The 27th Annual

Symposium

On

Chemical Physics

at the

University of Waterloo

November 4 -6, 2011

Acknowledgements

We are very grateful to the following sponsors
for their generous financial support of this conference.

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

SESSION I: Friday, November 4, 2011 — P.M. EIT-1015
Chair: **Pierre-Nicholas Roy**

7:30 – 8:15 **Jochen Autschbach**
(State University of New York at Buffalo)
Spectroscopy `In Silico'

8:15 – 8:30 **Sandra Rabi,** Toon Verstraelen, and Paul W. Ayers
(McMaster University)
An Efficient Method for Transition State Optimization Using Redundant Internal Coordinates

8:30 – 8:45 **Scott Hopkins**
(University of Waterloo)
Imaging Wavefunctions in Dissociative Photoionization

8:45 – 9:00 **Lee Huntington**, Andreas Hansen, Frank Neese, and Marcel Nooijen
(University of Waterloo and Max-Planck-Institut für Bioanorganische Chemie)
Accurate Thermochemistry from a Parameterized Coupled-Cluster Singles and Doubles Model and a Local Pair Natural Orbital Based Implementation for Applications to Larger Systems

SESSION II: Saturday, November 5, 2011 – A.M. EIT-1015
Chair: **Wing-Ki Liu**

9:00 – 9:45 **John Klassen**
(University of Alberta)
Structure and stability of protein-ligand complexes in the gas phase

9:45 – 10:00 **Aakash Ravi,** Susumu Kuma, Katsunari Enomoto, and Takamasa Momose
(University of British Columbia)
Superfluid response in He nanodroplets studied by high resolution spectroscopy of CH_4

10:00 – 10:15 **Etienne Garand,** Michael Z. Kamrath, Peter A. Jordan, Arron B. Wolk, Scott J. Miller, and Mark A. Johnson
(Yale University)
Isolating non-covalent linkages in peptidic host-guest complexes through gas phase cryogenic ion vibrational spectroscopy

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 5, 2011 – A.M. EIT-1015
Chair: **Jim Martin**

10:45 – 11:45 ***The Roger E. Miller Lecture*** : **Robert McKellar**
(National Research Council of Canada)
Spectroscopy of Molecular Clusters

11:45 – 12:00 **Michael Schuurman**
(National Research Council of Canada)
Ab Initio On-the-fly Excited State Dynamics: Dynamical Motifs at Carbon-Carbon Double Bonds

12:00 – 12:15 **Styliani Consta**
(University of Western Ontario)
Ion transfer in highly charged nanodroplets

12:15 – 1:30 **Lunch** – EIT Foyer

SESSION IV: Saturday, November 5, 2011 – P.M. EIT-1015
Chair: **Mikko Karttunen**

1:30 – 2:15 **Vladimir Mandelshtam**
(University of California at Irvine)
Simulations of Quantum Liquids and Clusters by Thermal Gaussian Molecular Dynamics

2:15 – 2:30 T. J. Reddish, A. Padmanabhan, **M. A. MacDonald**, L. Zuin, J. Fernández, A. Palacios and F. Martín
(Canadian Light Source)
Observation of interference between two distinct autoionizing states in dissociative photoionization of H_2

2:30 – 2:45 **F. Y. Naumkin** and D. J. Wales
(UOIT)
Be_n cluster cages encapsulating H_2 molecules: Towards light-metal nanofoams for hydrogen storage

2:45 – 3:00 **Shamus A. Blair** and Ajit J. Thakkar
(University of New Brunswick)
Which molecules have polarizabilities that violate a simple upper bound based on atomic additivity?

3:00 – 3:15 **John W. Tromp**
(Vanier College)
An investigation of boundary conditions in complex time quantum dynamics

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

The Roger E. Miller Lecture is 60 min. including 10 min for discussion.
Invited talks are 45 min. including 5 min. for discussion
Contributed talks are 15 min. including 3min. for discussion

SESSION V: Saturday, November 5, 2011 from 3:30 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 6, 2011 – A.M. EIT 1015
Chair: **Marcel Nooijen**

9:15– 10:00 **Albert Stolow**
(National Research Council of Canada)
CARS Microscopy Made Simple

10:00 – 10:15 **Jayashree Nagesh** and Edwin L. Sibert III
(University of Wisconsin-Madison)
Simulation of $\tilde{A}^2A_1 \rightarrow \tilde{X}^2E$ Laser Excitation Spectrum in CH_3O using iterative methods

10:15 – 10:30 **Christian Merten,** Yunjie Xu
(University of Alberta)
Vibrational Circular Dichroism of Matrix Isolated Molecules

10:30 – 11:00 **Coffee Break**

SESSION VII: Sunday, November 6, 2011 – A.M. EIT 1015
Chair: **Scott Hopkins**

11:00 – 11:45 **Jennifer van Wijngaarden**
(University of Manitoba)
High-Resolution Spectroscopy from the Microwave Through the Infrared Region

11:45 – 12:00 **Ismail Badran**, Yujun Shi
(University of Calgary)
Decomposition of 1-methyl-1-silacyclobutane on tungsten filament, competitive reactions of methyl radicals, silenes, and silylenes

12:00 – 12:15 **James Brown,** Xiao-Gang Wang, Tucker Carrington Jr., and Richard Dawes
(Queen's University)
The dynamics of the OCS dimer and the role of cross-shaped configurations

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: **Pierre-Nicholas Roy**

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) **Nabil F. Faruk**, Hui Li, Jing Yang, Robert J. Le Roy, Pierre-Nicholas Roy
(University of Waterloo)
Simulation Studies of the Vibrational Dynamics of para-Hydrogen Clusters

1(b) L. Jones and **J. D. D. Martin**
(University of Waterloo)
Modification Rydberg State Polarizabilities using mm-wave dressing fields

2(a) D. Forthomme, C. Linton, A. Read, **D. Tokaryk**, A. G. Adam, L. E. Downie, A. D. Granger and W. S. Hopkins
(University of Brunswick)
Unraveling the visible spectrum of strontium monomethoxide

2(b) Adrian Adamescu, **Ian Hamilton**, Hind Al-Abadleh
(Wilfrid Laurier University)
Thermodynamics of Dimethylarsinic Acid and Arsenate Interactions with Hydrated Iron-(oxyhydr)oxide Clusters: DFT Calculations

3(a) **Jennifer J. Le Roy**, Matthew Jeletic, Po-Heng Lin, Serge I. Gorelsky, Ilia Korobkov, and Muralee Murugesu
(University of Ottawa)
Building Block Approach to Dysprosium Single Molecule Magnets

3(b) **John Titantah** and Mikko Karttunen
(University of Western Ontario)
The iceberg model of hydration and its breakdown

4(a) **Matthew Schmidt,** Pierre-Nicholas Roy, Marcel Nooijen, Robert LeRoy, Tao Zeng, and Chris Ing
(University of Waterloo)
Weakly bound systems: Accurate interaction potentials and simulations of water clathrates and doped parahydrogen clusters

4(b) **F. X. Sunahori**, G. Yang, E. Kitova, J. S. Klassen, and Y. Xu
(University of Alberta)
Chiral Recognition Study of Protonated Serine Dimer and Octamer by Infrared Multiphoton Dissociation Spectroscopy and DFT calculations

5(a) **Stephen Walker**, **Jeff Crouse**, Hans-Peter Loock, Natalie Cann
(Queen's University)
Early Developments into a New Flexible Water Model to Study Photochemical Interactions Within Ice Surfaces

5(b) **Zi Jian Long**, Denys I. Bondar and Wing-Ki Liu
(University of Waterloo)
Electron dynamics under few-cycle laser pulse

6(a) X. Liu, **Ian Hamilton,** R. Krawczyk, and P. Schwerdtfeger
(Wilfrid Laurier University)
The Stability of Helical Gold Nanorods: A Relativistic Density Functional Study

6(b) **Mohammad Reza Poopari**, Zahra Dezhahang, Guochun Yang, Peiyang Zhu, Zhi Bie, and Yunjie Xu
(University of Alberta)
Do N-protected L-amino acids make zwitterions in aqueous solution? A comparative study of N-acetyl-L-Cysteine and Serine Molecules using Vibrational Circular Dichroism spectroscopy and Density Functional Theory simulations

7(a) **Zahra Dezhahang**, Christian Merten, Yunjie Xu
(University of Alberta)
Conformational Analysis of two Diphosphine Ligands and their corresponding Palladium complexes by Vibrational Circular Dichroism Spectroscopy

7(b) **Matthew Ian Hoopes**
(University of Waterloo)
Experimental and Computational Multiscale Studies of Model Cellular Lipid Bilayer Membranes: Additives, Supports, and Curvature

8(a) **A. Mkrtchyan**, T. Hynninen, C. L. Dias, V. Heinonen, M. Karttunen, A. S. Foster, and T. Ala-Nissila
(University of Western Ontario)
Molecular dynamics simulation of cold denaturation

8(b) **Hanna Omrani**, Hans-Peter Look, Helen Waechter, Klaus Bescherer
(Queen's University)
Characterization of Machinery Fluid Using Excitation-Emission Matrices (EEM) and Cavity Ring-Down Spectroscopy (CRDS)

9(a) **Ming Sun** and Jennifer van Wijngaarden
(University of Manitoba)
Transient molecules detected by a chirped-pulse Fourier transform microwave spectrometer with multiple-FID techniques

9(b) **Tokio Yukiya**, Nobuo Nishimiya, Masao Suzuki and Robert. J. Le Roy
(Tokyo Polytechnic University and University of Waterloo)
Direct-Potential-Fit Analysis for the $A^3\Pi_{1u} - X^1\Sigma_g^+$ System of Br_2

10(a) **Ziqiu Chen** and Jennifer van Wijngaarden
(University of Manitoba)
A synchrotron-based far infrared study of 3-oxetanone

10(b) R. Toukabri and **Y. J. Shi**
(University of Calgary)
Study of H_2 elimination mechanism during the decomposition of mehtylsilanes in a cat-cvd process

11(b) Cody van Dijk, Ming Sun and **Jennifer van Wijngaarden**
(University of Manitoba)
Microwave spectroscopic study of fluorinated pyridines

11(b) **Santa Rabi**, **Christopher Haddad**, Sandra Rabi, Toon Verstraelen and Paul Ayers
(McMaster University)
Finding an Initial Guess for a Transition State Using Redundant Internal Coordinates

12(a) **Xiao-Gang Wang**, Tucker Carrington Jr
(Queen's University)
Calculating the rovibrational levels of methane with a new basis

12(b) **G. Guillon**, M. Leino, A. Viel, A. Zanchet, R. E. Zillich
(Université de Rennes)
Quantum Monte Carlo studies of Rb and Rb2 (ground triplet) in helium environment*

13(a) **J. Saunders**, **W. Chen**, J. Barmes, H.-P. Loock, D.-X. Xu, R. Ma, S. Janz
(Queen's University and Institute of Microstructural Sciences, NRC)
Micro-optical Refractive Index Sensing of Volatile Organic Compounds

13(b) Ryan Zaari and **Alex Brown**
(University of Alberta)
Effect of diatomic molecular properties on binary laser pulse optimizations of $ACNOT_1$ and NOT_2 quantum gate operations

14(a) Markus Schröder, Meiyu Zhao, and **Alex Brown**
(University of Alberta)
Controlling quantum dynamics in polyatomic molecules: The OCT-MCTDH approach

14(b) **E. G. Schnitzler**, M. T. Parsons, K. M., McDonald, J. Tulip, W. Jäger
(University of Alberta)
Continuous secondary organic aerosol yields from photochemical reactions of toluene and p-xylene with hydroxyl radical

15(a) **Lisa Ugray** and Ralph Shiell
(Trent University)
The hydrogen atom in a spherical well: Calculating ionization rates for a free atom using bound-bound transition theory

15(b) Sida Zhou, **Omid Nourbakhsh**, Pavle Djuricanin, Takamasa Momose
(University of British Columbia)
Zeeman decelerator for making cold free radicals

16(a) F. Matsushima, T. Shiraishi, C. Shinozuka, **T. Amano**, R. Fujimori, K. Kawaguchi
(University of Toyama, University of Waterloo, and Okayama University)
THz Spectrum of H_2F^+

16(b) Hsuan-Chen Chen, Chung-Yun Hsiao, Jin-Long Peng, **Takayoshi Amano**, and Jow-Tsong Shy
(National Tsing-Hua University and University of Waterloo)
Saturation Spectroscopy of the Infrared Transitions of H_3^+ and HeH^+

17(a) **Chrisopher Ing**, Jing Yang, Konrad Hinsen, Toby Zeng, Hui Li, and Pierre-Nicholas Roy
(University of Waterloo)
Understanding Doped Helium Clusters with Path Integral Molecular Dynamics

17(b) **Yalina Tritzant-Martinez**, Tao Zeng, and Pierre-Nicholas Roy
(University of Alberta and University of Waterloo)
Potential of Mean Force Calculations of the Water Dimer and the Water Trimer

18(a) **Tao Zeng**, Hui Li, and Pierre-Nicholas Roy
(University of Waterloo)
Superfluidity in pH_2 cluster with a water dopant

18(b) **Jeffrey Philippson**, Robert Collister, and Ralph Shiell
(Trent University)
Long-range ionic-covalent coupling in alkali-alkali collisions

19(a) **R.M. Lees**, Li-Hong Xu, A.R.W. McKellar and B.E. Billinghurst
(University of New-Brunswick, National Research Council, and Canadian Light Source)
IR Spectroscopy at the Canadian Light Source: New States of Trans-Acrolein in the 1100-1200 cm^{-1} Region

19(b) **Paul Hockett**, Christer Z. Bisgaard, Owen Clarkin, and Albert Stolow
(National Research Council and University of Copenhagen)
Time-resolved Molecular Frame Photoelectron Angular Distributions as a Probe of Electronic Dynamics

20(a) **Prateek Goel** and Marcel Nooijen
(University of Waterloo)
A primer on vibronic coupling theory with applications of a double vibronic model to photo-detachment spectroscopy

20(b) **Julia Endicott** and Marcel Nooijen
(University of Waterloo)
The (routine) construction of vibronic models and their application to simulations of photo-electron spectra

21(a) **Yao Li,** Prateek Goel and Marcel Nooijen
(University of Waterloo)
On the use of (routinely) constructed vibronic models (using VIBRON and ACES II) in the Multi-Configurational Time-Dependent Hartree approach (MCTDH)

21(b) Satya Bulusu, **Sergey Kazachenko**, and Ajit J. Thakkar
(University of New Brunswick)
Structural transitions of methanol clusters

22(a) **Peter A. Limacher**, Hans-Peter Lüthi and Paul W. Ayers
(McMaster University)
Linearly conjugated chains exposed to an electric field: A closer look on the polarizabilities obtained with several quantum chemical methods

22(b) **Steven K. Burger**, Patrick Gunning and Paul W. Ayers
(McMaster University)
A Method for the Automated Parametrization of the AMBER force field for Metal containing systems

23(a) **Jing Yang**, Christopher Ing, and Pierre-Nicholas Roy
(University of Waterloo)
Effective Potential Approach to the Simulation of Large Para-hydrogen Clusters and Droplets

23 (b) **M. T. Parsons**, E. G. Schnitzler, W. Jäger, K. McDonald, J. Tulip
(University of Alberta)
Implementation of a smog chamber to continuously measure secondary organic aerosol yields from photochemical reactions

Notes

SUPPLEMENTARY INFORMATION

- **Poster Preservation**
  In past years posters left up after the poster session have been vandalized during the night. If you wish to avoid this possibility, take down your poster after the session Saturday afternoon, before leaving for the Conference Dinner.

- **Recycling**
  Before leaving on Sunday, please drop you plastic name-tag holder into the cardboard box by the entrance to the Registration area. This will allow recycling and reduced our costs for next year.

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  United Taxi: 519-888-0400
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