Friday, April 25, 2008 - Science Pavilion S110, Loyola Campus

17:00 Welcoming remarks
Graham Carr, Associate Dean, Research & Graduate Studies, Arts & Science
Louise Dandurand, Vice-President, Research & Graduate Studies, Concordia University

Discussion Leader: **Gilles Peslherbe** (Concordia University)

Dennis Salahub (University of Calgary)
Quantum Mechanics and Molecular Mechanics: Could They/Should They Play a Key Role in Systems Biology? What's Possible? What's Not?

18:15 Reception - Science Pavilion Atrium
Sponsored by ***Azuris Technologies*** and the ***Canadian Society for Chemistry*** (Division of Physical, Theoretical and Computational Chemistry)

Saturday, April 26, 2008 - De Sève Cinema, Library Building, SGW Campus

Discussion Leader: TBA

9:30 **Thanh-Tung Nguyen-Dang** (Université Laval)
Non-Variational TDMCSCF Method for Correlated Electron Dynamics in Ultrashort Intense Laser Pulses

10:10 **Philippe Rocheleau** and Matthias Ernzerhof (Université de Montréal)
Molecular Conductance in Terms of Orbital Densities

10:30 **Ian Hamilton** (Wilfrid Laurier University)
Charge Density and Decomposition of the Kinetic Energy into Classical and Purely Quantum Terms

10:50 Coffee Break - De Sève Cinema Foyer

Discussion Leader: TBA

11:10 **Pierre-Nicholas Roy** (University of Alberta)
Quantum Effects in Molecular Simulations

11:50 **Vibin Thomas** and Radu Iftimie (Université de Montréal)
Exploring the Chemical Nature of Weak Acid Dissociation Intermediates in Water

12:10 Thomas Lazzara, **Michael (Tony) Whitehead**, Theo van de Ven (McGill University)
Nanotube Self-Assembly Mechanism of Styrene and Maleic Anhydride Alternating Copolymers

12:30 **John Tromp** (Vanier College)
Finite Differences: An Approach That Has No Limits

12:50 Lunch - De Sève Cinema Foyer

Discussion Leader: TBA

14:00 **Mikko Karttunen** (University of Western Ontario)
Scale Hopping & Coarse Graining in Soft Matter Systems

14:40 **Jean-François Truchon** (Université de Montréal, Merck Frosst Canada), Anthony Nicholls (OpenEye Inc.), Radu Iftimie (Université de Montréal), Benoît Roux (University of Chicago), Christopher Bayly (Merck Frosst Canada)
Use of Continuum Electrostatics to Accurately Include Polarizability in Force Fields

15:00 **Nicolas Moitessier**, Christopher Corbeil, Jeremy Schwartzentruber (McGill University)
Computational Tools for Organic Chemists

15:20 **Monique Laberge** (Concordia University) and Takashi Yonetani (University of Pennsylvania)
Principal Components Analysis Applied to Describing Functionally Significant Hemoglobin

15:40 **Chun Mak**, Denise Koch and Gilles Peslherbe (Concordia University)
Theoretical Studies of Guanidinium Ions in Aqueous Clusters

16:00 Poster Session - Library Building Atrium

19:00 Banquet - Location TBA

Sunday, April 27, 2008 - De Sève Cinema, Library Building, SGW Campus

Discussion Leader: TBA

9:30 **Qadir Timerghazin**, Haley Carlson, Darrel Cotton, Robert Campbell and Alex Brown (University of Alberta)
Photoemission of Fluorescent Protein Chromophores

9:50 **Elena Ivanova** and Heidi Muchall (Concordia University)
A Computational Study of the Mechanisms of Syn-Anti Interconversion of N-sulfinyl Compounds

10:10 **Lei Zhang**, Gilles Peslherbe and Heidi Muchall (Concordia University)
Relationship Between The Geometry and Electronic Structure of Biphenyl Systems and Their Radical

10:30 Coffee Break - De Sève Cinema Foyer

Discussion Leader: TBA

10:50 **Paul Ayers** (McMaster University)
Sparse Integration Grids for Density Functional Theory

11:30 **Chunfeng Zhao** and Natalie Cann (Queen's University)
Enantioselective Mechanism of the Whelk-O 1 Chiral Stationary Phase from Molecular Dynamics

11:50 **Shihao Wang** and Natalie Cann (Queen's University)
Chiral Induction: The Transfer of Chirality from Chiral Solutes to Achiral Solvents

Poster Session

Saturday, April 26, 2008 - Library Building Atrium, SGW Campus

(1). **Samir Mushrif**, Alejandro Rey (McGill University) and Gilles Peslherbe (Concordia University)
First-Principles Calculations of the Palladium (II) Acetylacetonate Crystal Structure

(2). **Randall Dumont** (McMaster University)
Nonadiabatic Transition and Resonance

(3). **Tomasz Rog** (Helsinki University of Technology), Ilpo Vattulainen (Tampere University of Technology) and Mikko Karttunen (University of Western Ontario)
Modeling Lipid Rafts Components

(4). **François Goyer** and Matthias Ernzerhof, (Université de Montréal)
Using Complex Potentials to Calculate Electron Transmission in Molecules

(5). **Petrin Kamya** and Heidi Muchall, (Concordia University)
A Quantum Chemical Analysis on Sequence and Structural Effects of GU Mismatches on the Strength of H-bonds and Pi-Stacking in RNA

(6). **Denise Koch**, Ann English and Gilles Peslherbe (Concordia University)
Computational Investigation of Protein Chemistry: S-Nitrosohemoglobin

(7). **Yong Park**, David Wardlaw (University of Western Ontario) and Erwin Buncel (Queen's University)
A Density-Functional Theory Investigation of Spironaphthoxazine-merocyanine Interconversion: Metal Ion Stabilization

(8). **Abdul Latif**, Leon Jovner and M.C. Goh (University of Toronto)
Development of Mesoscale Models for Directed Protein Assembly

(9). **Xiaogang Wang** and Tucker Carrington (Queen's University)
A Discrete Variable Representation Treatment of the Rovibrational Quantum Dynamics of Molecules with More Than Three Atoms

(10). **Patrick Lague** and Sebastien Légaré (Université Laval)
Theoretical Study of the Influenza Hemagglutinin Fusion Peptide pKa Shifts

(11). **Pablo Englebienne**, Christopher Corbeil and Nicolas Moitessier (McGill University)
A New Platform for Drug Discovery

(12). **Peter Pawelek** (Concordia University)
Homology Modelling of the E. coli Enterobactin Efflux Transporter EntS

(13). **Nicolas Moitessier**, Christopher Corbeil, Jeremy Schwartzentruber and Pablo Englebienne (McGill University)
FITTED: A Docking-based Virtual Screening Tool for Flexible and Complex Systems

(14). **Devin Lee** and Nicolas Moitessier (McGill University)
Determination of the Effects of Protein Flexibility and Conserved Water Molecules in the Identification of Active Molecules in Large Databases: A Comparative Study of Virtual Screening Tools

(15). **Bilkiss Issack** and Gilles Peslherbe (Concordia University)
Transport of Small Molecules Across Lipid Membranes: A Molecular Dynamics Study

(16). **Murat Tamer Ataol** and Gilles Peslherbe (Concordia University)
Use of DFTB for Methane Intermolecular Potential Modeling

(17). **Alexandre Foisy-Geoffroy** and Gilles Peslherbe (Concordia University)
Cluster Size Effects on the Reactivity of Vanadium Oxides: Reaction of CH2F2 With V2O4+ and V4O8+