The 30th Annual

Symposium

On

Chemical Physics

at the

University of Waterloo

November 7-9, 2014

Acknowledgements

We are very grateful to the following sponsors
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AB SCIEX

Symposium on Chemical Physics

at the University of Waterloo

November 7-9, 2014

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

SESSION I: Friday, November 7, 2014 — P.M. EIT-1015

Chair: **Marcel Nooijen**

7:30 – 8:15 **David Cory**
(University of Waterloo)
Quantum Sensors and Computers

8:15 – 8:30 **Tao Zeng**, Nandini Ananth, and Roald Hoffmann
(Cornell University)
Seeking small molecules for singlet fission: a heteroatom substitution strategy

8:30 – 8:45 **John Saunders**, McGregor Clayton, Sean Chen, Weijian Chen, Chris Brauer, Michaela Thomas, Sogol Borjian, Scott Yam, Jack Barnes and Hans-Peter Loock
(Queen's University)
Chemical Sensing with Thin Films by Optical Interferometric Refractometry

8:45 – 9:00 **Prateek Goel** and Marcel Nooijen
(University of Waterloo)
A proposed new vibrationally resolved Spectroscopy: prp-cw-pes

SESSION II: Saturday, November 8, 2014 – A.M. EIT-1015

Chair: **Pierre-Nicholas Roy**

9:00 – 9:45 **Lai-Sheng Wang**
(Brown University)
Electrospray Photoelectron Spectroscopy: From Multiply Charged Anions to Ultracold Anions

9:45 – 10:00 **Nikesh S. Dattani** and Mariusz Puchalski
(Kyoto University and Adam Mickiewicz University)
Using spectroscopy of HeH^+ and 3rd order QED to determine the Boltzmann constant with an order of magnitude greater precision

10:00 – 10:15 **Paweł Tecmer**
(McMaster University)
Ab Initio Modeling of Excited States of Uranium Compounds: Dissecting the Interplay of Electron Correlation and Relativistic Effects

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 8, 2014 – A.M. EIT-1015
Chair: **Pierre-Nicholas Roy**

10:45 – 11:45 ***The Roger E. Miller Lecture*** : David Ceperley
(University of Ilinois)
Dense hydrogen: what we can calculate, implications for density functionals, and multi scale approaches

11:45 – 12:00 **Pierre-Alexandre Turgeon**, Jonathan Vermette, Patrick Ayotte, Oren Ofer and Gil Alexandrowicz
(Université de Sherbrooke)
Demonstration of Ortho-Water Enrichment Using a Novel Magnetic Focusing Methodology and REMPI (2+1) Spectroscopy

12:00 – 12:15 **Anastasia Gunina**, Samer Gozem, and Anna I. Krylov
(University of Southern California)
Dyson Orbitals for Calculating Photoionization Cross-sections

12:15 – 1:30 **Lunch** – EIT Foyer

SESSION IV: Saturday, November 8,2014 – P.M. EIT-1015
Chair: **James Martin**

1:30 – 2:15 **Anna Krylov**
(University of Southern California)
A Fresh Look at Resonances: An Equation-of-Motion Coupled-Cluster Based Approach

2:15 – 2:30 **Phillip S. Thomas** and Tucker Carrington, Jr.
(Queen's University)
Vibrational Energy Level Calculations for High-Dimensional Systems Using Tensor Formats

2:30 – 2:45 **Samuel Beaulieu**, Heide Ibrahim, Benji Wales, Bruno E Schmidt, Nicolas Thiré, Emmanuel P Fowe, Éric Bisson, Christoph T Hebeisen, Vincent Wanie, Mathieu Giguère, Michael Spanner, André D Bandrauk, Joseph Sanderson, Michael S Schuurman and François Légar
(Centre Énergie Matèriaux et Télécommunications, University of Waterloo, Université de Sherbrooke, National Research Council of Canada)
Table-top imaging of the non-adiabatically driven isomerization in the acetylene cation

2:45 – 3:05 ***The 2013 'D.J. Le Roy Prize' Lecture***: **Salil Bedkihal**
(University of Toronto and McGill University)
Magnetotransport in Aharonov-Bohm interferometers using numerically exact path integrals

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

SESSION IV: Saturday, November 8 2014 – P.M. … continued … EIT-1015
Chair: **James Martin**

3:05 – 3:25 ***The 2014 'D.J. Le Roy Prize' Lecture***: **C.C. Jumper**, J.M. Anna, A. Stradomska, J. Schins, M. Myahkostupov, V. Prusakova, D.G. Oblinsky, F.N. Castellano and G.D. Scholes
(University of Toronto)
Excited State and Energy Transfer Dynamics in Natural and Synthetic Light-Harvesting Systems

3:25 – 6:00 **Refreshments and Poster Session**

SESSION V: Saturday, November 8, 2014 from 3:20 P.M. EIT Foyer
POSTER SESSION
Chair: **Marcel Nooijen**

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
8:30 P.M.	Informal Discussions	Graduate Club

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 VI: Sunday, November 9, 2014 – A.M. EIT 1015
Chair: **German Sciaini**

9:15– 10:00 **Amy Mullin**
(University of Maryland)
Dynamics of Molecular Gyroscopes

10:00 – 10:15 **Li-Hong Xu**, J.T. Hougen, S. Belov, V. Ilyushin, L.H. Coudert
(University of New Brunswick, NIST, NNOV, Kharkov, Lisa)
Spin-rotation hyperfine splittings at moderate to high J values in methanol

10:15 – 10:30 **Hong-Xing Zhang**
(Jilin University)
Excited States of Transition Metal Complexes

10:30 – 11:00 **Coffee Break**

SESSION VII: Sunday, November 9, 2014– A.M. EIT 1015
Chair: **Scott Hopkins**

11:00 – 11:45 **Guillaume Lamoureux**
(Concordia University)
Molecular modeling of proton cotransport in proteins

11:45 – 12:00 **Loïc Joubert-Doriol**, Ilya G. Ryabinkin, and Artur F. Izmaylov
(University of Toronto Scarborough)
A problem-free time-dependent variational principle for open quantum systems

12:00 – 12:15 Guillaume Marcotte, Patrick Marchand, Stèphanie Pronovost, **Patrick Ayotte**, Carine Laffon, and Philippe Parent
(Université de Sherbrooke)
Ionization and Enhanced Photochemistry of Nitric Acid on Ice

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

POSTER SESSION: Saturday, November 8, 2014 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) L. Aissaoui, **M. Bouledroua**, and K. Alioua
(Badji Mokhtar University, Algeria)
Quantum-mechanical mobility of $C^+(^2P)$ and $C^+(^4P)$ ions evolving in cooled helium gas

1(b) **Bin Liu**, Matthew Hoopes, Mikko Karttunen
(University of Waterloo)
Molecular Dynamics Simulations of Daptomycin's Antimicrobial Activity

2(a) **Gustavo Avila-Blanco** and Tucker Carrington Jr.
(Queen's University)
Using high-dimensional Smolyak interpolation to solve the Schrödinger equation and represent potentials

2(b) **Myong In Oh** and Styliani Consta
(University of Western Ontario)
Release and Ejection Mechanisms of Poly(ethylene glycol) in Charged Aqueous Droplets

3(a) Suk Kyoung Lee, Yun Fei Lin, Fadia Cudry, **Steven Lingenfelter**, Fan Lin and Wen Li
(Wayne State University)
Coincidence Ion Imaging with a Fast Frame Camera

3(b) **Lindsay Orr** and Pierre-Nicholas Roy
(University of Waterloo)
Centroid dynamics in curved spaces

4(a) **Yoany Rodriguez García**
(Queen's University)
Optical Fibre pH Sensor Using PAA Electrospan Nanowebs

4(b) **Alexander H. Winney**, Thushani Herath, Yun Fei Lin, Pradip Adhikari, Cun Shun Huang, Suk Kyoung Lee and **Wen Li**
(Wayne State University)
Three Dimensional Attosecond Electron-Ion Coincidence Measurements

5(a) **Hanieh Farkhondeh**, Fatemeh R. Rahsepar, Lei Zhang and Tong Leung
(University of Waterloo)
STM and XPS Investigation of Small Biomolecules on Ag/Si(111)$\sqrt{3}\times\sqrt{3}$ for Biosensing Applications

5(b) **Corinne Duperrouzel**, Paweł Tecmer, Katharina Boguslawski, Gergerly Barcza, Örs Legeza, Paul W. Ayers
(McMaster University)
A quantum informational approach for dissecting chemical reactions

6(a) W. Scott Hopkins, Chuantian Zhan, **Patrick J. Carr** , Michael Burt, Terry B. McMahon, Vincent Steinmetz and Eric Fillion
(University of Waterloo)
Mode-selective Ligand Scrambling in Palladium Catalysts

6(b) **J. Fan**, N.L.P. Andrews, N. Henning, M.C. Chen, and H-P. Loock
(Queen's University)
Remaining lifetime evaluation using excitation emission matrix spectroscopy

7(a) **N.L.P Andrews**, D. Munzke, C. van Horne, J.A. Barnes, and H-P. Loock
(Queen's University)
Interferometry effects with ammonia in hollow core photonic crystal fibres

7(b) **Tina Lee,** Ce Zhou, and W. Scott Hopkins
(University of Waterloo)
Enantiomeric Separation of Quaternary Ammonium Salt Catalysts

8(a) **Zhebing Liu** and Marcel Nooijen
(University of Waterloo)
Multireference Equation-of-Motion coupled Cluster study of atomic excitation spectra of first row transition metal atoms Cr, Mn, Fe and Co

8(b) **Amy MacLean**, Michaela Thomas, Sean Stuart, Jack Barnes, Carlos Escobedo, and Hans-Peter Loock
(Queen's University)
Design of a surface plasmon resonance imaging system for the monitoring of chemical kinetics

9(a) **Annica I. Freytag**, **Ian M. Bergeron**, Jack A. Barnes, Amy G. MacLean, Tamina Schneider, and Hans-Peter Loock
(Queen's University)
Quantitative Photoacoustic Concentration Measurements of Aqueous Phosphates using Fiber Optic Detection

9(b) **Geoffrey S. Sinclair**, Graham K. Murphy, and W. Scott Hopkins
(University of Waterloo)
Based Catalyst Effects on an Iodoarene Difluorination Reaction

10(a) **Johnathan Steffen**, J. Larry Campbell, and W. Scott Hopkins
(University of Waterloo)
Developing a Model For DMS Trajectories

10(b) **Ariel Petruk**, Kostyantyn Pichugin, and German Sciaini
(University of Waterloo)
Atomically-Resolved Dynamics & Ultrafast Imaging

11(a) **Philip Myatt,** Pat Carr, Denzel Huang, Michael Burt, Eric Fillion, Terry McMahon and W. Scott Hopkins
(University of Waterloo)
IRMPD of Boron Fluoride Clusters

11(b) **Weiqiang Fu** and W. Scott Hopkins
(University of Waterloo)
Exploring Structures and Properties of Ionic Amino Acid Clusters

12(a) **Jingfei Yao** and W. Scott Hopkins
(University of Waterloo)
Chemical Bonding in the Cobalt Dimer Cation

12(b) **R.M. Lees,** Li-Hong Xu, B.E. Billinghurst, and M. Mollabashi
(University of New Brunswick Saint John, CLS, & Iran U. of Science and Technology)
FTIR Synchrotron Spectroscopy of CD_3OH: The Tau of Methanol

13(a) **J. Crouse**, N. M. Cann, H.-P. Loock, S. Walker, and S. Takahashi
(Queen's University)
Photodynamics in Ice: Simulating Ice Photochemistry Using Molecular Dynamics

13(b) Ruijie Xue, **Hui Li**, and Jiali Gao
(Jilin University, Jilin, People's Republic of China)
A New Method for Linear or Two-Dimensional Vibrational Spectroscopy Calculation and Its Application in $HCl(H_2O)_n$ Clusters

14(a) **Lena Semine** and Dvira Segal
(University of Toronto)
Electron transport through nano-scale junctions with local an-harmonic modes

14(b) *Paper withdrawn*

15(a) **James Brown** and Tucker Carrington Jr.
(Queen's University)
Calculating rovibrational energies using phase-space localized basis functions in polyspherical coordinates

15(b) **Bohdan Kulchytskyy**, Stephen Inglis, and Roger Melko
(University of Waterloo)
Detecting Goldstone Modes via Entanglement Entropy

16(a) Allan Adam, **Ryan Hall**, Robbie Weale and Dennis Tokaryk
(University of New Brunswick)
An Analysis of the $^4\Pi-^4\Sigma^-$ Transition of Rhenium Monocarbide

16(b) **Young-Sang Cho** and Robert J. Le Roy
(University of Waterloo)
Full empirical potential curves and improved dissociation energies for the $X\,^1\Sigma^+$ *and* $A\,^1\Pi$ *states of* CH^+

17(a) **Ilya G. Ryabinkin**
(University of Toronto Scarborough)
When and how does the geometric phase affect non-adiabatic excited-state dynamics through conical intersections?

17(b) **Rami Gherib**, Ilya G. Ryabinkin and Artur F. Izmaylov
(University of Toronto Scarborough)
Capturing geometric phase effects by mixed quantum-classical methods

18(a) **Ryan J. MacDonell**, Michael S. Schuurman
(University of Ottawa and National Research Council of Canada)
Photoinitiated excited state dynamics of cyclopropenylidene and chlorocyclopropenylidene

18(b) Tracy W. Liu, Juan Chen, Laura Burgess, Brian C. Wilson, Gang Zheng, Lixin Zhan, **Wing-Ki Liu**, and Bae-Yeun Ha
(University of Waterloo)
Activation Kinetics of Zipper Molecular Beacons

19(a) **Xiao-Gang Wang** and Tucker Carrington Jr.
(Queen's University)
The Vibration-rotation-tunnelling levels of N_2-H_2O *and* N_2-D_2O

19(b) **Kai Slaughter** and Robert J. Le Roy
(University of Waterloo)
Direct-Potential-Fit Analyses of the $B\,^1\Pi_u$ *Barrier States of* Li_2 *and* Rb_2

20(a) **Kevin Bishop** and Pierre-Nicholas Roy
(University of Waterloo)
Quantum mechanical free energy profiles of the water dimer

20(b) **Nabil Faruk**, Matthew Schmidt, Robert Le Roy, and Pierre-Nicholas Roy
(University of Waterloo)
Quantum Effects in Sugar and para-H_2 *cluster Systems*

21(a) **Spencer Yim** and Pierre-Nicholas Roy
(University of Waterloo)
Quantum Properties of Confined Systems

21(b) **Lecheng Wang**, Robert J. Le Roy and Pierre-Nicholas Roy
(University of Waterloo)
Quantum Monte Carlo Simulation of Vibrational Frequency Shift in Pure and Doped Solid para-Hydrogen

22(a) **Matthew Schmidt**, Dmitri Iouchtchenko, Nabil Faruk, Kevin Bishop, Steve Constable, and P.-N. Roy
(University of Waterloo)
A Molecular Dynamics Approach to Calculating Equilibrium and Dynamic Ground State Properties

22(b) **C. M. Herdman**, S. Inglis, P.-N. Roy, R. G. Melko, and A. Del Maestro
(University of Waterloo)
Entanglement entropies of interacting bosons via path-integral Monte Carlo

23(a) **Sung Hong,** Pawel Tecmer and Paul W. Ayers
(University of Waterloo)
Dissecting the cation-cation interactions in uranium oxides: A view from Ab initio quantum chemistry

23(b) **Neil Raymond**, Dmitri Iouchtchenko, and Pierre-Nicholas Roy
(University of Waterloo)
Semiclassical time correlation functions: Path-Integral Ground State (PIGS) and Initial Value Representation (IVR)

24(a) **Lee Huntington** and Marcel Nooijen
(University of Waterloo)
Orbital Selection Scheme in Multi-Reference Equation-of-Motion Coupled-Cluster Theory: Application to Transition Metal Complexes

24(b) **Yilin** Zhao and Paul W. Ayers
(McMaster University)
A theoretical Study on the Decomposition of 1,1-dimethyl-1-silacyclobutane

25(a) **Dongbin (Artus) Zhang** and Pierre-Nicholas Roy
(University of Waterloo)
Path Integrals With Tsallis Propagators

25(b) **Chunying Rong**, Tian Lu, Shubin Liu, and Paul W. Ayers
(McMaster University)
Developing Density Functional Reactivity Theory with Shannon Entropy and Fisher Information

26(a) **Saurabh Srivastava**, Joseph Palathinkal Thomas, Md. Anisur Rahman, Marwah Abd-Ellah, Nina Heinig, and Kam Tong Leung
(University of Waterloo)
Size-Dependent Photoelectrochemical Water splitting Performances for Ultra-small TiO_2 Nanoclusters

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.

- **Phone Numbers**:

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