The 25th Annual

Symposium

On

Chemical Physics

at the

University of Waterloo

November 6 - 8, 2009

Symposium on Chemical Physics

at the University of Waterloo

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REGISTRATION begins at 6:30 p.m. (coffee & cookies available) EIT Room 1015

SESSION I: Friday, November 6, 2009 — P.M. EIT 1015

Chair: **Marcel Nooijen**

7:30 – 8:15 **Kevin Lehmann**
(University of Virginia)
Cavity Ring-Down Spectroscopy

8:15 – 8:30 **Steven K. Burger**, David Thompson and Paul Ayers
(McMaster University)
Cytochrome C Peroxidase: QM/MM Docking Calculations To Distinguish Between Binders and Decoys

8:30 – 8:45 **Lee Huntington** and Marcel Nooijen
(University of Waterloo)
Parameterized Coupled Cluster Methods

8:45 – 9:00 **Sergey Kazachenko** and Ajit J. Thakkar
(University of New Brunswick)
Global Minima of Water Clusters: Comparison of TIP4P, TTM2.1-F and AMOEBA

9:30 P.M. Informal Discussions Graduate Club

SESSION II: Saturday, November 7, 2009 – A.M.
Chair: **James Martin**

9:00– 9:45 **Jeremy Hutson**
(University of Durham)
Ultracold Molecules and Ultracold Collisions

9:45 – 10:00 **Sergei Manzhos**, Koichi Yamashita, Tucker Carrington
(University of Tokyo and Queen's University)
Calculation of Vibrational Spectra from Discrete Samples of the Potential Energy Surface and an Ultra-Small Basis, Obviating Quadratures and the Need for a Potential Function

10:00 – 10:15 **Jonathan Baugh**, J. S. Fung, R. R. LaPierre, Y. Song and J. Mracek
(University of Waterloo)
Building a Spin Quantum Bit Register Using Semiconductor Nanowires

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, 2009 – A.M. EIT 1015
Chair : **Robert Le Roy**

10:45 – 11:45 ***The Roger E. Miller Lecture*** : **Marsha Lester**
(University of Pennsylvania)
Dynamical Outcomes of Quenching: Reflections on a Conical Intersection

11:45 – 12:00 **Richard Dawes** and Ahren W. Jasper
(Sandia National Labs)
Methods for Construction of ab initio PESs Describing Large Amplitude Motion

12:00 – 12:15 **Rogelio Cuevas-Saavedra** and Paul W. Ayers
(McMaster University)
Ornstein-Zernike-Like Models for the Exchange-Correlation Hole in the Homogeneous Electron Liquid

12:15 – 1:30 **Lunch** – EIT Foyer

SESSION IV: Saturday, November 7, 2009 – P.M. EIT 1015
Chair: **John Hepburn**

1:30 – 2:15 **Giacinto Scoles**
(International School for Advanced Studies, Trieste)
Nanomedicine: Towards New Definitions, Diagnostics and Cure of Illness in Modern Medicine

2:15 – 2:30 **Thomas C. Preston** and Ruth Signorell
(University of British Columbia)
Growth and Optical Properties of Gold Nanoshells Prior to the Formation of a Continuous Metallic Layer

2:30 – 2:45 **Fedor Y. Naumkin** and Gurpaul Kochhar
(University of Ontario Institute of Technology)
Un/Usual Coordination of Carbon in Hyper/Metallide CM_n Species

2:45 – 3:30 **Robert J. Le Roy**
(University of Waterloo)
Adventures in 'Potentiology'

3:30 **Refreshments and Poster Session** EIT Upper Foyer

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 7, 2009 from 3:30 P.M. EIT Upper 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 8, 2009 – A.M. EIT 1015
Chair: **Tong Leung**

9:15 – 10:00 **Wolfgang Jäger**
(University of Alberta)
Doped Superfluid Clusters

10:00 – 10:15 **Bryan van der Ende**, Linda Aarts, Ramon Muller and Andries Meijerink
(Utrecht University)
Photon Management for Solar Cells: Conversion of the Solar Spectrum Using High-Efficiency Near-Infrared Quantum Cutting

10:15 – 10:30 **Alexandre Foisy-Geoffroy**, Bilkiss B. Issack and Gilles H. Peslherbe
(Concordia University)
Computational Investigation of the Thermal Stability of Zeolites: Silicalite and ZSM-5 as Case Studies

10:30 – 11:00 **Coffee Break**

SESSION VII: Sunday, November 8, 2009 – A.M. EIT 1015
Chair: **Pierre-Nicholas Roy**

11:00 – 11:45 **Roman Krems**
(University of British Columbia)
Ultracold Chemistry

11:45 – 12:00 **Soran Jahangiri** and Gilles H. Peslherbe
(Concordia University)
Theoretical Investigation of Solvation in Aqueous Clusters: The Nitrate and Nitrite Ions

12:00 – 12:15 **Fumie Sunahori**, Guoshun Yang, Elena N. Kitova, John S. Klassen & Yunjie Xu
(University of Alberta)
FTICR-IRMPD Spectroscopy of Serine Clusters

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

POSTER SESSION

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) **Chun C. Mak**, Qadir K. Timerghazin and Gilles H. Peslherbe
(Concordia University)
Theoretical Studies of Electron Solvation Dynamics in Photoexcited Iodide-Water Clusters

1(b) D. Forthomme, **C. Linton**, D. W. Tokaryk, A. G. Adam and A. D. Granger
(University of New Brunswick)
High Resolution Laser Spectroscopy of $Mg^{12}C^{12}CD$, $Mg^{13}C^{13}CH$, $Mg^{12}C_4H$ and $Mg^{12}C_6H$

2(a) Noureddin E.-B. Kassimi and **Ajit J. Thakkar**
(University of New Brunswick)
Polarizabilities are Additive: 19th Century Ideas Come to the Aid of 21st Century Computations

2(b) **A. Kuleshov**, M. Khorunzhiy, S. I. Khomenko and Boris P. Yefimov
(Institute of Radiophysics and Electronics of NAS of Ukraine)
Excitation of Long-Living Plasma in Open Air, and Doppler Radar Method for Investigation of Plasma Parameters

3(a) **F.P.Temme**
(Queen's University)
Quantal Completeness of Indistinguishable Point-Sets via G-Action-Based Projective Maps \& Reduced Littlewood Polynomial Invariant Theory in NMR: TR-Invariance-derived G-Invariant Cardinality of (X)@ $^{13}C_{60}$ Fullerenes as Isochronous -defined Nano-Systems Beyond the Remit of R-W Algebra

3(b) James Thomas, Katie Lower and **Craig Murray**
(University of Bristol)
Exploring C-N Bond Fission Pathways in Methylamine Photodissociation

4(a) **P. A. Johnson** and P.W. Ayers
(McMaster University)
N-Representability of the 2nd-Order Reduced Density Matrix: Necessary Diagonal Conditions

4(b) **Ben S. Carver** and Nicholas J. Mosey
(Queen's University)
Olefins Under Stress: Effects of Mechanochemistry on Reactions at Carbon-Carbon Double Bonds

5(a) **Luan T. Nguyen**, George C. McBane and Reinhard Schinke
(Grand Valley State University and Max Planck Institute for Dynamics and Self-Organization)
Trajectory Surface Hopping Study of Energy Disposal in the Triplet Channel of Ozone Photodissociation in the Hartley Band

5(b) Carolyn J. Carkner and **Nicholas J. Mosey**
(Queen's University)
First Principles Simulations of Tribochemical Reactions

6(a) **Denis J. Gendron**
(Claire Lasers Corporation)
Production of Metal/Metal-Oxide Nanoparticles on Aluminum Surfaces Within a Laser Excited Plasma: Application to Laser Based Photographic Reproduction

6(b) **Gurpaul Kochhar**, Adrian Bailey, Nicholas J. Mosey
(Queen's University)
Dependence of Mechanochemical Effects on the Locations of Pulling Points

7(a) **C.Y. Yang**, X.K. Hu, A.V. Loboda and R.H. Lipson
(University of Western Ontario)
A Useful Binary Matrix for Visible-MALDI of Low Molecular Weight Analytes

7(b) Sabine A. Weyand, Joanne McNeish, **Nicholas J. Mosey**
(Queen's University)
Extending the Time-Scales Accessible in Molecular Dynamics Simulations of Chemical Reactions

8(a) **Adrian Adamescu**, Holly Gray, I. P. Hamilton and Hind A. Al-Abadleh
(Wilfrid Laurier University)
Quantum Chemical Calculations of Geometry, Atomic Charges and Infrared Frequencies of As(V)-containing Compounds Important in Geochemistry

8(b) **Wei Guo**, Piyumie Wickramasinghe, Stephen Walker, Jeff Crouse and Hans-Peter Loock
(Queen's University)
Velocity Map Imaging to Investigate Photochemistry of Water Ice

9(a) **Bryan Linford**, J. Mark Parnis, and Matthew G. K. Thompson
(Trent University)
A Matrix Isolation Investigation of the Fragmentation Products Following Charge Transfer Ionization of Vinyl Fluoride

9(b) **Piyumie Wickramasinghe**, Wei Guo, Hans-Peter Loock; Tetsuya Hama, Masaaki Yokoyama, Akihiro Yabushita, Masahiro Kawasaki; Michael.N.R.Ashfold, and Colin M.Western
(Queen's University, Kyoto University, and University of Bristol)
Translational and Internal Energy Distributions of Methyl and Hydroxyl Radicals Produced by 157 nm Photodissociation of Amorphous Solid Methanol

10(a) **Paul Raston** and Wolfgang Jäger
(University of Alberta)
Rotational Spectra Study of (para-Hydrogen)$_N$-Carbon Monoxide Clusters

10(b) H. Waechter, **K. Bescherer**, J. Barnes, R.D. Oleschuk and H.-P. Loock
(Queen's University)
Microfluidic Detection using Cavity Ring-Down Spectroscopy at 405nm and Implementation of Liquid Core Waveguides as Cavity Medium

11(a) **Hui L**i, Robert J. Le Roy, Pierre-Nicholas Roy and A.R.W. McKellar
(University of Waterloo)
Measurement of Superfluid Response in CO_2-(p-H_2)$_N$ Clusters: Experiment and Theory

11(b) W. Al-Basheer, **Z. J. Cai**, M. Heden and Y. J. Shi
(University of Calgary)
Study of Two-photon Resonant Four-wave Sum Mixing (TPR-FWSM) in Atomic Xenon

12(a) **G. Avila-Blanco** and Tucker Carrington Jr.
(Queen's University)
Non-Product Quadrature Grids for Solving the Vibrational Schrödinger Equation

12(b) **Z. J. Cai** and Y. J. Shi
(University of Calgary)
Effect of Methyl Substitution on the Structures and Electronic Transitions of Three Monosilacyclobutane Molecules Using ab initio Calculations

13(a) **S. S. Farvid**, K.G. Stamplecoskie, N. Dave, L. Ju and P.V. Radovanovic
(University of Waterloo)
The Effect of Dopant Ions on the Morphology, Structure, and Properties of Nanomaterials

13(b) **Ebrahim Najafi**, Jian Wang, Adam Hitchcock, Carmen Andrei, Gianluig Botton, Jingwen Guan and Benoit Simard
(McMaster University and S.I.M.S. NRC)
X-ray Absorption and Electron Energy Loss Spectroscopy of Individual Carbon Nanotubes

14(a) **Debajit Chakraborty** and Paul W. Ayers
(McMaster University)
Linear Fitting of Diatomic Potential Energy Curves by Orthogonal Polynomials

14(b) **Sergei Manzhos** and Koichi Yamashita
(University of Tokyo)
Reconstruction of a Potential Energy Surface of a Molecule-Surface Reaction from Extremely Sparse ab initio Samples Using Neural Network Dimensionality Reduction

15(a) **Jason Tao**, Carl Haugen, Robert J. Le Roy
(University of Waterloo)
Potentiology Leads to Compact and Robust Analytic Potential Energy Functions for the Ground States of Ca_2, NaCs, NaRb and Rb_2 (and probably almost anything!)

15(b) **Samir Mushrif**, Alejandro Rey and Gilles Peslherbe
(Concordia University and McGill University)
Towards Understanding Palladium Doping of Carbon Supports: A First Principles Molecular Dynamics Investigation

16(a) **J. Saunders**, J. Barnes, H.-P. Loock and D.-X. Xu
(Queen's University)
Chemical Detection using Polymer Coated Micro-optical Devices

16(b) **Allan Runstedtler** and Javier Giorgi
(Natural Resources Canada and University of Ottawa)
Surfaces of Yttria-Stabilized Cubic Zirconia: a Computational Study

17(a) **R.M. Lees**, Li-Hong Xu, D.R.T. Appadoo and Brant Billinghurst
(University of New Brunswick, and Canadian Light Source)
FIR and IR Spectroscopy of Methanol Isotopologues at the Canadian Light Source

17(b) **Galen Sedo**, Jennifer van Wijngaarden, and Steven T. Shipman
(University of Manitoba and New College of Florida)
The New Chirped-Pulse Fourier Transform Microwave Spectrometer at the University of Manitoba

18(a) **Debabrata Pradhan**, Zhengding Su, Shrey Sindhwani, John F. Honek and Tong Leung
(University of Waterloo)
Realization of Active Nanobiocomposite of ZnO Nanobelts an Glucose Oxidase

18(b) **Ziqiu Chen** and Jennifer van Wijngaarden
(University of Manitoba)
Synthesis and Microwave Spectroscopic Characterization of Silacyclopentane

19(a) **Susumu Kuma,** Aakash Ravi and Takamasa Momose
(University of British Columbia)
Infrared Spectroscopy of CH_4-$(H_2)_N$ in Superfluid ^{4}He Droplets

19(b) **Xunchen Liu**, Yunjie Xu, Wai Shun Tam, and Igor Leonov
(University of Alberta)
Application of a Room Temperature Quantum Cascade Laser with Rapid Scan and Wavelength-Modulation Techniques

20(a) Eric Vyskocil, Watheq Al-Basheer, Susumu Kuma and **Takamasa Momose**
(University of British Columbia)
Generation of a Cold Pulsed Molecular Beam at 100 mK

20(b) **Samad Bazargan** and Kam Tong Leung
(University of Waterloo)
Photoluminescence in Eu--Doped Tin (IV) Oxide Nanostructured Thin Films

21(a) **Shahidul M. Islam**, Pierre-Nicholas Roy and Todd L. Lowar
(University of Waterloo)
Conformational Study on a Series of Arabinofuranosides using Long Molecular Dynamics and Umbrella Sampling Simulations

21(b) **A. Chatterjee**, L. Zhang and K. T. Leung
(University of Waterloo)
Adsorption of Glycine on Si(111)7x7: An STM Investigation

22(a) **Xiujuan Yang**, X. K. Hu and R. H. Lipson
(University of Western Ontario)
Metal-Based Substrates for Soft Laser Desorption-Ionization Mass Spectrometry

22(b) M. Bakhtvar, **N. Moghimi** and A. Hojabri
(Islamic Azad University, Iran)
The UV-barrier Properties of Al Thin Film on PET (Polyethylene Terephthalate)

23(a) **Xiao-Gang Wang** and Tucker Carrington Jr.
(Queen's University)
A Theoretical Study of Rovibrational Levels of H_2O-H_2

23(b) **Yalina Tritzant Martinez** and Pierre-Nicholas Roy
(University of Waterloo)
Influence of Flexibility on the Stability of Water Clusters: Modeling of the Long-Range Interaction

24(a) **Xiao-Gang Wang** and Tucker Carrington Jr.
(Queen's University)
Rovibrational energy levels of CH_5^+

24(b) **Qadir K. Timerghazin** Pierre-Nicholas Roy and Alex Brown
(University of Waterloo and University of Alberta)
Mechanism for the Ground-State Isomerization of the Green Fluorescent Protein Chromophore: A Computational Study

25(a) Robert A. Collister, **Jeffrey N. Philippson** and Ralph C. Shiell
(Trent University
A Study of Long-Range Valence-Ion-Pair Coupling in Rb_2 and a Comparison with Li_2

25(b) **Gregory J. Bubnis** and Howard R. Mayne
(University of New Hampshire)
Modeling the Self-Assembly of Derivatized Fullerenes on Au(111)

26(a) **Chris Ing,** Konrad Hinsen and Pierre-Nicholas Roy
(University of Waterloo)
Path Integral Molecular Dynamics Implementation in MMTK

26(b) Jose-Luis Carreon-Macedo, Markus Schroeder and **Alex Brown**
(University of Alberta)
Ab Initio Potential Energy and Dipole Moment Surfaces for CS_{2}: Towards Optimal Control of a CARS Process Using the OCT-MCTDH Approach

27(a) **Denise M. Koch**, Soran Jahangiri and Gilles H. Peslherbe
(Concordia University)
New Insights into Ion Hydration: The Halide Series as a Case Study