Symposium on Chemical Physics

at the University of Waterloo

October 25-27, 2002

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

SESSION I: Friday, October 25, 2002 - P.M. Davis Centre Room 1351
Chair: **James Martin**

7:30 – 8:15 Nicholas Bigelow (University of Rochester)
Photoassociation of Molecules in Laser-Cooled Atomic Gases: Precision Spectroscopy, Photoionization and Molecule Formation

8:15 – 8:30 Alex Plyukhin and Jeremy Schofield (University of Toronto)
Microscopic Models of Nonlinear Langevin Dynamics

8:30 – 8:45 Massimo Boninsegni (University of Alberta)
Theoretical Study of H_2 Adsorption on Alkali Metal Substrates

8:45 – 9:00 Simon G. Cox and Iain R. McNab (University of Newcastle upon Tyne)
Zeeman Spectroscopy of a Molecular Dication (DCl^{++})

9:15 Grad Club - Informal Discussions

SESSION II: Saturday, October 26, 2002 - A.M. Davis Centre Room 1351
Chair: **Peter Bernath**

9:00 – 9:45 Grenfell Patey (University of British Columbia)
Forces Between Immersed Objects: A Discussion of Interactions on Different Length Scales

9:45 – 10:00 XiaGeng Song, P. N. Roy, Yunjie Xu and Wolfgang Jäger (University of Alberta)
Rotational Spectrum, Energy Levels and Wavefunctions of the Weakly Bound Complex He-N_2O

10:00 – 10:15 Darren Anderson and M. Cynthia Goh (University of Toronto)
Detecting Interfacial Events - a New Spin on Diffraction

10:15 – 10:45 **Coffee Break**

SESSION III: Saturday, October 26, 2002 - A.M. Davis Centre Room 1351
Chair: **Terry McMahon**

10:45 – 11:45 John Maier (University of Basel)
Electronic Spectroscopy of Carbon Chains and their Relevance to Astrophysics

11:45 – 12:00 J. Tang and A.R.W. McKellar (Steacie Institute for Molecular Sciences, National Research Council)
High Resolution Spectroscopy of Helium Clusters: He_N - CO, with N = 1 to ~20

12:00 – 12:15 Hannah H. Chang, Anirban Hazra and Marcel Nooijen (Princeton University)
Examination of Ethylene UV-Vis Spectrum: Vibronic Coupling and Non-Adiabatic Dynamics

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

SESSION IV: Saturday, October 26, 2002 - P.M. Davis Centre Room 1351
Chair: **Bob Le Roy**

1:30 – 2:15 Colan Linton (University of New Brunswick)
Laser Spectroscopy of Lanthanide Molecules: Past, Present and Future

2:15 – 2:30 Alexandre Trottier and R.L. Brooks (University of Guelph)
Mid-IR Spectroscopy of Proton-Irradiated CO Ice Films

2:30 – 2:45 Mark Cybulski (Miami University)
A Critical Note on DFT Studies of Biomolecules

2:45 – 3:00 Kevin Liu,[1] Li-Hong Xu,[1] R.D. Suenram,[2] D.F. Plusquellic,[2] F.J. Lovas,[2] A.R. Hight Walker,[2] J.O. Jensen[3] and A.C. Samuels[3] ([1]University of New Brunswick, [2]NIST, [3]Aberdeen Proving Ground)
Rotational Spectra, Conformational Structures and Dipole Moments of Hydroxyethyl Ethyl Sulfide by Jet-Cooled FTMW and Ab Initio Calculation

3:00 – 3:15 Qadir K. Timerghazin and Gilles H. Peslherbe (Concordia University)
Relaxation Dynamics of Photoexcited Iodide-Solvent Clusters: A Theoretical Study

3:15 **Refreshments and Poster Session**

SESSION V: Saturday, October 26, 2002 – from 3:30 P.M. Davis Centre Lobby

POSTER SESSION AND SPONSOR'S DISPLAY

6:00 P.M.	Poster session ends Depart for Conrad Grebel University College	
6:30 P.M.	Cash Bar	Conrad Grebel University College
7:00 P.M.	**DINNER**	Conrad Grebel University College

SESSION VI: Sunday, October 27, 2002 – A.M. Davis Centre Room 1351
Chair: **Fred McCourt**

9:15 – 10:00 James Lisy (U. Illinois at Urbana-Champaign)
Competition between Non-Covalent Interactions: Surprising Size-Selectivity

10:00 – 10:15 Y. Hu, M. Case, G. McLendon, T.K. Vanderlick and G. Scoles (Princeton University)
Playing with Proteins: Bouncing them off a Nanowall or Smearing Them on It

10:15 – 10:30 Nicholas V. Blinov and Pierre-Nicholas Roy (University of Alberta)
A Simplified Model for Superfluid Environments

10:30 – 11:00 **Coffee Break**

SESSION VII: Sunday, October 27, 2002 - A.M. Davis Centre Room 1351
Chair: **Jim Sloan**

11:00 – 11:45 Frank De Lucia (Ohio State University)
Spectroscopy, Collisions and Energy in the Submillimeter

11:45 – 12:00 Sergey Dobrin, Javier B. Giorgi, Tae Geol Lee, Hong He, Fedor Y. Naumkin, John C. Polanyi, Sergei A. Raspopov and Jiaxi Wang (University of Toronto)
Photoinduced Charge-Transfer Reactions Between Sodium Clusters and HF, HBr Adsorbed on LiF

12:00 – 12:15 Eli Barkai, YounJoon Jung and Robert J Silbey (Notre Dame University)
Theory of Time Dependent Fluctuations in Single Molecule Spectroscopy

POSTER SESSION

Chair: **Bob 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.**

1a) David B. Pedersen and Benoit Simard (Steacie Institute for Molecular Sciences, NRC)
Metal-DNA Base Complexes in the Gas Phase

1b) M. J. Dick,[1] C. Linton,[1] J.L. MacGregor,[1] A. G. Adam,[1] P. Crozet[2] and A. Ross[2] ([1]University of New Brunswick, [2]Université Lyon)
Laser Spectroscopy of Holmium Monochloride

2a) Sergei Manzhos, Dmitrii Boldovsky, Hans-Peter Loock and Constantin Romanescu (Queen's University)
Reconstruction of Superexcited State Potentials from Photoelectron VM Images

2b) Allan G. Adam, Scott Hopkins and Scott A. Shepard (University of New Brunswick)
High Resolution Laser Spectroscopy of Hafnium Monofluoride

3a) Marjan Mohammadi and Robert J. Le Roy (Guelph-Waterloo Centre for Graduate Work in Chemistry and Biochemistry, University of Waterloo)
Improved Potential Energy Curve and Molecular Constants for the $A^3\Pi_{1u}$ State of I_2

3b) Denise M. Koch, Qadir K. Timerghazin, Gilles H. Peslherbe and James T. Hynes (Concordia University)
Nonadiabatic Trajectory Studies of the Photodissociation Dynamics in $NaI(H_2O)_n$ Clusters

4a) Marcel Nooijen and Hannah Chang (Princeton University)
From Electronic Structure To Spectroscopy: Short-Time Dynamics and Vibronic Coupling

4b) Mouna Sbata and Gilles H. Peslherbe (Concordia University)
Quantum Monte Carlo Simulations: Studies of Iodide-Water Clusters

5a) A.Yu. Zasetsky,[1] J.J.Sloan[1] and T.P. Kurosu[2] ([1]University of Waterloo, [2]Harvard-Smithsonian Center For Astrophysics)
Characterisation of Condensed Phases in Stratosphere from IR Measurements: A Random Walk Among Equally Good Solutions

5b) Jeff Seabrook, Clark Richards and Dennis Tokaryk (University of New Brunswick)
Trace Gas Detection Using a High Finesse Optical Cavity

6a) Naila Siddique, Lucas J. Neil, Daniel R. Flaming and James J. Sloan (University of Waterloo)
Characterization of Particulate Matter by Raman Spectroscopy

6b) Liza Liu,[1] Li-Hong Xu,[1] R.M. Lees,[1] M.Yu. Tretyakov[2] and I. Yakovlev[2]

([1]University of New Brunswick, [2]Institute of Applied Physics, Nizhny Novgorod, Russia)
External Cavity Tunable Diode Laser NH_3 Spectra in the 1.5 μm Region - A Test Case

7a) Li-Hong Xu,[1] J.T. Hougen,[2] R.M. Lees[1] and M.A. Mekhtiev[2] ([1]University of New Brunswick, [2]NIST)
Torsional Angle Definitions and Linear and Quadratic Force Field Variations along the Torsional Coordinate for CH_3OH and CH_3CHO

7b) Alexei Khalizov,[2] Pascal Larregaray,[1] Balakrishnan Viswanathan[2] and Parisa Ariya[2] ([1]Concordia University, [2]McGill University)
Role of Halogens in the Transformation of Atmospheric Mercury: Experiment and Theory

8a) Mandy Hennip, Stefan Kilyanek, George McBane and Stephanie Schaertel (Grand Valley State University)
Frequency Modulation and Cavity Ringdown Spectroscopy for Isotope Ratio Determination

8b) Pascal Larregaray and Gilles H. Peslherbe (Concordia University)
On the Statistical Nature of Collision- and Surface-Induced Dissociation: A Theoretical Investigation of Aluminum Clusters

9a) Aude Simon, Pierre Boissel, Joel Lemaire and Philippe Maitre (Université de Paris XI)
IR Spectroscopy of Reactive Intermediates in the Gas Phase: Probing the Stepwise Activation of Methane by Ta^+ and W^+

9b) Matthew G. K. Thompson and J. Mark Parnis (Trent University)
Interaction of Ethene with Early First and Second Row Transition Metal Atoms Characterized by Matrix Isolation Spectroscopy

10a) Zhaoguo Tong, Alex Wright, Michael Jakubinek and Hans-Peter Loock (Queen's University)
Characterization of Loss Mechanisms in Fiber-Loop Ring-Down Spectroscopy

10b) Anguang Hu and Tom K. Woo (University of Western Ontario)
A Method for the Evolution of the Kohn-Sham Electron Density in the Real-time Domain with a Finite Basis Expansion

11a) J. Tang and A.R.W. McKellar (Steacie Institute for Molecular Sciences, National Research Council)
Infrared Studies of He, H_2 and Ne Clusters Seeded with CO, OCS, or N_2O

11b) Nicholas J. Mosey, Anguang Hu and Tom. K. Woo (University of Western Ontario)
Electronic Structure-Based Bias Potentials for the Acceleration of Ab Initio Molecular Dynamics Simulations

12a) Hans Osthoff and Wolfgang Jäger (University of Alberta)
Mid-Infrared Spectrum of the CO_2-SO_2 van der Waals Complex

12b) Emma E. Rennie and Paul M. Mayer (University of Ottawa)
The Ionisation Energy of the Transient Neutral N_4 Species Measured Using Neutralisation Reionisation Mass Spectrometry

13a) Jose Amado Dinglasan and Al-Amin Dhirani (University of Toronto)
Electrical Measurements of Azomethine-Modified Aluminum Oxide Tunnel Junctions

13b) Alireza Shayesteh, Keith Tereszchuk, Peter Bernath and Reginald Colin (University of Waterloo)
Fourier Transform Infrared Emission Spectra of BeH/BeD and BeH_2/BeD_2

14a) Wendy C. Topic, Aiko Huckauf, XiaoGeng Song and Wolfgang Jäger (University of Alberta)
The Microwave Rotational Spectrum of the He-HCCCN van der Waals Complex

14b) Kaley A. Walker, Treana Parekunnel, Iouli Gordon, Keith Tereszchuk and Peter F. Bernath (University of Waterloo)
Fourier Transform Emission Spectroscopy of SrH and SrD

15a) P. Wahnon, C. Tablero, J.J. Fernandez and P. Palacios (Universidad Politecnica Madrid)
Optoelectronic Transition Calculations of Alloy Semiconductors by DFT within a LCAO Scheme

15b) I. Gordon,[1] M. Dick,[2] K. Tereszchuk,[1] C. Linton[2] and P. Bernath[1] ([1]University of Waterloo, [2]University of New Brunswick)
Fourier Transform Emission Spectroscopy of Gas-Phase YbH and YbD in the Infrared Region

16a) P.-E. Trudeau and A.-A. Dhirani (University of Toronto)
Competitive Transport and Percolation in Disordered Arrays of Molecularly-Linked Au Nanoparticles

16b) R. Nassar and P. Bernath (University of Waterloo)
Laboratory Hot Methane Spectra for Astrophysical Applications

17a) Wai-To Chan and I.P. Hamilton (Wilfrid Laurier University)
Complexes of Coinage Metal Clusters with Hydrogen Sulphide

17b) Dominique Appadoo,[1] Richard Morrisson[2] and Don McNaughton[2] ([1]University of Waterloo, [2]Monash University)
High Resolution FT Study of the Jet Emission Spectrum of the CN Radical

18a) Z.D. Sun,[1] M. Yu. Tretyakov,[2] Vladimir Doroskikh,[2] Li-Hong Xu[1] and R.M. Lees[1] ([1]University of New Brunswick, [2]Institute of Applied Physics, Nizhny Novgorod, Russia)
Precision Frequency Stabilized CO_2-Laser/Microwave Sideband as a Broadband Tunable Mid-Infrared Source

18b) Alexander Auer[1] and Juergen Gauss[2] ([1]Princeton University, [2]Institut fuer Physikalische Chemie Mainz)
Highly Accurate Calculations of NMR-Parameters

19a) Denise M. Koch and Gilles H. Peslherbe (Concordia University)
Thermodynamics of Surface- vs. Interior Solvation in Halide-Water Clusters

19b) Richard Brezina and Wing-Ki Liu (University of Waterloo)
Control of Bond Excitation in HCN Using Laser Pulses

20a) Yoshinori Suganuma and Al-Amin Dhirani (University of Toronto)
Hysteretic Single Charge Effects in Nanometallic Tunnel Junctions in Air

20b) Kevin J. Crowell, Randall S. Dumont and Peter M. Macdonald (McMaster University)
Simultaneous Measurement of Multiple Phospholipid Lateral Diffusion Coefficients in Lipid Bilayers via ^{31}P Slow Spinning MAS EXSY NMR

21a) Robert C. Mawhinney[1] and John D. Goddard[2] ([1]Concordia University, [2]University of Guelph)
S_2N_2: A Theoretical Assessment of the Mechanism of Polymerization and the Identification of a Recently Observed Isomer

21b) Y. Suganuma, P.-E. Trudeau, B. Leathem, B. Shieh and A. Dhirani (University of Toronto)
Single Electron Forces in a Nanoparticle Tunnel Junction System Observed by Hybrid Scanning Tunneling-Atomic Force Microscopy

22a) George C. McBane[1] and Kirk Peterson[2] ([1]Grand Valley State University, [2]Washington State University)
A New He-CO Potential Energy Surface with Vibrational Coordinate Dependence: Calculations of Vibrational Relaxation Cross Sections

22b) Travis D. Fridgen, Jami L. Burkell, Ashraf N. Wilsily, Vicki Hoffman, Josh Wasylycia and Terry B. McMahon (University of Waterloo)
High-Pressure Mass Spectrometric Studies of the Potential Energy Surfaces of Gas-Phase S_N2 Reactions Involving Substituted Nitriles

23a) Vatche B. Deyirmenjian, John E. Sipe and R.J. Dwayne Miller (University of Toronto)
Coherent Electron Diffraction Using Ionized Image States