*The 31st Annual*

# Symposium

# On

# Chemical Physics

*at the*

*University of Waterloo*

*November 6-8, 2015*

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## Acknowledgements

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

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# Symposium on Chemical Physics

*at the University of Waterloo*

November 6-8, 2015

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

**SESSION I**: Friday, November 6, 2015 — P.M. EIT-1015

Chair: **Pierre-Nicholas Roy**

7:30 – 8:15 **Rebecca Jockush**
(University of Toronto)
*Combined Mass Spectrometry and Fluorescence Studies to Separate Intrinsic Behavior from Environmental Effects: from Fundamental Investigations of Fluorescent Probes to FRET for Gas-phase Protein Conformation*

8:15 – 8:30 **Darya Komsa** and Viktor N. Staroverov
(Western University)
*Elimination of spurious fractional charges in dissociating molecules by correcting the shape of approximate Kohn-Sham potentials*

8:30 – 8:45 **Xiao-Gang Wang** and Tucker Carrington, Jr.
(Queen's University)
*A numerically exact full-dimensional calculation of rovibrational levels of water dimer*

8:45 – 9:00 **Styliani Consta** and Mahmoud Sharawy
(University of Western Ontario)
*Toward the understanding of the stability of non-covalent complexes of Macromolecules in charged droplets*

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

Chair: **Marcel Nooijen**

9:00 – 9:45 **Artur Izmaylov**
(University of Toronto, Scarborough)
*Role of Topology in Chemical Dynamics Beyond Born-Oppenheim er Approximation*

9:45 – 10:00 **Elijah Schnitzler** (S), Courtenay Badran and Wolfgang Jäger
(University of Alberta)
*The Two Most Stable Oxalic Acid Monohydrates Identified by Rotational Spectroscopy: Significant Effect of Conformation on Decarboxylation*

10:00 – 10:15 **Li-Hong Xu**, S.P. Belov, G. Yu Golubiatnikov, A.V. Lapinov, V.V. Ilyushin, E.A. Alekseev, A.A. Mescheryakov and J.T. Hougen
(University of New Brunswick)
*Torsionally mediated spin-rotation hyperfine splittings at moderate to high J values in Methanol - modeled to experimental accuracy!*

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 7, 2015 – A.M. EIT-1015
Chair: **German Sciaini**

10:45 – 11:45 ***The Roger E. Miller Lecture*** : **Dwayne Miller**
(University of Toronto and Max Planck Institute, Hamburg)
*Mapping Atomic Motions with Ultrabright Electrons:*
*The Chemists' Gedanken Experiment Enters the Lab Frame*

11:45 – 12:00 **Simon Neville** and Michael Schuurman
(University of Ottawa)
*Core-excitation as a probe of non-adiabatic dynamics: a theoretical study*

12:00 – 12:15 **Hui Li**
(Jilin Uninersity)
*A New Approach to Simulate Infrared Probe Spectra*

12:15 – 1:30 **Lunch** – EIT Foyer

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

1:30 – 2:15 **Gary Douberly**
(University of Georgia)
*Laser Spectroscopy of Reactive Intermediates in Superfluid Helium Droplets*

2:15 – 2:30 **Robert Wodraszka** and Tucker Carrington
(Queen's University)
*Using a non-direct product single particle function basis within the multi-configurational time-dependent Hartree (MCTDH) approach*

2:30 – 2:50 ***The 2015 'D.J. Le Roy Prize' Lecture***: **Yin Song** and Gregory D. Scholes
(University of Toronto)
*Vibrational coherence probes the mechanism of ultrafast electron transfer in polymer-fullerene blends*

2:50 – 3:05 **Toon Verstraelen**
(Ghent University)
*Minimal Basis Iterative Stockholder (MBIS): a Self-Consistent Hirshfeld Method Tailored to Force-Field Development*

3:05 – 3:20 Javix Thomas, Xunchen Liu, Wolfgang Jäger and **Yunjie Xu**
(University of Alberta)
*The H-bond topologies in the 2-fluoroethanol and trifluoroethanol trimers*

3:25 – 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
Contributed talks are 15 min. including 3min. for discussion
Invited talks are 45 min. including 5 min. for discussion

**SESSION V**: Saturday, November 7, 2015 from 3:25 P.M. EIT Upstairs Foyer
POSTER SESSION
Chair: **Marcel Nooijen**

6:00 P.M. Poster sessions ends
Depart for Large Conference Room, ***Federation Hall*** (*check your maps!*)

6:30 P.M. Cash Bar: Large Conference Room, ***Federation Hall***

7:00 P.M. **DINNER:** Large Conference Room, ***Federation Hall***

8:30 P.M. - … Informal Discussions: Large Conference Room, ***Federation Hall***

**SESSION VI**: Sunday, November 8, 2015– A.M. EIT 1015
Chair: **Terry McMahon**

9:15– 10:00 **Erin Johnson**
(Dalhousie University)
*Properties of molecular crystals from density-functional theory*

10:00 – 10:15 **Jayashree Nagesh**, Ilya Ryabinkin, Artur Izmaylov and Paul Brumer
(University of Toronto)
*Application of localized operator to study electronic energy transfer in bi-chromophoric systems*

10:15 – 10:30 **N.L.P. Andrews** (S), R.J. Ross, D. Munzke, A-S. Lehnert, J.A. Barnes, and H-P.Loock
(Queen's University)
*Interferometric Analysis of a Gas filled Hollow-Core Photonic Crystal Fibre*

10:30 – 11:00 **Coffee Break**

**SESSION VII**: Sunday, November 8, 2015– A.M. EIT 1015
Chair: **Wing-Ki Liu**

11:00 – 11:45 **Valeria Molinero**
(University of Utah)
*Crystallization of water: a molecular perspective*

11:45 – 12:00 **Stijn Fias**, Paul W. Ayers and Paul Geerligns
(Free University of Brussels and McMaster University)
*A Perspective on the Transferability of Functional Groups From the Nearsightedness of Electronic Matter*

12:00 – 12:15 **Chang Liu**, J. C. Yves Le Blanc, Jefry Shields, John S. Janiszewski, Christian Ieritano, Gene Ye, Gillian Hawes, Moaraj Hasan, W. Scott Hopkins and J. Larry Campbell
(SCIEX and University of Waterloo)
*Understanding the Roles of Electronic and Steric Effects in Separating Isomers Using Differential Mobility Spectrometry*

12:15 – 1:30 Light **Lunch & Coffee** – EIT Foyer

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

**POSTER SESSION:** Saturday, November 7, 2015 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) **S. Walker**, J. Crouse, S. Takahashi, and H.P. Loock
(Queen's University)
*Photochemical Reaction Dynamics of Condensed Nitrogen Dioxide-Argon Systems, Using Resonance Enhanced Multiphoton Ionization Spectroscopy and Fragment Time of Flight Profiles*

1(b) **V. C. Saheer**
(Indian Institute of Technology Madras, India)
*Quantum dynamical studies on elastic and charge transfer processes in* $H^+ + O_2$ *system*

2(a) **Omar Mahassneh** and Jennifer van Wijngaarden
(University of Manitoba)
*Synchrotron-Based Infrared Spectroscopy of Oxetane*

2(b) **Wenhao Sun** and Jennifer van Wijngaarden
(University of Manitoba)
*Microwave spectra and geometries of cis- and trans-2-fluorothiophenol*

3(a) **Michael Kilgour** and Dvira Segal
(University of Toronto)
*Charge transport in molecular junctions: From tunneling to hopping with the probe technique*

3(b) **N. Moazzen-Ahamdi** and J. Norooz Oliaee
(University of Calgary)
*The* $\nu_6$ *band of ethane around 7 micron: Frequency analysis of the* $\nu_6$ *band*

4(a) **Xiaoli Cai**, Yuefei Zhang, Mohammad Reza Poopari, Aliaksandr Savin, Zahra Dezhahang and Yunjie Xu
(University of Alberta)
*Vibrational circular dichroism spectroscopy as a power tool for stereochemical analysis of Chinese herbal medicines*

4(b) **Myong In Oh** and Styliani Constas
(University of Western Ontario)
*Flexible Linear Macromolecule Confined in a Nanodroplet*

5(a) **G.X. Stewart**, N.L.P. Andrews, N. Henning, O. Reich, A. Dudelzak and H-P. Loock
(Queen's University)
*Multiplexed Excitation Emission Matrix Spectrometry*

5(b) **Ronald M. Lees, Li-Hong Xu, Bishnu Thapaliya, David Perry**, Sylvestre Twagirayezu and Brant Billinghurst
(University of New Brunswick, University of Akron, Brookhaven National Lab, and Canadian Light Source Inc.)
*High Resolution Spectroscopy of Methyl Mercaptan at the Canadian Light Source: a Perplexity of Perturbations*

6(a) S. Sheybani-Deloui, **A. J. Barclay**, K.H. Michaelian, A. R. W. McKellar and N. Moazzen-Ahmadi
(University of Calgary)
*Spectroscopic observation of the O-bonded T-shaped isomer of the $CO_2$ dimer and two of its intermolecular frequencies*

6(b) **Amy MacLean**, Michaela Thomas, Jack Barnes and Hans-Peter Loock
(Queen's University)
*An SPR imaging spectrometer to optically study self-assembling films*

7(a) **R. L. Forward**, J. Z. Fan, N.L.P. Andrews, M. Chen and H-P. Loock
(Queen's University)
*Watching the $SNO^+$ melt 2.O*

7(b) **Annica I. Freytag**, Jack A. Barnes and Hans-Peter Loock
(Queen's University)
*Fiber-optic vibration sensing of cantilevers immersed in viscous fluids*

8(a) **James Brown** and Tucker Carrington Jr.
(Queen's University)
*Phase-space localized basis functions applied to sum-of-products potentials*

8(b) **Johnathan Steffen**, J. Larry Campbell and W. Scott Hopkins
(University of Waterloo and AB SCIEX)
*Developing a Model for Differential Mobility Spectrometry (DMS) Trajectories*

9(a) **Shadman Zaman**, W. Scott Hopkins, Chang Liu, J.C. Yves LeBlanc, Subhakar Dey, Subhashish Purkayastha and J. Larry Campbell
(University of Waterloo and AB SCIEX)
*DMS Solvent Clustering of Testosterone Derivatives*

9(b) **Ahdia Anwar**, Shadman Zaman, W. Scott Hopkins, Chang Liu, J.C. Yves LeBlanc, Subhakar Dey, Subhashish Purkayastha, and J. Larry Campbell
(University of Waterloo and AB SCIEX)
*Differential Mobility Spectrometry (DMS) of Solvated Steroid Derivatives*

10(a) **Jingfei Yao**, Marcel Nooijen and W. Scott Hopkins
(University of Waterloo)
*Theoretical photodissociation of $Co^+Rg$ species*

10(b) **Alison Mark**, Chang Liu, Larry Campbell and W. Scott Hopkins
(University of Waterloo and AB SCIEX)
*Microsolvation of Gas Phase Protonated Aniline Tautomers*

11(a) **Ce Zhou**, Amy Yang, Mike Lecours, Rick A. Marta, Eric Fillion,
Terry McMahon, W. Scott Hopkins
(University of Waterloo)
*Structures and properties of serine clusters*

11(b) **Weiqiang Fui**, Shabna Mohideen, Dalia Naser,Patrick Carr, Mike Lecours,
Christian Ieritano, Michael Burt, Eric Fillion, Vincent Steinmetz, Terry McMahon,
and W. Scott Hopkins
(University of Waterloo)
*Exploring the Properties and Structures of Ionic Amino Acid Clusters*

12(a) **Sviataslau V. Kohut** and Viktor N. Staroverov
(University of Western Ontario)
*Origin of the step structure of the exact exchange-correlation potential*

12(b) **Sarah Bicker**, Micheal J. Lecours, Rick A. Marta, Eric Fillion, W. Scott Hopkins
and Terry B. McMahon
(University of Waterloo)
*Growing Gas-Phase Salt Clusters: Lithium Formate Ion and Sodium Formate Ion Species*

13(a) **Derrick. X. T. Yang** and P. W. Ayers
(McMaster University)
*Flat-Planes Conditions and Spin-Reactivity Indicators for Atoms and Ions*

13(b) **Anand Patel**, Farnaz Heidar-Zadeh, Ralph E. Pudritz and Paul W. Ayers
(McMaster University)
*Tools for solving simultaneous equillibria in astrochemical reaction networks*

14(a) **Farnaz Heidar-Zadeh**, Paul W. Ayers, Carlos Cedenas Valencia
(McMaster University)
*Pairwise Comparison Methods and Electronegativity*

14(b) Supriya Ghosh (S), Javix Thomas, Yunjie Xu and **Wolfgang Jäger**
(University of Alberta)
*Rotational Spectra of Methyl Salicylate - Water Conformers*

15(a) P. Carr, **M. Lecours**, E. Fillion, T.B. McMahon and W. Scott Hopkins
(University of Waterloo)
*IR-induced Chemistry of Palladium Catalysts*

15(b) **Evan Shepherdson**, Theodore Chow and Scott Hopkins
(University of Waterloo)
*Interactions of Carbonyl Sulfide with Cationic Rhodium Nanoclusters of Increasing Size*

16(a) **Siyuan Wu** and Marcel Nooijen
(University of Waterloo)
*"EPV"-Balanced Approximation to Coupled Cluster Singles and Doubles (CCSD)*

16(b) **Nathan Seifert**, Jiao Gao and Wolfgang Jaeger
(University of Alberta)
*The Cyclohexanone - Water Complex: A Microwave and ab initio Study*

17(a) **John E. Saunders**, Connor Sanders, Sean Chen, Jack A. Barnes and Hans-Peter Loock
(Queen's University)
*Near Infrared Refractive Index Measurements of Solvents, Solutions and Films using Large-Angle Refractometry*

17(b) **Lecheng Wang**, Robert J. Le Roy, and Pierre-Nicholas Roy
(University of Waterloo)
*A Priori Prediction of Equation of State and Vibrational Shift in Solid para-$H_2$*

18(a) **C. M. Herdman**, P.-N. Roy, R.G. Melko and A. Del Maestro
(University of Waterloo)
*Entanglement in the Lieb-Liniger model*

18(b) **Tao Zeng**, Roald Hoffmann, Reinhard Nesper, N. W. Ashcroft, Timothy A. Strobel, and Davide M. Proderpio
(Carleton University and Cornell University)
*Li-Filled, B-Substituted Carbon Clathrates*

19(a) **Cristina E. González-Espinoza**, Jacek Karwowski, Andreas Savin and Paul W. Ayers
(McMaster University)
*Energy Extrapolation: Finding a systematic way to correct model energies*

19(b) **Kevin P. Bishop** and Pierre-Nicholas Roy
(University of Waterloo)
*Quantum free energy calculations of the water dimer*

20(a) **Philip Myatt**, Pragna Chandresekhar, Ashok Dham, Frederick R.M. McCourt and Robert J. Le Roy
(University of Waterloo)
*An Accurate New Empirical Potential for $Ar_2$*

20(b) **Caitlin Lanssens**, Paul. W. Ayers and Patrick Bultinck
(McMaster University)
*Methods for making response reduced density matrices approximately N-representable*

21(a) **Matthew Schmidt**, Dmitri Iouchtchenko, Nabil Faruk, Kevin Bishop, and Pierre-Nicholas Roy
*Comparing Quantum Molecular Dynamics Calculations To Experimental Observations*

21(b) **Hanqing Zhao** and Viktor Staroverov
(University of Western Ontario)
*Reconstruction of Energy Functionals by Integration of Orbital-Dependent Potentials*

22(a) **Ryan J. MacDonell** and Michael S. Schuurman
(University of Ottawa)
*Chemical control of the nonadiabatic dynamics of acrylonitrile: An ab initio and time-resolved photoelectron spectroscopic study*

22(b) **Phillip S. Thomas** and Tucker Carrington, Jr.
(Queen's University)
*Computing Vibrational Spectra of Polyatomic Molecules Using Wavefunctions in Low-Rank Tensor Format*

23(a) **S. Walker**, J. Crouse, S. Takahashi, and H.P. Loock
(Queen's University)
*Photochemical Reaction Dynamics of Condensed Nitrogen Dioxide-Argon Systems, Using Resonance Enhanced Multiphoton Ionization Spectroscopy and Fragment Time of Flight Profiles*

23(b) **Hao Chen**, John Saunders, Sogol Borjian, Connor Sanders, Jack Barnes and Hans-Peter Loock
(Queen's University)
*Detection of aqueous lead using periodic mesoporous organosilica films on SOI micro-optical device*

24(a) **Ilya G. Ryabinkin** (P) and Artur F. Izmaylov
(University of Toronto – Scarborough)
*Electron-induced dissociation of molecules on metallic surfaces: The role of electronic friction*

24(b) **Gabriel Hanna** (F) and Farnaz Shakib
(University of Alberta)
*New insights into the nonadiabatic dynamics of model proton-coupled electron transfer reactions from the mixed quantum-classical Liouville approach*

25(a) **Neil Raymon** Pierre-Nicholas Roy
(University of Waterloo)
*Investigating the feasibility of graphics processing unit (GPU) matrix-vector products*

25(b) Aimee Bell, James Singer and **Jennifer van Wijngaarden**
(University of Manitoba)
*Analysis of the Far-IR Rovibrational Spectrum of 2-Fluorophenol Using Synchrotron Techniques*

26(a) **S. Kervazo**, S. Kahlal, B. Le Guennic, J-Y. Saillard
(McMaster University)
*Title: $d^{10}$-$d^{10}$ interactions in the Group 11 metals series: A comparative theoretical analysis*

26(b) **Matthew Chan**, Toon Verstraelen, Kasia Boguslawski, Cristina Gonzales, Farnaz Heidar Zadeh, Tae Won Kim, Pawel Tecmer, and Paul W. Ayers
(McMaster University)
*HORTON: Open Source Quantum Chemistry For Idea Development*

27(a) **Taewon Kim**, Farnaz Heidar-Zadeh, Patrick Bultinck and Paul W. Ayers
(McMaster University)
*Basis Set Independent Mulliken Analysis: Retaining Atomic Features of Diffuse Basis Functions Through Quasiatomic Orbitals*

27(b) **Rayner B. Mendes** and Viktor N. Staroverov
(University of Western Ontario)
*Simulation of Stokes Shifts in Diflouride Formazanate Complexes*

28(a) **Ayse Kumru Dikmenli**
(McMaster University)
*Investigation of Interaction Energies of Topoisomerase 1 Inhibitor: Topotecan*

28(b) **Michael Richer**
(McMaster University)
*Coarse-grained Monte Carlo Simulation of Solvent-Exposed, Surface Adsorbed Polymer Brushes at Different Packing Densities and Geometries*

29(a) **Dmitri Iouchtchenko** , Matthew Schmidt, Chris Herdman, Pierre-Nicholas Roy
(University of Waterloo)
*Numerical Approaches for Entanglement and Semiclassical Dynamics*

29(b) Nicolas Castro-Folker, Caroline Allen, **Ariel Petruk**, Kostyantyn Pichugin and German Sciaini
(University of Waterloo)
*A new Ultrafast Electron Imaging Lab*