The 23rd Annual

Symposium

On

Chemical Physics

at the

University of Waterloo

November 9 - 11, 2007

Acknowledgements

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for their generous financial support of this conference.

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

SESSION I: Friday, November 9, 2007 — P.M. Davis Centre Room 1351

Chair: **Marcel Nooijen**

7:30 – 8:15 **Paul Ayers**
(McMaster University)
Chemical Reaction Mechanism Prediction and Elucidation with the Fast-Marching Method

8:15 – 8:30 Akihiro Yabushita,[1] Noboru Kawanaka,[1] Daisuke Iida,[1] Tetsuya Hama,[1] Masahiro Kawasaki,[1] Naoki Watanabe,[2] Michael N. R. Ashfold[3] and **Hans-Peter Loock**[4] ([1]Kyoto University, [2] Hokkaido University, [3] University of Bristol, [4] Queen's University)
State-Selective Detection of Hot Molecular Hydrogen Following Photolysis of Water Ice at 157 nm

8:30 – 8:45 **J. N. Philippson**, M Ugray, T J Toai and R.C. Shiell
(Trent University)
Development of a Compact Angle-Resolved Optical Spectrum Analyzer

8:45 – 9:00 **Dominika Zgid** and Marcel Nooijen (University of Waterloo)
Orbital Optimization with Density Matrix Renormalization Group Method

SESSION II: Saturday, November 10, 2007 – A.M.
Chair: **Pavle Radovanovic**

9:00– 9:45 **Alex Brown**
(University of Alberta)
Laser Control of Polyatomic Molecules: The Optimal Control Theory Multi-Configuration Time-Dependent Hartree Approach

9:45 – 10:00 **Nicole Borho** and Yunjie Xu
(University of Alberta)
A Microscopic Lock-and-Key Model System: Hydrogen Bonding in the Propylene Oxide ···Ethanol and Propylene Oxide ··· 2-Fluoroethanol Dimers

10:00 – 10:15 **Bijoy Krishna Dey**
(University of Waterloo)
Optimal reduced dimensional representation of classical molecular dynamics

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 10, 2007 – A.M. Davis Centre Room 1351
Chair : **Robert Le Roy**

10:45 – 11:45 ***The Roger E. Miller Lecture*** : **Frédéric Merkt**
(ETH Zurich)
Rydberg Stark Deceleration and Zeeman Deceleration of Atoms and Molecules

11:45 – 12:00 **Bilkiss Issack** and Pierre-Nicholas Roy
(University of Alberta)
Semiclassical Dynamics With Constraints

12:00 – 12:15 Nader Dehghani,[1] Mahin Afshari,[1] A.R.W. McKellar[2] and **N. Moazzen-Ahmadi**[1]
([1] University of Calgary, [2] National Research Council)
Laser Spectroscopy of Clusters of Linear Triatomic Molecules Using a Rapid-Scan Pulsed Supersonic Jet Expansion Source

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

SESSION IV: Saturday, November 10, 2007 – P.M. Davis Centre Room 1351
Chair: **Tong Leung**

1:30 – 2:15 **Alec Wodtke**
(University of California Santa Barbara)
Do We Have a Theory for Reactions at Metal Interfaces? The Unsolved Problem of Electronic Non-Adiabaticity

2:15 – 2:30 **Fedor Y. Naumkin**
(University of Ontario Institute of Technology)
Dividing the Charge and Conquering the Valence: Novel Trapped-Molecule Complexes with Pentavalent Carbon

2:30 – 2:45 **David Proctor** and H. Floyd Davis
(Cornell University)
Mode-specific Reactivity of the Methane Antisymmetric Stretch in an Insertion Reaction: $Y + CH_4 \rightarrow YCH_2 + H_2$

2:45 – 3:00 **Dvira Segal**
(University of Toronto)
Non-Equilibrium Quantum Dissipation: Marcus Rate in Electronic Environments

3:00 – 3:15 **X.-G. Wang** and T. Carrington Jr.
(Queen's University)
A Full Angular DVR Based on Extended Spherical Harmonics: Vibrational Calculations for Four-Atom Molecules

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 10, 2007 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 11, 2007 – A.M.
Chair: **Fred McCourt**

9:15– 10:00 **Ed Grant**
(University of British Columbia)
Spectroscopic Manifestations of High-Rydberg Dynamics (Intra- and Intermolecular)

10:00 – 10:15 **Norberto Castillo**, Todd L. Lowary and Pierre-Nicholas Roy
(University of Alberta)
Are Sugars Quantum?

10:15 – 10:30 **Ronghu Wu** and Terry B. McMahon
(University of Waterloo)
Non-Covalent Interactions and Structures of Amino Acids and Peptides in the Gas Phase

10:30 – 11:00 **Coffee Break**

SESSION VII: Sunday, November 11, 2007 – A.M. Davis Centre Room 1351
Chair: **Takayashi Amano**

11:00 – 11:45 **James Martin**
(University of Waterloo)
Resonant Electric Dipole-Dipole Interactions Between Ultra-Cold Rydberg Atoms

11:45 – 12:00 **J.R. Cooper** and T. Carrington
(Queen's University)
Exact Wavepacket Propagation in a Dynamically Pruned Simultaneous Diagonalization Basis

12:00 – 12:15 **Julie M. Michaud** and Wolfgang Jaeger
(University of Alberta)
High Resolution Microwave Spectroscopy of Doped Hydrogen Clusters: $(H_2)_N$ – OCS and $(H_2)_N$ – HCCCN for N = 2-7

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) **I. E. Gordon** and L.S. Rothman
(Harvard-Smithsonian Center for Astrophysics)
HITEMP Reloaded

1(b) **Jack Barnes**, Stephen Brown, Judy Cipot-Wechsler, Cathy Crudden, Hans-Peter Loock, Marian Dreher, Jenny Du, Krista Plett and Gabriela Rappell
(Queen's University)
Water Contamination Sensing using Polymer Coated Long-Period Gratings and Fibre-Loop-Ring-Down Spectroscopy

2(a) **Hui Li** and Robert J. Le Roy
(University of Waterloo)
An Analytic Three-Dimensional Potential Energy Surface for CO_2-He and Its Predicted Infrared Spectrum

2(b) **Brett Kamino**, Klaus Bescherer, Jessica Litman, Sydney Dias, Ben Carver, Anthony Tong, Jack Barnes and Peter Loock
(Queen's University)
Fibre-Loop Ring-Down Spectroscopy for Capillary Flow Systems

3(a) **Hui Li**,[1] Tsuneo Hirano,[2] Takayoshi Amano[1] and Robert J. Le Roy[1]
([1] University of Waterloo, [2] Ochanomizu University, Yokyo)
Theoretical Investigation of Formation Dynamics and Intra-molecular Energy Transfer for HCO^+

3(b) **Klaus Bescherer**, Brett Kamino, Sydney Dias, Nick Trefiak, Scott Yam, Gianluca Gagliardi and Peter Loock
(Queen's University)
Phase-Shift Cavity Ring-Down of Multiexponential Decays

4(a) **Karine Le Bris**, Kimberly Strong and Stella Melo
(University of Toronto)
Temperature-Dependent Fourier Transform Spectroscopy of HCFC-142b

4(b) A. Hermann, R.P. Krawczyk, M. Lein, P. Schwerdtfeger, **I.P. Hamilton** and J.J.P. Stewart
(Massey University, New Zealand, Wilfrid Laurier University, Stewart Computational Chemistry, USA)
Convergence of the Many-Body Expansion of Interaction Potentials: From van der Waals to Covalent and Metallic Systems

5(a) **Liguo Kong** and Marcel Nooijen
(University of Waterloo)
Internally-contracted Multireference Coupled Cluster Method & Computer-aided Implementation

5(b) **Allan G. Adam** and Aaron D. Granger
(University of New Brunswick)
High Resolution Laser Spectroscopy of Iridium Monophosphide

6(a) **Xiangzhu Li** and Josef Paldus
(University of Waterloo)
Real and Artifactual Symmetry Breaking in Linear Triatomic Molecules

6(b) **A.R.W. McKellar**
(National Research Council)
H*igh Resolution Infrared Spectra of Seeded Helium Clusters*

7(a) **Reza Rajaie khorasani** and Randall S. Dumont
(McMaster University)
Lanczos Scattering Calculations

7(b) **Kaori Kobayashi**, Takanori Matsui, Norimichi Mori, Shozo Tsunekawa, and Nobukimi Ohashi
(University of Toyama)
Microwave Spectroscopy of Trans-ethyl Methyl Ether in the Asymmetric Torsionally Excited State

8(a) **F. Temme**
(Queen's University)
Group-branching: SU(m ≤ 5) x S_{20} ↓ A_5 Spin Symmetries Revisited

8(b) **Shanshan Yu**, T. Hirao and T. Amano
(University of Waterloo)
Submillimeter-wave Spectroscopy of HCO^+ and DCO^+ in Excited Vibrational States: Extensive Analysis and Implications of the Observed Population Inversion

9(a) **F. Temme**
(Queen's University)
Invariant Theory in $\{T^k_v\}$ Dual Tensorial Set Quantal Basis-Completeness: Limitations of R-W Algebra

9(b) **Jun Chen**, Clarice Kelleher, Onur Tokel and Paul Houston
(Cornell University)
Product Imaging in the Study of O (1D) Reactions/Deactivations with NO, N_2 and O_2

10(a) **Qingxin Yang**, John A. Barnes, Jonathan Saari, Steven Weinberg, Scott Hopkins, Nick Trefiak, Igor Kozin, Hans-Peter Loock, David Pedersen
(Queen's University)
Fiber Bragg Grating Acoustic Transducers

10(b) B.D. Eustergerling, M. Heden and **Y. J. Shi**
(University of Calgary)
Deposition Chemistry in the Hot-Wire Chemical Vapor Deposition Process with SiH_4-NH_3 Gas Mixtures

11(a) **Stephanie Y. Wong**, Alex Brown and Pierre-Nicholas Roy
(University of Alberta)
Electronic Structure Study and Direct Dynamics Simulations of the Ground and Excited States of CH_3OCl

11(b) **Denise M. Koch**, Gilles H. Peslherbe and James T. Hynes
(École Normale Superieure, Paris, and Concordia University)
Ion-Molecule Reaction Routes to the Formation of Amino Acid Precursors in the Interstellar Medium

12(a) **Qin Ran**,[1] Daniel Matsiev,[1] Daniel J. Auerbach[2] and Alec M. Wodtke[1]
([1] University of California, Santa Barbara; [2] Gas Reaction Technologies, Inc., Santa Barbara CA)
Molecular Beam-Surface Scattering: Observation of Vibrational Excitation in HCl Collisions with Au(111)

13(a) **Lisandro Hernández de la Peña**, Ramses van Zon, Jeremy Schofield and Gilles H. Peslherbe
(Concordia University and University of Toronto)
Quantum Free Energy Differences From Non-Equilibrium Path Integral Methods

13(b) **Javier E. Cuervo** and Pierre-Nicholas Roy
(University of Alberta)
Ground State Structure and Energetics of $(p\text{-}H_2)_N$ (N = 8-37) Clusters Doped with $(o\text{-}D_2)_3$

14(a) **Alireza Shayesteh**, Robert D.E. Henderson, Robert J. Le Roy, and Peter F. Bernath
(University of Waterloo)
Dissociation Energy of MgH with Sub-Wavenumber Accuracy

14(b) **Sergei Manzhos** and Tucker Carrington
(Queen's University)
Molecule-Independent and Dynamics-Friendly Methodology to Build High-Dimensional Potential Energy Surfaces

15(a) **C. Linton**, D. W Tokaryk, A. G. Adam, A. D. Granger, L. E. Downie and W. S. Hopkins
(University of New Brunswick)
Population Depletion Spectroscopy of the Calcium and Strontium Mono-Methoxide Radicals

15(b) **R. H. Lipson**, C. Lu and S. S. Dimov
(University of Western Ontario)
Synthetic Strategies for Nonlinear Photonic Devices using β-BBO

16(a) Tuan Hoang, Scott Cowen and **Hind A. Al-Abadleh**
(Wilfrid Laurier University)

Spectroscopic Investigations of the Surface Interactions of p-Arsanilic Acid with Iron (Oxyhydr)oxides

16(b) **Cheng Lu**, Shaun Leong, Fengping Wang, Zhingfeng Ding and Robert Lipson
(University of Western Ontario)
Oxidation Evolution of $VO(acac)_2$ to Vanadium Oxides

17(a) **Kris Eldridge** and Terry McMahon
(University of Waterloo)
The Hunt for Gas Phase Zwitterion Stability of Glycine Through the Addition of One and Two Methanol Molecules

17(b) **Jennifer van Wijngaarden**[1] and Dennis Tokaryk[2]
([1] University of Manitoba, [2] University of New Brunswick)
A Synchrotron-Based Study of the Rotationally-Resolved Infrared Spectrum of Thiophene

18(a) **Jonathan K. Martens**, Richard A. Marta and Terry McMahon
(University of Waterloo)
A Study of Sodium-Methanol Cluster Ions by High Pressure Mass Spectrometry and Computational Methods

18(b) Gilles H. Peslherbe, **Chun Chi Mak**, Denise M. Koch
(Concordia University)
Solvation Structure and Thermodynamics of Guanidinium Ions in Aqueous Clusters

19(a) **Richard A. Marta**, Jonathon K. Martens and Terry B. McMahon
(University of Waterloo)
Expanding the Realm of High Pressure Mass Spectrometry: Electrospray Ionization

19(b) **C.A. Ryan**, O. Moussa, J. Baugh and R. Laflamme
(University of Waterloo)
A Spin Based Heat Engine: Multiple Rounds of Algorithmic Cooling

20(a) **Dejian Fu**, Chris D. Boone, Peter F. Bernath, Debra K. Weisenstein, Curtis P. Rinsland and Kaley Walker
(University of Waterloo and University of Toronto)
First Global Observations of Atmospheric COClF from the Atmospheric Chemistry Experiment (ACE) Mission

20(b) **Guochun Yang** and Yunjie Xu
(University of Alberta)
The Effects of Self-Aggregation and Solvents on the Vibrational Circular Dichrosim and Oprical Rotation Measurements of Glycidol

21(a) **Rudolf Lehnig**, Paul Raston, and Wolfgang Jäger
(University of Alberta)
Microwave Spectroscopy of NH_3 and OCS in Helium Droplets

21(b) **Mark Cybulski**
(Miami University)
Critical Assessment of Performance of Empirical Force Fields for Modeling DNA Interactions

22(a) **Zi Jian Long** and Wink-Ki Liu
(University of Waterloo)
Interaction of Model Atoms and Molecular Ions with a Few-Cycle Laser Pulse

22(b) M. Ortiz-Suarez, M. Witinski and **F. Davis**
(Cornell University)
Reaction Dynamics of Simple Free Radicals Using H and O Atom Rydberg TOF Spectroscopy

23(a) **Samad Bazargan** and Tong K. Leung
(University of Waterloo)
Growth and Characterization of Nanostructured Thin Films of SnO_2 on Silicon and Glass Substrates

23(b) **M.T. Ataol**, S. Roy and F. Mueller-Plathe
(Concordia University and Technische Universität Darmstadt)
A New Force Field for Heptyl Phosphonic Acid and its Structural and Dynamical Properties Through MD Simulations

24(a) **Zi Jian Long** and Wing-Ki Liu
(University of Waterloo)
Interaction of Model Atoms or Molecular Ions with Few-Cycle Laser Pulses