

*The 26th Annual*  
**Symposium**  
**On**  
**Chemical Physics**  
*at the*  
*University of Waterloo*  
*November 5 -7, 2010*

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**Acknowledgements**

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

Vice President Academic & Provost, University of Waterloo  
Faculty of Science, University of Waterloo  
Department of Chemistry, University of Waterloo

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# Symposium on Chemical Physics

at the University of Waterloo

November 5 - 7, 2010

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

**SESSION I:** Friday, November 5, 2010 — P.M. EIT-1015

Chair: **Pierre-Nicholas Roy**

7:30 – 8:15 **Arthur Suits**  
(Wayne State University)  
*Roaming Radicals! Results from High-Resolution Imaging Studies*

8:15 – 8:30 **Dipayan Datta** and Marcel Nooijen  
(University of Waterloo)  
*A Partially Internally Contracted Multireference Coupled-Cluster Approach*

8:30 – 8:45 **Jesse Greener**, Clement Scholl, Bardia Abbasi, Dan Voicu, and  
Eugenia Kumacheva  
(University of Toronto)  
*Spectroscopy on a Chip: a New Tool for Studying Chemical Kinetics of  
Microfluidic Reactions*

8:45 – 9:00 **Nikesh S. Dattani**  
(Oxford University)  
*Numerical Feynman Integrals with Master Equation Interpolants Allow for  
Faster Convergence and Significant Reduction in Computational Cost.  
Application to GaAs Quantum Dots and the FMO Photosynthetic Complex*

**SESSION II:** Saturday, November 6, 2010 – A.M. EIT-1015

Chair: **Takayoshi Amano**

9:00– 9:45 **Yujun Shi**  
(University of Calgary)  
*Catalytic Chemical Vapor Deposition Chemistry in the Gas Phase and  
on the Catalyst Surface*

9:45 – 10:00 **Prakash Dayal** and Nicholas J. Mosey  
(Queen's University)  
*A Highly Efficient and Improved Temporal QM/MM: Extending the Time-Scales  
Accessible in Molecular Dynamics Simulations of Reactions*

10:00 – 10:15 **Ruth Signorell**  
(University of British Columbia)  
*Hydrocarbon Aerosols in Titan's Troposphere*

10:15 – 10:45 **Coffee Break**

**SESSION III:** Saturday, November 6, 2010 – A.M.

EIT-1015

Chair : **Robert Le Roy**

10:45 – 11:45 **The Roger E. Miller Lecture : Tom Ziegler**

(University of Calgary)

*The Description of Excited States by Density Functional Theory*

11:45 – 12:00 **M. Peters**, T.T. Nguyen-Dang, C. Cornaggia, S. Saugout, E. Charron, A. Keller

and O. Atabek

(Université Laval and Université de Paris-Sud, Saclay)

*Ultrafast Molecular Imaging by Laser-Induced Electron Diffraction*

12:00 – 12:15 **S.K. Burger**, S. Liu and P. Ayers

(McMaster University)

*Practical Calculation of Molecular Acidity with Reactive Indicators*

12:15 – 1:30 **Lunch** – EIT Foyer

**SESSION IV:** Saturday, November 6, 2010 – P.M.

EIT-1015

Chair: **Jim Martin**

1:30 – 2:15 **Andrey Vilesov**

(University of Southern California)

*Growing Clusters in He Droplets: From Nano- to Micro-Droplets*

2:15 – 2:30 **Gustavo Avila-Blanco** and Tucker Carrington, Jr.

(Queen's University)

*Using Non-Product Quadrature Grids to Solve the Vibrational Schrödinger Equation in 12D*

2:30 – 2:45 **Etienne Garand**, Michael Z. Kamrath, Rachael A. Relph,

Christopher M. Leavitt, and Mark A. Johnson

(Yale University)

*Infrared Predissociation Spectroscopy of Collisionally-Cooled Electrosprayed Ions: Towards Characterization of Complex Reaction Intermediates*

2:45 – 3:00 **Jérémy Viau Trudel** and T.T. Nguyen-Dang

(Université Laval)

*Quantum Dynamics of Many-Electron Systems in Intense Laser Fields: A Multi-Scale Approach*

3:00 – 3:15 **John W. Tromp** and Randall S. Dumont

(Vanier College and McMaster University)

*The Thermal Flux-Flux Correlation Function and Classical-Quantum Correspondence*

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 6, 2010 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 7, 2010 – A.M.

EIT 1015

Chair: **Marcel Nooijen**

9:15– 10:00 **Nick Mosey**  
(Queen's University)  
*First-Principles Simulations of Tribological Processes*

10:00 – 10:15 **Xunchen Liu** and Yunjie Xu  
(University of Alberta)  
*Infrared Spectra of Ar-H<sub>2</sub>O and Higher-Order Complexes with a CW Mode-Hop-Free External Cavity Quantum Cascade Laser*

10:15 – 10:30 Dipayan Paul, Charles A. Odame-Ankrah, Sahar Da'er, Robert D. Thaler,  
and **Hans Osthoff**  
(University of Calgary)  
*In Situ Measurements of Atmospheric Nitrogen Oxides by Broadband Diode Laser Cavity Ring-Down Spectroscopy*

10:30 – 11:00 **Coffee Break**

**SESSION VII:** Sunday, November 7, 2010 – A.M.

EIT 1015

Chair: **Tong Leung**

11:00 – 11:45 **Kaley Walker**  
(University of Toronto)  
*Using Spectroscopy to Study Atmospheric Composition*

11:45 – 12:00 **Alex P. Gaiduk** and Viktor N. Staroverov  
(University of Western Ontario)  
*Toward Density-Functional Theory Based on Model Kohn-Sham Potentials*

12:00 – 12:15 **Helen Wächter**, Dorit Munzke, Jessica Litman, Hengameh (Hanna) Omrani,  
Jack A. Barnes and Hans-Peter Loock  
(Queen's University)  
*Fiber-cavity Enhanced Absorption Detector for Picoliter to Nanoliter-Sized Samples of Liquids and Gases*

Chair: **Robert Le 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) **Randall S. Dumont**  
(McMaster University)  
*Two-channel Conduction Through Polycenes -- Extension of the Source-Sink Potential Method to Multichannel Coupling to Leads*
- 1(b) **Debajit Chakraborty** and Paul A. Ayers  
(McMaster University)  
*Linear Fitting of Diatomic Potential Energy Curves by Orthogonal Polynomials*
- 2(a) **Carl Haugen** and Ajit Thakkar  
(University of New Brunswick)  
The Determination of Structures of Aluminum Nanoparticles, Al<sub>n</sub> Using an Evolutionary Algorithm
- 2(b) **Greg Wentworth**, Greg Casey, Hind Al-Abadleh and Ian Hamilton  
(Wilfrid Laurier University)  
*Kinetics of Photochemical Reactions and Water Uptake in Organic-Containing Aerosols*
- 3(a) **Paul A. Johnson** and Paul W. Ayers  
(McMaster University)  
*A Kohn-Sham-Like Model for the 1-Body Reduced Density Matrix from a Strongly-Correlated Reference*
- 3(b) **Pei Yan Zhu**, Guochun Yang and Yunjie Xu  
(University of Alberta)  
*Leucine in Solution: A Vibrational Circular Dichroism and Density Functional Theory Study*
- 4(a) **Rogelio Cuevas** and Paul Ayers  
(McMaster University)  
*A New Approach to Non-Local Exchange-Correlation Functionals*
- 4(b) **Mohammad Reza Poopari, Zahra Dezhahang**, Guochun Yang and Yunjie Xu  
(University of Alberta)  
*Probing Hydrogen Bonding Interaction of N-acetyl-L-Cysteine in Solution using Vibrational Circular Dichroism Spectroscopy, and Density Functional Theory and Molecular Dynamics Calculations*

- 5(a) **Gurpaul S. Kochhar**, Adrian Bailey and Nicholas J. Mosey  
(Queen's University)  
*Competition between Orbitals and Stress in Mechanochemistry*
- 5(b) **Adrian Adamescu**, William Mitchel, I. P. Hamilton and Hind A. Al-Abadleh  
(Wilfrid Laurier University)  
*Insights into the Surface Complexation of Dimethylarsinic Acid on Iron (Oxyhydr)oxides from ATR-FTIR Studies and Quantum Chemical Calculations*
- 6(a) J. Norooz Oliaee, M. Dehghany, N. Moazzen Ahmadi, and **A.R.W. McKellar**  
(University of Calgary and National Research Council)  
*Spectroscopic Identification of Carbon Dioxide Clusters: (CO<sub>2</sub>)<sub>6</sub> to (CO<sub>2</sub>)<sub>13</sub>*
- 6(b) Javix Thomas, Fumie X. Sunahori, Nicole Borho and **Yunjie Xu**  
(University of Alberta)  
*A Microscopic Induced Fit Example: Chirality Recognition in the Glycidol...Propylene Oxide Complex*
- 7(a) **Francis P. Temme**  
(Queen's University)  
*Disjoint Sums over  $S_n$  G-Invariant-Labelled terms as Transformation-like Forms within TR-invariance-constrained Automorphisms for Invariant-Theoretic  $\chi^{(\lambda)}$  Char-sum Modelling in Establishing the IPS Quantal Completeness of all  $3 \leq n \leq 48, (60)$ -indexed (Endohedral) Spin Systems*
- 7(b) **Oleksandr Sukhorukov**, Steve Dempster, Qi-Yi (Tracey) Lei, and Wolfgang Jäger  
(University of Alberta)  
*A Chirped Pulse Fourier Transform Microwave Spectrometer for the Study of Weakly Bound Complexes and Clusters*
- 8(a) Luca Evangelisti and **Jennifer van Wijngaarden**  
(University of Manitoba)  
*Experimental Determination of the Structure and Internal Rotor Dynamics of 1,1,1-Trifluoro-2-Butanone*
- 8(b) **Steve Dempster**, Oleksandr Sukhorukov, Qi-Yi (Tracey) Lei, and Wolfgang Jäger  
(University of Alberta)  
*Study of (He)<sub>N</sub>-HCN Clusters using Rotational Spectroscopy*
- 9(a) Adam Grabowiecki, Luca Evangelisti and **Jennifer van Wijngaarden**  
(University of Manitoba)  
*Rotational Spectra of 2,2,2-Trifluoroethylformate*
- 9(b) **Gregory Casey**, Gregory R. Wentworth, I.P. Hamilton and Hind A. Al-Abadleh  
(Wilfrid Laurier University)  
*Quantum Chemical Calculations on Solvation effects for Selected Photoreactive Aromatic Organic Molecules of Atmospheric Relevance*
- 10(a) **Farnaz Heidar Zadeh** and Shant Shahbazian  
(McMaster University)  
*Quasi-Atoms within the Context of the Quantum Theory of Atoms in Molecules*

- 10(b) **Hongjuan Zhu** and Nicholas J. Mosey  
(Queen's University)  
*The Tensile Strengths of Polymer-Containing Interfaces: A Comparison of Static and Dynamic First-Principles Calculations*
- 11(a) **Allan Adam**, Thomas Allen, Laura Downie, Aaron Granger and Michelle Jacobs  
(University of New Brunswick)  
*Studies of Two Transition Metal Containing Diatomic Molecules: RhBr and IrH*
- 11(b) **N. Moghimi** and T. K. Leung  
(University of Waterloo)  
*Application of Hybrid Fe Nano-Structures*
- 12(a) **James D. D. Martin**  
(University of Waterloo)  
*Modifying Rydberg State Polarizabilities using an RF Dressing Field*
- 12(b) **Sandra Rabi**, Toon Verstraelen, Steven Burger and Paul Ayers  
(McMaster University)  
*An Efficient Method for Transition State Optimization Using Redundant Internal Coordinates*
- 13(a) Svetoslav Rashev and **David C. Moule**  
(Bulgarian Academy of Sciences and Brock University)  
*Vibrational Calculations in Formaldehyde: The CH stretch System*
- 13(b) **Otman Abida**, Hans D. Osthoff and Todd C. Sutherland  
(University of Calgary)  
*Photochemical Transformation of Nitrate in Frozen Solutions*
- 14(a) **Jeffrey Philippson**, Steven McMurtry, Matthew Romerein and Ralph Shiell  
(Trent University)  
*Observation and Modelling of Uneven Mode Spacing and Frequency-Pulling in a Helium-Neon Laser*
- 14(b) **Rim Toukabri** and Y. J. Shi  
(University of Calgary)  
*Effect of Pressure and Filament Materials on the Activation Energy of Hot-Wire Decomposition of Di- and Trimethylsilane*
- 15(a) **Zi Jian Long** and W.K. Liu  
(University of Waterloo)  
*Strong Field Ionization of the Hydrogen Molecular Ion*
- 15(b) **Natalie Cann** and Shihao Wang  
(Queen's University)  
*Chirality Transfer in Solution and at Interfaces*



- 16(a) **Lee Huntington** and Marcel Nooijen  
(University of Waterloo)  
*Accurate Thermochemistry from a Parameterized Variant of CCSD*
- 16(b) **Christopher D. Daub** and Natalie M. Cann  
(Queen's University)  
*Molecular Dynamics Simulations of Phenyl-Pyrimidine Liquid Crystal Phase*
- 17(a) **Shahid M. Islam**, Todd L. Lowary and Pierre-Nicholas Roy  
(University of Waterloo and University of Alberta)  
*Simulation Studies of Biologically Relevant Oligo-arabinofuranosides*
- 17(b) **Mohammad Ashtari** and Natalie M. Cann  
(Queen's University)  
*Modelling Proline-Based Chiral Stationary Phases*
- 18(a) **Paul Raston**, Chrissy Knapp and Wolfgang Jäger  
(University of Alberta)  
*Laser Spectroscopy of Hydrogen Peroxide in Helium Nanodroplets*
- 18(b) **J. Saunders**, G. Ongo, M. Dreher, J.A. Barnes, C. Crudden, J. Du, H.-P. Loock,  
D.-X. Xu, A. Densmore, R. Ma, S. Janz, M. Vachon, J. Lapointe, A. Delâge, J. Schmid,  
and P. Cheben  
(Queen's University)  
*Refractive Index Detection of Environmental Contaminants using Silicon-on-Insulator  
Microdevices*
- 19(a) **Rick A. Marta**, Sabrina M. Martens, Jon K. Martens, and Terry B. McMahon  
(University of Waterloo)  
*Simultaneous Dual Action Spectra of Protonated Clusters of Trimethylamine and  
Substituted Phenylalanines: Charge-Solvated and Zwitterionic Isomers Revealed*
- 19(b) **Blake Ziegler** and Terry McMahon  
(University of Waterloo)  
*Hydrogen/Deuterium Exchange Mechanisms of Gas Phase Peptides*
- 20(a) **Sabrina M. Martens**, Rick A. Marta, Jonathan K. Martens and Terry B. McMahon  
(University of Waterloo)  
*Infrared Multiple Photon Dissociation Spectroscopy of Ferulic Acid: a Unique  
Fragmentation Mechanism*

## 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 your plastic name-tag holder into the cardboard box by the entrance to the Registration area. This will allow recycling and reduce our costs for next year.

- **Phone Numbers:**

*Comfort Inn:* 519-747-9400 190 Weber Street N, Waterloo

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*Waterloo Inn:* 519-884-0220 485 King Street N., Waterloo

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*United Taxi:* 519-888-0400

*City Cab:* 519-747-7777

R.J. Le Roy: 519-885-1198 (home)

519-589-4051 (mobile)