistics, McMaster University  

In 1923, Dulac published a proof of the claim that every real analytic vector field on the plane has only finitely many limit cycles (now known as Dulac’s Problem). In the mid-1990s, Ilyashenko completed Dulac’s proof; his completion rests on the construction of a quasianalytic class of functions. We are attempting to extend this construction in various ways to obtain a uniform version of Dulac’s problem, known as Roussarie’s conjecture, for a generic family of vector fields. (Joint work with Zeinab Galal (Paris), Tobias Kaiser (Passau), Jean-Philippe Rolin (Dijon) and Tamara Servi (Paris))
Facility Tours

**MCMASTER UNIVERSITY**
Wednesday, February 7th

14:00 – 15:30  **Canadian Centre of Electron Microscopy**
A. N. Bours Building (ABB), Room B161

OR

14:00 – 15:30  **Centre for Emerging Device Technologies**
John Hodgins Engineering (JHE) Building, Room A318

14:00 – 15:30  **McMaster Nuclear Reactor**
Nuclear Research Building

OR

14:00 – 15:30  **McMaster Manufacturing Research Institute**
John Hodgins Engineering (JHE) Building, Room 109A

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**UNIVERSITY OF WATERLOO**
Thursday, February 8th

9:00  **Bus departure from Visitor’s Inn**

10:30  **Arrival and Tour /Presentation/Lab tour at WIN**
Sushanta Mitra, Executive Director, Waterloo Institute for Nanotechnology
Matthew Rae, Communication and Events Coordinator, Waterloo Institute for Nanotechnology

12:30  **Lunch at Conference Foyer, RAC 2**
Drew Knight, Director, Global Research & Strategic Alliances, Office of Research (co-host)
Ni Jadon, Senior Project Manager/International Liaison Officer, Office of International Affairs, McMaster University (co-host)

13:30  **Overview Presentation and Discussion (IQC & Transformative Quantum Technologies), RAC 2**
Tracey Forrest, Program Director, Transformative Quantum Technologies

14:30  **Lab tour, Transformative Quantum Technologies, RAC 2**
Tracey Forrest, Program Director, Transformative Quantum Technologies

15:30  **Return**
## Participant List

<table>
<thead>
<tr>
<th>Materials sciences</th>
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### Pure and applied mathematics

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<tbody>
<tr>
<td>Peter Mascher</td>
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## Department of Physics and Astronomy

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<tr>
<th>Name</th>
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<tbody>
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## Department of Chemistry and Chemical Biology

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## Department of Mathematics and Statistics

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General Information

Le Centre National de la Recherche Scientifique (CNRS) and McMaster University

1. Visitor’s Inn
2. McMaster Innovation Park/CANMET
   Tuesday February 6
3. Faculty Club (also named University Club)
   All days
4. CIBC Hall (3rd floor Student Centre)
   Wednesday, February 7
5. Bus stop
   Any – 1, 1A, 5A, 5C, 51

Accommodation

VISITOR’S INN

Your entire stay has been booked at the Visitor’s Inn by our office as per the dates which you have previously provided. The Office of International Affairs at McMaster University will cover the cost of your stay from February 4th to 8th. If you still for additional days outside of this time, you will be required to provide a credit card upon check-in to cover the cost of the stay for those additional days.

649 Main St W
Hamilton, ON | L8S 1A2
905-529-6979
reservations1@visitorsinn.com
www.visitorsinn.com
Transportation

AIRPORT
McMaster has reserved 1 shuttle travelling from Terminal 1 of Toronto Pearson International Airport at 17:00. The limo-bus will be held under the name of Gérald Ferblantier (who happens to have the latest arrival time before the bus departs that day). The shuttle will be at Section A of Terminal 1 on the Arrivals level inside the glass doors. YOU MUST check in with the commissionaire in the booth, if there are any problems please call toll free 1-877-387-6464 for assistance.

VBL Luxury Coach & Limousine
1-905-667-8020 ext 1.
1-877-387-6464
admin@vblbus.com

Airways Transit: Hamilton
905-689-4460
infohamilton@airwaystransit.com

Airways Transit: Waterloo
519-886-2121
infowaterloo@airwaystransit.com
http://www.airwaystransit.com/

WATERLOO
If you are going on the University of Waterloo tour, a limo-bus will pick you up at 9:00 am at the Visitor’s Inn and will return you to the hotel around 16:30.

OTHER OPTIONS
TAXI
Hamilton Cab (905) 777-7777
Blue Line Taxi (905) 525-0000

UBER
If you have this app installed on your smartphone, it works quite well in Hamilton

HSR (public transit)
There are numerous buses which can be caught 2 blocks from the hotel to get to the McMaster University’s main campus. Buses can also be easily caught from the university to the hotel and stop directly beside the hotel.

VISITOR’S INN TO McMaster UNIVERSITY MAIN CAMPUS TRAVEL
There will be a limo-bus from the Visitor’s Inn to get participants to and from McMaster’s main campus. See below for times and drop points. The shuttle will make multiple trips if necessary but can seat 18 and up to 10 people standing. The drive is only 10 minutes. Please note that participants will walk to and from the McMaster Innovation Park and the Visitor’s Inn which is about 600m from the hotel.

February 4 | 6:45 pm | Visitor’s Inn to Faculty Club
February 4 | 9:00 pm | Faculty Club to Visitor’s Inn

February 5 | 7:30 am | Visitor’s Inn to Faculty Club
February 5 | 9:00 pm | Faculty Club to Visitor’s Inn

February 6 | 6:30 pm | Visitor’s Inn to Faculty Club
February 6 | 9:00 pm | Faculty Club to Visitor’s Inn

February 7 | 7:30 am | Visitor’s Inn to Student Centre
February 7 | 5:15 pm | Student Centre to Visitor’s Inn
Meals

**ON-CAMPUS**
All meals will be provided during the Joint Workshop from breakfast on January 5th until lunch February 7th. Light refreshments will also be served during the evening reception on February 4th.

**OFF-CAMPUS**
Hamilton’s downtown has been experiencing quite a wonderful rejuvenation in recent years; if you are curious we would encourage you to travel to some of the restaurants downtown to try some of the excellent local casual restaurants which can be found in the areas of James St. North, King William St. and James Street South.

For more information
http://tourismhamilton.com/tasty-restaurants-hamilton

Emergency Contacts

Jean-Pierre Landesman  289-489-4543
Paul Leegsma  289-683-5627
McMaster University Campus

1. Faculty Club
2. MUSC – CIBC Hall
   3rd floor
3. MUSC – Front Door
   Bus pick up/drop off area
4. CCEM – ABB B161
5. CEDT – JHE A318
6. MMRI – JHE 109A
7. McMaster Nuclear Reactor (MNR) Building
McMaster Innovation Park

PARKING
McMaster Innovation Park

CONFEERENCE – LEVEL 1

1. Breakout Session 1
   Room 1B
2. Breakout Session 2
   Room 1A
3. Breakout Session 3
   Room 2