Symposium on Chemical Physics

at the University of Waterloo

November 1-3, 2013

REGISTRATION begins at 7:00 p.m. EIT Foyer

SESSION I: Friday, November 1, 2013 — P.M. EIT-1015

Chair: **Robert J. Le Roy**

7:30 – 8:15 **Travis Fridgen**
(Memorial University of Newfoundland)
Gas Phase Structures and Energetics of Metal Cationized Non-Covalent Complexes of DNA Bases

8:15 – 8:30 **Michael Schuurman**
(National Research Council of Canada)
The ab initio simulation of spectroscopic probes for excited state non-adiabatic molecular dynamics

8:30 – 8:45 **Maxim Ivanov**, Marat Talipov and Qadir Timerghazin
(Marquette University)
Point charge fitting of electrostatic potentials: New insights from genetic algorithm optimizations

8:45 – 9:00 Jack A. Barnes, Gianluca Gagliardi, and **Hans-Peter Loock**
(Queen's University)
Quantitative overtone absorption measurements of sub-monolayers on a microsphere resonator

SESSION II: Saturday, November 2, 2013 – A.M. EIT-1015

Chair: **Marcel Nooijen**

9:00 – 9:45 **Matthias Ernzerhof**
(Université de Montréal)
Kekuè formulae, Hückel theory, and Dirac's equation: Combining various concepts to better understand electron transport in conjugated systems

9:45 – 10:00 Mahesh B Dawadi, **David S. Perry**, Sylvestre Twagirayezu and Brant E. Billinghurst
(University of Akron and Canadian Light Source)
High-Resolution Infrared Spectra of Different Bands and Tortion-Rotation-Vibration Coupling in the Asymmetric NO Stretch of Nitromethane

10:00 – 10:15 **Farnaz Heidar Zadeh** and Paul W. Ayers
(McMaster University)
Information Theoretic Approach to Optimally Transfer Atoms to Molecules

10:15 – 10:45 **Coffee Break**

Invited talks are 45 min. including 5 min. for discussion
Contributed talks are 15 min. including 3 min. for discussion

SESSION III: Saturday, November 2, 2013 – A.M. EIT-1015
Chair: **Scott Hopkins**

10:45 – 11:45 ***The Roger E. Miller Lecture*** : M**ichael Ashfold**
(University of Bristol)
Molecular Photofragmentation Dynamics in the Gas and Liquid Phase: Parallels and Differences

11:45 – 12:00 **Ilya G. Ryabinkin** and Artur F. Izmaylov
(University of Toronto Scarborough)
Capturing the geometric phase in the quantum-classical Liouville approach

12:00 – 12:15 **Michael Burt**, Kathleen Wilson, Rick Marta, Moaraj Hasan, Scott Hopkins and Terry McMahon
(University of Waterloo)
Identifying anion-Π interactions in halide-bound phenylalanine derivatives using IRMPD spectroscopy

12:15 – 1:30 **Lunch** – EIT Foyer

SESSION IV: Saturday, November 2, 2013 – P.M. EIT-1015
Chair: **James Martin**

1:30 – 2:15 **Kirk Madison**
(University of British Columbia)
Production and Study of Ultra-Cold Molecules from Laser-Cooled Atoms: A New Regime for Ultracold Chemistry and Physics

2:15 – 2:30 **G. Guillon**, T. Zeng, P.-N. Roy
(University of Waterloo)
A post-quantization constrained propagator for path integral simulations

2:30 – 2:50 ***The D.J. Le Roy Prize Lecture***: **Lena Simine** and Dvira Segal
(University of Toronto)
Vibrational cooling, heating, and instability in molecular conducting junctions: full counting statistics and path integrals simulations

2:50 – 3:05 **Yunjie Xu**
(University of Alberta)
Solvation of Chiral Molecules: a 'Clusters-in-Liquid' Approach for Simulating Vibrational CD Spectra

3:05 – 3:20 **Stephen Walker**, Jeff Crouse, Meghan Beattie, Natalie Cann, Hans-Peter Loock
(Queen's University)
Using Velocity Map Imaging to Investigate Condensed Phase Photochemistry

3:15 – 6:00 **Refreshments and Poster Session**

The Roger E. Miller Lecture is 60 min. including 10 min for discussion.
The D.J. Le Roy Prize Lecture is 20 min including 5 min for duscussion
Invited talks are 45 min. including 5 min. for discussion
Contributed talks are 15 min. including 3min. for discussion

SESSION V: Saturday, November 2, 2013 from 3:00 P.M. EIT Foyer

POSTER SESSION

6:00 P.M. Poster sessions ends
Depart for Festival Room, South Campus Hall

6:30 P.M.	Cash Bar	Festival Room, South Campus Hall
7:00 P.M.	**DINNER**	Festival Room, South Campus Hall
9:30 P.M.	Informal Discussions	Graduate Club

SESSION VI: Sunday, November 3, 2013 – A.M. EIT 1015
Chair: **Pierre-Nicholas Roy**

9:15– 10:00 **Bill Poirier**
(Texas Tech University)
Ten Thousand Quantum States of Acetonitrile

10:00 – 10:15 **J. Larry Campbell**, Yves Le Blanc, Bradley Schneider, Eva Duchoslav, Mabel Zhu, and W. Scott Hopkins
(AB SCIEX and University of Waterloo)
Using Differential Ion Mobility to Explore (and Exploit?) the Solvation of Ions

10:15 – 10:30 **James Brown**, Xiao-Gang Wang, Tucker Carrington Jr.
(Queen's University)
Calculating and assigning rovibrational energies of four N_2O dimer isotopologues

10:30 – 11:00 **Coffee Break**

SESSION VII: Sunday, November 3, 2013– A.M. EIT 1015
Chair: **Takayoshi Amano**

11:00 – 11:45 **Nikolay Blinov**
(National Institute for Nanotechnology and University of Alberta)
Bridging the gap between Explicit and Implicit Solvation: Perspective of the Molecular Theory of Solvation

11:45 – 12:00 **Gavin S. Heverly-Coulson** and Nicholas J. Mosey
(Queen's University)
Development of a Predictive Model for Static Friction Coefficients

12:00 – 12:15 **Paul Hockett**, Enrico Ripani, Andrew Rytwinski, and Albert Stolow
(National Research Council of Canada)
Probing Ultrafast Dynamics with Time-resolved Multi-dimensional Coincidence Imaging: Butadiene

Invited talks are 45 min. including 5 min. for discussion
Contributed talks are 15 min. including 3min. for discussion

POSTER SESSION EIT Upstairs Foyer

Chair: **Marcel Nooijen**

To give people presenting papers in this session an opportunity to both present their work and visit other posters, this session is divided into two time slots:

3:30 – 4:45 Those whose papers were given (a) labels (1a, 2a, 3a, etc.) should attend their posters.

4:45 – 6:00 Those whose papers were given (b) labels (1b, 2b, 3b, etc.) should attend their posters.

1(a) **Zeb Kramer**, Barry K. Carpenter, Stephen Wiggins, Gregory S. Ezra
(Cornell University)
Non-statistical dynamics and selectivity in the ring-opening of the cyclopropyl radical

1(b) **Jack Barnes**, Hans-Peter Loock, Gianluca Gagliardi
(Queen's University and INO, Naples)
Rayleigh Back-Scatter Phase-Shift Cavity Ring-Down Measurements on a Silica Microsphere

2(a) **Iain Wilkinson**, Jochen Mikosch, Andrey E. Boguslavskiy, Julien B. Bertrand, Hans-Jakob Woerner, David M. Villeneuve, Michael Spanner, Serguei Patchkovskii and Albert Stolow
(National Research Council of Canada)
Probing the Excited State Dynamics of SO_2 Using Weak and Strong Laser Fields

2(b) **Cristina E. González-Espinoza**, Matthew Chan, Toon Verstraelen and Paul W. Ayers
(McMaster University and Ghent University
Energy Decomposition Analysis with occupation constraints

3(a) **Mabel Zhu**, W. Scott Hopkins, J. Larry Campbell and John E. Lape
(University of Waterloo)
Asymmetric Microsolvation of Alkylated Ammonium

3(b) **Patrick Carr**, Dr. W.S. Hopkins, M. Lecours and B. Drouillard
(University of Waterloo)
Exploring Sulphur-Poisoning of Rhodium Cluster Surface Reactions

4(a) **Mike Lecours**, Theodore Chow, and Scott Hopkins
(University of Waterloo)
The Effects of Sulphur Absorption on Rhodium Clusters

4(b) **Kevin Bishop**, Pierre-Nicholas Roy
(University of Waterloo)
Quantum Mechanical Free Energy Calculations on the Water Dimer

5(a) **Gene Fay Ye**, Scott Hopkins
(University of Waterloo)
Structures and Properties of Lanthanum Clusters

5(b) **N.L.P. Andrews**, J. Litman, D. Stroh, J.A. Barnes, H-P. Loock
(Queen's University)
Amplified Fibre Cavity Ring-down Spectroscopy

6(a) Wei_Jo Ting and **Takayoshi Amano**
(National Tsing Hua University, Taiwan, and University of Waterloo)
Submillimeter-wave Spectroscopy of NeD^+, XeH^+, and XeD^+: The Dunham Ananlysis

6(b) **Myong In Oh**, Styliani Consta
(University of Western Ontario)
Release Mechanism of a Polyethylene Glycol from a Highly Charged Aqueous Droplet

7(a) **Jeremy Viau Trudel**, Thanh-Tung Nguyen-Dang and Osman Atabek
(Université Laval et Université de Paris-Sud)
Molecular ionization by an XUV attosecond pulse: Is the Franck-Condon Principle acceptable?

7(b) **Ahdia Anwar**, Scott Hopkins
(University of Waterloo)
Density Functional Theory Studies of Monoisotopic Lanthanide Clusters

8(a) **A.G. Adam**, R.M. Hall, D.W. Tokaryk and R. Weale
(University of New Brunswick)
High Resolution Laser Spectroscopy of Rhenium Monocarbide

8(b) **T.Yukiya**, N. Nishimiya, M.Suzuki, and R. J. Le Roy
(Tokio Polytechnic University and University of Waterloo)
Direct-Potential-Fit Analysis for the $A\,^3\Pi_1$ and $X\,^1\Sigma^+$ States of IBr

9(a) **A.G. Adam**, L.M. Esson, A.M. Smith, C. Linton and D.W. Tokaryk
(University of New Brunswick)
High Resolution Laser Spectroscopy of Hafnium Monofluoride

9(b) **Elena Ivanova** and Qadir Timerghazin
(Marquette University)
An efficient computational treatment of dipole-bound anions with a diffuse electron corrective potential

10(a) **John Saunders**, Weijian Chen, McGregor Clayton, Chris Brauer, Amy MacLean, Jack A. Barnes, Scott S.-H.Yam, and Hans-Peter Loock
(Queen's University)
Interferometric Refractometry: A Technique for Chemical Sensing using Thin Films

10(b) **Loïc Joubert-Doriol**, Ilya G. Ryabinki, and Artur F. Izmaylov
(University of Toronto Scarborough)
Dynamics of macrosystems in the presence of a conical intersection: diabatic vs. adiabatic picture

11(a) **Gustavo Avila-Blanco** and Tucker Carrington
(Queen's University)
Solving the Schroedinger equation using Smolyak interpolants

11(b) **Prateek Goel**, and Marcel Nooijen
(University of Waterloo)
Fundamental considerations in time-resolved spectroscopy

12(a)

12(b) **Silvija C. Smith** and Ian P. Hamilton
(Wilfrid Laurier University)
Hydrogen atom transfer in alkane thiol-gold cluster complexes: A density functional theory study

13(a) Ismail Badran and **Yujun Shi**
(University of Calgary)
Gas-phase Reaction Chemistry of 1,3-disilacyclobutane and Filament Aging in Catalytic Chemical Vapor Deposition

13(b) **Zach Johnston**, Michael Burt, Scott Hopkins and Terry McMahon
(University of Waterloo)
Exploring the Serial Addition of Water to p-hydroxybenzoic acid using Computational Techniques

14(a) **Josh Featherstone**, Michael Burt, Kathleen Wilson and Terry McMahon
(University of Waterloo)
Influence of Solvent on Chloride-Bound Phenylalanine using Computational Chemistry

14(b) **Lecheng Wang**, Robert J Le Roy, Pierre-Nicholas Roy and Daiqian Xie
(University of Waterloo and Nanjing University)
Quantum Simulations of Molecular Hydrogen: From Point-Like to Stick-Like Particles

15(a) Travis Ko, Michael Burt, Nabeel Quasimuddin, Rick Marta, Moaraj Hasan,
W. Scott Hopkins, and Terry McMahon
(University of Waterloo)
Gas-Phase Structures of Chloride-Bound Phenylalanine Derivatives Determined by IRMPD Spectroscopy and Computational Chemistry

15(b) **Kathleen Wilson** and Terry B. McMahon
(University of Waterloo)
Examining Fluorination Effects on Phenylalanine Anion-Π Interactions using Computational Chemistry

16(a) **Dmitri Iouchtchenko**, Matthew Schmidt and Pierre-Nicholas Roy
(University of Waterloo)
Particle Entanglement in Quantum Clusters: Rényi Entropy via the SWAP Operator

16(b) **Mahmoud Sharawy** and Styliani Constas
(University of Western Ontario)
Counter Ions on the Release Mechanisms of Charged Macromolecules from Nanodroplets

17(a) Sepideh Soltani and Styliani Constas
(University of Western Ontario)
Solvation of PEG in queous Nanodroplets

17(b) **Gabriel L. C. de Souza** and Alexander Brown
(University of Alberta)
Structures, Energetics, Vibrational Frequencies and Infrared Intensities of HOOCl, HOClO and HClOO

18(a) **Lindsay Orr**, Pierre-Nicholas Roy, Gregoire Guillon and Tao Zeng
(University of Waterloo)
Centroid Dynamics in Curved Spaces

18(b) **Ahrar Monsur**, Kevin Bishop and Pierre-Nicholas Roy
(University of Waterloo)
Potential Energy Surfaces Gradients, and Path Integral Simulations

19(a) **Xiao-Gang Wang** and Tucker Carrington, Jr.
(Queen's University)
Quantum dynamics of a Van der Waals Dimer with Flexible Monomers: A Case Study of Water Chloride Anion

19(b) **Harold Hodgins** , Ian Hamilton, Jay Foley, Stephen Gray
(Wildrid Laurier University and Argonne National Laboratory, USA)
Electronic Excitation Spectra of Gold Clusters: Time Dependent Density Functional Requirements

20(a) **Nabil Faruk, Matthew Schmidt**, Hui Li, Robert Le Roy, and Pierre-Nicholas Roy
(University of Waterloo)
First-Principles Prediction of the Vibrational Raman Shifts in paraHydrogen Clusters

20(b) **Nabil F. Faruk**, Kevin P. Bishop, Stephen J. Constable and Pierre-Nicholas Roy
(University of Waterloo)
Conformational analysis of sugars using graphics processing unit-accelerated Path-integral molecular dynamics

21(a) **Matthew Schmidt**, Stephen Constable, Chris Ing, Tao Zeng, P.N. Roy
(University of Waterloo)
Path-Integral Methods to Simulate the Ground-State and Dynamics of Weakly Bound Clusters

21(b) **Sadru-Dean Walji**, Katherine Sentjens and Robert J.Le Roy
(University of Waterloo)
Improved Dissociation Energy and Potential Energy Functions for the Ground $X\,^1\Sigma^+$ *and "Avoided-Crossing"* $A\,X\,^1\Sigma^+$ *States of NaH and NaD*

22(a) Stephanie Y.Y. Wong, **Alexander Brown** and Pierre-Nicholas Roy
(University of Alberta and University of Waterloo)
Ab initio SC-IVR: Implementation in MMTK and benchmarks

22(b) **Katharina Boguslawski**, (P), Paweł Tecmer and Paul W. Ayers
(McMaster University)
Towards an efficient description of strongly correlated systems

23(a) **Paweł Tecmer**, Katharina Boguslawski, Örs Legeza, Markus Reiher and Paul W. Ayers
(McMaster University)
Unravelling the quantum-entanglement effect of noble gas coordination on the spin ground state of CUO