The 24th Annual

Symposium

On

Chemical Physics

at the

University of Waterloo

November 7 - 9, 2008

Symposium on Chemical Physics

at the University of Waterloo

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REGISTRATION begins at 7:00 p.m. Davis Centre Room 1301

SESSION I: Friday, November 7, 2008 — P.M. Davis Centre Room 1351

Chair: **Fred McCourt**

7:30 – 8:15 **Peter Bernath**
(University of York)
Molecular Astronomy

8:15 – 8:30 ***Shahidul M. Islam*** and Raymond A. Poirier
(Memorial University)
Can Kinetic Isotope Effects be Used to Determine Substituent Effects on the Structure of S^N2 Transition States?

8:30 – 8:45 **Maryam Ebrahimi** and Kam Tong Leung
(University of Waterloo)
Selective Chemisorption and Thermal Evolution of Carboxylic Acids on Si(100)2: From Experiment to DFT Calculations

8:45 – 9:00 Cody van Dijk, Ziqiu Chen, Samantha van Nest and **Jennifer van Wijngaarden**
(University of Manitoba)
Fourier Transform Microwave and Infrared Study of Silacyclobutane

SESSION II: Saturday, November 8, 2008 – A.M.
Chair: **Pierre-Nicholas Roy**

9:00– 9:45 **Ruth Signorell**
(University of British Columbia)
Vibrational Excitons in Aerosol Spectroscopy

9:45 – 10:00 **Jean Christophe Tremblay** and Peter Saalfrank
(Universität Potsdam)
Controlling Vibrational Dynamics of Adsorbates at Metal Surfaces

10:00 – 10:15 **Sergei Manzhos** and Koichi Yamashita
(University of Tokyo)
Dynamics-Friendly High-Dimensional Potential Energy Surfaces to Streamline the Modeling of Heterogeneous Catalysis: an N_2O/Cu(100) Example

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, 2008 – A.M. Davis Centre Room 1351
Chair : **Robert Le Roy**

10:45 – 11:45 ***The Roger E. Miller Lecture*** : **Joel Bowman**
(Emory University)
Reaction and Vibrational Dynamics on Full-Dimensional ab initio-Based Potential Energy Surfaces

11:45 – 12:00 **Xunchen Liu**, Nicole Borho and Yunjie Xu
(University of Alberta)
Molecular Self-Recognition: Rotational Spectra of the Dimeric 2-Fluoroethanol Conformers

12:00 – 12:15 **Hui Li**, Robert J. Le Roy, N. Blinov and P.-N. Roy
(University of Waterloo and NRC National Institute for Nanotechnology)
Shortcomings of a Reduced-Dimension Potential Energy Surface: PIMC Simulation of v_3 Vibrational Shifts for CO_2 in He_N Clusters

12:15 – 1:30 **Lunch** – Davis Centre 1301

SESSION IV: Saturday, November 8, 2008 – P.M. Davis Centre Room 1351
Chair: **Pavle Radovanovic**

1:30 – 2:15 **Tong Leung**
(University of Waterloo)
Spintronics: Emerging Nanotechnology or just Applied Chemical Physics?

2:15 – 2:30 Masaaki Tsubouchi and **Takamasa Momose**
(University of British Columbia)
Rovibrational Wavepacket Manipulation by Shaped Femtosecond Pulses: Simulation and Experiments

2:30 – 2:45 **Markus Schröder** and Alex Brown
(University of Alberta)
Quantum Gate Operations in 6D Ammonia using the OCT-MCTDH Approach

2:45 – 3:00 **Yujun Shi**, B. D. Eustergerling and M. Heden
(University of Calgary)
Development of a New Laser Induced Electron Impact Ionization Source and its Application

3:00 – 3:15 **Mark Cybulski**
(Miami University)
The Importance of Secondary Interactions in DNA

3:15 **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 8, 2008 from 3:30 P.M. Davis Centre Lobby

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 9, 2008 – A.M.
Chair: **Marcel Nooijen**

9:30– 10:15 **Garnet Chan**
(Cornell University)
Strongly Interacting Electrons in Chemistry

10:15 – 10:30 **Chun C. Mak**, Qadir K. Timerghazin, and Gilles H. Peslherbe
(Concordia University)
Theoretical Studies of the Relaxation Dynamics of Photoexcited Iodide-Water Clusters

10:30 – 10:45 Natalie Weigum, Clare McElcheran, **Kaley A. Walker**, Chris Boone, Peter F. Bernath, Geoffrey C. Toon, Gloria Manney, Susan Strahan, Bryan Duncan, Yasuko Yoshida, and Yuhang Wang
(University of Toronto, University of Waterloo, Jet Propulsion Laboratory, University of Maryland, Institute of Technology)
Global Distribution of CH_3Cl from ACE-FTS Solar Occultation Measurements

10:45 – 11:15 **Coffee Break**

SESSION VII: Sunday, November 9, 2008 – A.M. Davis Centre Room 1351
Chair: **Tong Leung**

11:15 – 12:00 **Dennis Tokaryk**
(University of New Brunswick)
Rings and Things at the Ring: FTIR Spectroscopy of Moderately Lage Molecules at the Canadian Light Source

12:00 – 12:15 **Xiaogang Wang** and Tucker Carrington Jr.
(Queen's University)
A Discrete Variable Representation Treatment of the Rovibrational Quantum Dynamics of Molecules with More Than Three Atoms

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) **George C. McBane**
(Grand Valley State University)
***PMP Molscat**: A Parallel Version of the Molscat Quantum Inelastic Scattering Program*

1(b) **Francis P. Temme**
(Queen's University)
Time-Reversal & Weyl-Schur Duality in Littlewood $\mathcal{GL}_n$-like Hooklength-realised Character-Sums for Direct Realisation of $\mathcal{S}_n$ G-Invariants Defining MR Indistinguishable Tensorial Point Sets and their Quantal-Completeness

2(a) K. Tono, Jer-Lai Kuo and **K. Tsukiyama**
(Tokyo Univeristy of Science, Scholl of Physical and Mathematical Sciences, and Nanyang Technological University)
Photodissociation Spectroscopy of Protonated Methanol Cluster Ions in the Middle Infrared Region: Solvation Structures of the Excess Proton

2(b) **Jesse Greener**, Tibert Hendrik van der Loop, Chantal Paquet, Gregory Scholes and Eugenia Kumacheva
(University of Toronto)
"Photo-Patterning of Semi-Conductor Nanocrystals and Alignment of Nanorods

3(a) **Cheng Lu** and Robert H. Lipson
(University of Western Ontario)
Oxidization-Induced Dipole Interaction for the Formation of Ultralong V_2O_5 Ribbons

3(b) **Bilkiss B. Issack** and Gilles H. Peslherbe
(Concordia University)
Free energy of Permeation Across Hydrated Lipid Bilayers: Comparison of Computational Techniques

4(a) **J. Li**, X.K. Hu, C. Lu and R.H. Lipson
(University of Western Ontario)
The Preparation of Porous Microcolumn Arrays of Silicon, and Post-Ionization of Neutral Particles from DIOS-MS

4(b) **Jeffrey N. Philippson**, Ralph C. Shiell, Elmar Reinhold and Wim Ubachs
(Trent University and Vrije Universiteit Amsterdam)
Using Hyperfine Structure to Investigate Perturbations Between Highly Excited States: The HF(C-X) Spectrum

5(a) **Chunyan Yang**, Xiaokun Hu and Rober H. Lipson
(University of Western Ontario)
Visible-MALDI Mass Spectrometry Using Rhodamine Dyes as Matrices

5(b) **Helia Jalili,** Nina Heinig and Tong Leung
(University of Waterloo)
X-ray Photoemission Study of Sr_2FeMoO_6 and $SrMoO_4$ Films Epitaxially Grown on MgO(100): Near-Surface Chemical-State Composition Analysis

6(a) **Xiaojing Liu**, Ian Hamilton, Robert Krawczyk and Peter Schwerdtfeger
(Wilfrid Laurier University and Massey University, NZ)
Helical Gold Nanowires

6(b) **Farheen Shenaz Kinoo** and K. T. Leung
(University of Waterloo)
FTIR Reflection Absorption Spectroscopy of Alanine Nanodeposits on Ice Nanolayers

7(a) **David Moule**
(Brock University)
A Study of the Intersystem Crossing and Intramolecular Vibrational Redistribution in Thiophosgene

7(b) **Xiangzhu Li** and Josef Paldus
(University of Waterloo)
Energetics of Naphthynes: Performance of Reduced Multireference Coupled-Custer Methods for Diradicals

8(a) **Yang Liu**, Martin Losada and Yunjie Xu
(University of Alberta)
Vibrational Circular Dichroism and Matrix Isolation Infrared Spectroscopy of {Methyl Lactate}--{Methanol}$_n$ Clusters

8(b) A.G. Adam, **Aaron D. Granger**, M.E. Slaney, L.E. Downie, D.W. Tokaryk and C. Linton
(University of New Brunswick)
High Resolution Laser Spectroscopy of Iridium Monophosphide

9(a) **Xunchen Liu** and Yunjie Xu
(University of Alberta)
Preliminary Experimental Results With a Room-Temperature Broadband Mode-Hop-Free Quantum Cascade Laser

9(b) **Yujun Shi** and Watheq Al-Basheer
(University of Calgary)
Second Harmonic Generation of 124.8 nm VUV Radiation in Xeon Gas

10(a) **Abdullah Radi**, Youngku Sohn, Deb Pradhan and Tong Leung
(University of Waterloo)
Growing and Controlling the Shape, Size and Number Density of Cu Core-Shell Nanoparticles on a p-Si(100) Surface by Electrochemical Deposition

10(b) **Ronghu Wu** and Terry B McMahon
(University of Waterloo)
Investigation of the Dissociation Mechanism of Peptides

11(a) **Paul Raston** and Wolfgang Jäger
(University of Alberta)
Infrared-Microwave Double Resonance Spectroscopy of Molecules Embedded in Superfluid Helium Nanodroplets

11(b) **Gustavo Avila-Blanco** and Tucker Carrington Jr.
(Queen's University)
Using Pruned Basis and a Smolyak Quadrature to Solve High-Dimensional Vibrational Problems

12(a) **Scott Cowen** and Hind A. Al-Abadleh
(University of Guelph)
DRIFTS Studies on the Role of Light in the Heterogeneous Reactions of Model HULIS

12(b) **Yalina Tritzant Martinez** and Pierre-Nicholas Roy
(University of Alberta)
Effect of Flexibility on the Classical Stability of Water Clusters

13(a) **Alex P. Gaiduk** and Viktor N. Staroverov
(University of Western Ontario)
How to Tell When a Model Kohn-Sham Potential is Not a Functional Derivative

13(b) **Jeff Crouse** and Dennis Tokaryk
(University of New Brunswick)
Measuring the Temperature of a Neutral Plasma Using the $C\,^3\Pi_u \rightarrow B\,^3\Pi_g$ *Emission Spectrum of Molecular Nitrogen*

14(a) **Jessica A. Thomas**, David W. Pratt, Eric Gloaguen, François Piuzzi and Michel Mons
(University of Pittsburgh and Laboratoire Francis Perrin)
A β-Lactoglobulin Folding Nucleus in the Gas Phase: UV/IR Spectroscopy of Ac-Trp-Tyr-NH_2 *and Ac-Trp-Tyr-Ser-*NH_2

14(b) **Iouli Gordon** and Laurence Rothman
(Harvard-Smithsonian Center for Astrophysics)
The New Edition of the HITRAN Database

15(a) **Damien Forthomme** and Colan Linton
(CLAMS, University of New Brunswick)
High Resolution Laser Spectroscopy of Samarium Monoxide

15(b) **Jonathan K. Martens**, Richard A. Marta, Sabrina M. Martens, Cveta L. Manassieva and Terry B. McMahon
(University of Waterloo)
Examining the Effects of Fluorination on Hydrogen Bonding Using an Improved High Pressure Mass Spectrometer and High Level Computational Methods

16(a) Susumu Kuma, Hiroko Nakahara, and **Takamasa Momose**
(University of British Columbia)
Non-Rigidity of Hydrogen Clusters at 0.4 K

16(b) **Rick Marta**, Ronghu Wu, Kris Eldridge, Jon Martens and Terry McMahon
(University of Waterloo)
IRMPD Spectroscopy and Quantum Chemical Calculations as a Demonstration of Why Ammonium will Bind to Theophylline and Not to Caffeine

17(a) **K. Bescherer**, H. Waechter, J. Barnes, R.D. Oleschuk and H.P. Loock
(Queen's University)
Cavity Ring-Down Spectroscopy Based Microfluidic Detector: Fibre Loops and Liquid Core Waveguides

17(b) **Samad Bazargan** and Tong Leung
(University of Waterloo)
Structural Evolution of SnO_2 Films Synthesized by Solution Coating on Glass Substrates and its Effect on the Resistivity of the Films

18(a) **J.Barnes**, B. Carver, J. Fraser, G. Gagliardi, H.-P. Loock, Z. Tian, M. Wilson, S. Yam, and O. Yastrubhak
(Queen's University)
Loss Determination in Microsphere Resonators by Phase-Shift Cavity Ring-Down Measurments

18(b) **A. Chatterjee**, L. Zhang and K. T. Leung
(University of Waterloo)
Scanning Tunneling Microscopy of Glycine and Diglycine on Si(111)7x7 Surface

19(a) J. Barnes, **A. Cheung**, H.-P. Loock, G. Mackey and K. Plett
(Queen's University)
Chemical Sensing Using a Polymer Coated Long-Period Fiber Grating Interrogated Using Ring-Down Spectroscopy

19(b) **Dominika Zgid**, Debashree Ghosh, Eric Neuscamman and Garnet Chan
(Cornell University)
Approximations to N-Electron Valence Perturbation Theory with a Density Matrix Renormalization Group Reference

20(a) **S. Jahangiri** and G. H. Peslherebe
(Concordia University)
Theoretical Investigation of Nitrate Ion in Water Clusters

20(b) **Stephen W. C. Walker**, Matthew G. K. Thompson and J. Mark Parnis
(Trent University and Queen's University)
Hydrogenation of Propene from Reaction with Vanadium Atoms via M-H Bond Insertion

21(a) **Denise M. Koch**, Tao-Nhan Nguyen and Gilles H. Peslherbe
(Concordia University)
Theoretical Investigation of the Photo-Ionization of Ion Pairs in Solvent Clusters

21(b) **Blake E. Ziegler**, Rick A. Marta, Jonathan Martens and Terry B. McMahon
(University of Waterloo)
Experimental and Theoretical Investigations of H/D Exchange Between Protonated Triglycine and ND_3

22(a) **Katherine Stewart**, Holly Gray, Adrian **Adamescu**, Ian Hamilton, and
Hind A. Al-Abadleh
(Wilfrid Laurier University)
Trends in the Infrared Frequencies of $V(AsO_x)$ [x=2,3] in Selected As(V)-Containing Compounds Investigated using Quantum Chemical Calculations

22(b) **Zi Jian Long** and Wing-Ki Liu
(University of Waterloo)
Keldysh's Theory of Intense Laser-Atom Interaction

23(a) **Matthew Chabot**, Tuan Hoang and Hind A. Al-Abadleh
(Wilfrid Laurier University)
Binding Mechanism of p-Arsanilic Acid to Iron (oxyhydr)oxides Studied by ATR-FTIR

23(b) **L. Zhang**, A. Chatterjee and K. T. Leung
(University of Waterloo)
Reversible Hydrogen Bonding-Mediated Adsorption of Biological Molecules on Si(111)7x7

24(a) A.G. Adam, **A.D. Granger**, L.E. Downie, D.W. Tokaryk, and C. Linton
(CLAMS, University of New Brunswick)
High *Resolution Laser Spectroscopy of Iridium Monofluoride*

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.

- **Phone Numbers**:
  Comfort Inn: 519-747-9400 190 Weber Street N, Waterloo
  Destination Inn: 519-884-0100 547 King Street N., Waterloo
  Waterloo Inn: 519-884-0220 485 King Street N., Waterloo
  Airways Transit: 519-886-2121 https://secure.airwaystransit.com
  R.J. Le Roy: 519-885-1198 (home)
  519-589-4051 (mobile)