

# Symposium on Chemical Physics

at the University of Waterloo

November 3 - 5, 2000

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

**SESSION I:** Friday, November 3, 2000 - P.M.

Davis Centre Room 1302

Chair: **John Hepburn**

- 7:30 – 8:15     Roger Miller (University of North Carolina)  
*Exploring Potential Energy Landscapes: Cluster Growth in He Nanodroplets*
- 8:15 – 8:30     M. Abouti Tamsamani, Li-Hong Xu and R.M. Lees (University of New Brunswick)  
*Intramolecular Dynamics in the 3- $\mu$ m CH-Stretching Fundamental Region of Methanol*
- 8:30 – 8:45     R.A. Dresser (US Air Force Research Lab.), Y. Chiu, D.J. Levandier (Boston College) and C.Y. Ng (Iowa State University)  
*Dynamics of Collision-induced Dissociation in Interactions of  $O_2^+$  with Ne, Ar*
- 8:45 – 9:00     Denise M. Koch, Nam Huan Khieu and Gilles H. Peslherbe (Concordia University)  
*Glyoxal Unimolecular Dissociation: Reconciling Experiment and Theory at Last!*
- 9:00 – 9:15     André D. Bandrauk, Francois Légaré and Szczepan Chelkowski (Université de Sherbrooke)  
*Carp-chirped Adiabatic Raman Passage and the Laser Control and Manipulation of Molecules*

9:30 Grad Club - Informal Discussions

**SESSION II:** Saturday, November 4, 2000 - A.M.

Davis Centre 1351

Chair: **Bob Le Roy**

9:00 – 9:45 Michael Klein (University of Pennsylvania)

*Computer Simulation Studies of Biophysical Systems: From Micelles to Model Membranes and Membrane-Proteins*

9:45 – 10:00 Raul Martinez and Kevin Lehmann (Princeton University)

*Vibrational Spectroscopy up to 4 eV Sequential Overtone Excitation*

10:00 – 10:15 U. Valbusa (University of Genoa, Italy)

*The Ion Sandblasting: A New Method to Nanostructuring Surfaces*

10:15 – 10:45 **Coffee Break**

10:45 - 11:45 Giacinto Scoles, (Princeton University)

*He Atom Reflectivity Studies of Chemical Dynamics on Metal Surfaces*

11:45 - 12:00 Raluca Voicu, Bruce Lennox, Antonella Badia and Thomas Ellis (Université de Montréal)

*Self-Assembled Metal-Alkanethiolate Materials: Taking Monolayers to New Dimensions*

12:00 - 12:15 Kaley A. Walker and A.R.W. McKellar (S.I.M.S., NRC Canada)  
*Millimeter Wave Spectroscopy of van der Waals Complexes Using a Coaxial Jet Spectrometer*

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

**SESSION III:** Saturday, November 4, 2000 - P.M.

Davis Centre 1351

Chair: **Jim Sloan**

1:30 - 2:15 Lorenzo Mattera, (Universita di Genova)  
*Correlation Between Growth Conditions and Magnetic Behavior at the Surface of Ultrathin Films*

2:15 - 2:30 Wolfgang E. Ernst (Penn State University)  
*Alkali Trimers – The Smallest Pieces of Metal?*

2:30 - 2:45 Jennifer van Wijngaarden and Wolfgang Jaeger (University of Alberta)  
*Microwave Spectra of the Ar-ND<sub>3</sub> van der Waals Complex and its Partially Protonated Isotopomers*

2:45 - 3:00 T. Toccoli, A. Boschetti, S. Iannotta (CeFSA-CNR, Italy)  
*Growth of Films of Thiophene Oligomers by Seeded Supersonic Beams to Improve Control on their Quality and Properties*

3:00 - 3:15 Erik Kerstel (University of Groningen, Netherlands)  
*Accurate Determination of Isotope Abundance Ratios in Water by Means of Infrared Laser Spectroscopy*

3:15 – 3:30 Patrick Ayotte, Greg A. Kimmel, Zdenek Dohnalek, R. Scott Smith, John L. Daschbach, Bruce D. Kay (Pacific Northwest National Laboratory)

*A Molecular Beam Study of the Helium Bulk Uptake by Ice*

3:30 **Refreshments**

**SESSION IV:** Saturday, November 4, 2000 - from 3:30 P.M.

Davis Centre Lobby

POSTER SESSION AND SPONSOR'S DISPLAY

6:00 P.M. Poster session ends.

Depart for Conrab Grebel College

6:30 P.M. Cash Bar Conrab Grebel College

7:00 P.M. **DINNER** Conrab Grebel College

**SESSION V:** Sunday, November 5, 2000 - A.M.

Davis Centre 1302

Chair: **Terry McMahon**

9:00 – 9:45 Udo Buck (MaxPlanckInstitut fuer Stroemungsforschung)

*Photodissociation and Caging in Different Cluster Environments*

9:45 – 10:00 Bill Poirier and John C. Light (University of Chicago)

*Accurate Rovibrational Spectroscopy Calculations Using Semiclassical Basis Optimization*

- 10:00 – 10:15 R. Burcl, P. Piecuch, V. Spirko and O. Bludsky (Michigan State University)  
*Bound and Quasi-bound States of the Li • FH van der Waals Molecule: The Effect of the Potential Energy Surface*
- 10:15 – 10:30 Xiao-Gang Wang and Tucker Carrington Jr. (Université de Montréal)  
*A Symmetry-adapted Lanczos Method for Calculating Energy Levels with Different Symmetries from a Single Set of Iterations*
- 10:30 - 11:00 **Coffee Break**
- 11:00 - 11:45 Paul Rowntree (Université de Sherbrooke)  
*Electron-Induced Processes In (and On) Self-Assembled Organic Monolayers*
- 11:45 - 12:00 Thomas Schultz, S. Lochbrunner, M. Schmitt, J.P. Shaffer, M.Z. Zgierski, A. Stolow (S.I.M.S., NRC Canada)  
*Investigation of Proton Transfer Reactions by Time-Resolved Photoelectron Spectroscopy*
- 12:00 - 12:15 A.D.J. Critchley, A.N. Hughes, Iain R. McNab (University of Newcastle upon Tyne)  
*Measurement of an Orth-Para Pure Rotation Transition in H<sub>2</sub><sup>+</sup>*

## POSTER SESSION

Chair: **John Hepburn**

**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) E. Kratz, R. Burcl and P. Piecuch (Michigan State University)

*Ab initio Studies of the Li • FCH<sub>3</sub> van der Waals Complex*

1b) Bill Poirier and Tucker Carrington Jr. (Université de Montréal)

*Calculating Energy Levels with Preconditioned Spectral Transform Techniques, as Applied to H<sub>2</sub>O*

2a) H.K. Srivastava, A. Conjusteau, H. Mabuchi, A. Callegari, K.K. Lehmann, G. Scoles, (Princeton University), M.L. Silva and R.W. Field (Massachusetts Institute of Technology)

*Rovibrational Spectroscopy of the  $v = 6$  Manifold in <sup>12</sup>C<sub>2</sub>H<sub>2</sub> and <sup>13</sup>C<sub>2</sub>H<sub>2</sub>*

2b) André Conjusteau, Iris Scheele, Carlo Callegari, Kevin K. Lehmann and Giacinto Scoles (Princeton University)

*Infrared Spectroscopy in Mixed H<sub>2</sub> - <sup>4</sup>He Droplets*

3a) C. Linton, A.G. Adam, M.J. Dick (University of New Brunswick), T.C. Melville, J.A. Coxon (Dalhousie University), P. Crozet and A.J. Ross (Université de Lyon)

*Laser Spectroscopy of Lanthanide Diatomics: Recent Results*

3b) J. Mark Parnis, Rick D. Lafleur, Eric Escobar-Cabrera, J. Paul Jacula and David M. Rayner (Trent University) (Queen's University) (S.I.M.S., NRC Canada)

*Product Distribution Studies of Nb Cluster Reactions with Small Hydrocarbons*

4a) M. Schmitt, V. Blanchet, S. Lochbrunner, J.P. Shaffer, T. Schultz, J.G. Underwood, M.Z. Zgierski and A. Stolow (S.I.M.S., NRC Canada)

*Electronic Continua in Time-Resolved Photoelectron Spectroscopy: Complementary and Corresponding Ionization Correlations*

- 4b) A.G. Adam, S. Hopkins and C. Richards (University of New Brunswick)  
*High Resolution Laser Spectroscopy of HfF and TiBr*
- 5a) Jeff Paci and David Wardlaw (Queen's University)  
*The Kinetic Energy Distribution of Dissociating Diatomic Molecules in an Intense Laser Field*
- 5b) James P. Shaffer, Thomas Schultz, Michael Schmitt and Albert Stolow (S.I.M.S., NRC Canada)  
*Untangling  $\pi-\pi^*/n-\pi^*$  Orbital Interactions Via Ultrafast Time-Resolved Photoelectron Spectroscopy*
- 6a) Richard Ochran and Paul M. Mayer (University of Ottawa)  
*Isomerization of Small Proton-Bound Dimers of Acetonitrile and Alcohols*
- 6b) Kaori Kobayashi, Greg Hall and Trevor J. Sears (Brookhaven National Laboratory)  
*Application of Frequency-Modulated Laser Absorption Spectroscopy to Transition Metal-Containing Radicals*
- 7a) Trevor J. Sears, Andrew J. Marr, James T. Muckerman and Tomas Gonzalez-Lezana (Brookhaven National Laboratory)  
*Further Studies of the Near-IR Spectrum of HCB<sub>r</sub>*
- 7b) Travis D. Fridgen, Jonathan D. Keller and Terry B. McMahon (University of Waterloo)  
*Experimental Barrier Heights for Methyl Cation Transfer Reactions by Fourier Transform Ion Cyclotron Resonance Mass Spectrometry*
- 8a) Travis D. Fridgen and Terry B. McMahon (University of Waterloo)  
*Temperature Effects on the Low-Pressure Radiative Association Reaction of Dimethyl Ether with Protonated Dimethyl Ether: An FTICR-MS Study*

- 8b) Keith Tereszchuk, Tsuyoshi Hirao and Peter F. Bernath (University of Waterloo)  
*Fourier Transform Emission Spectroscopy of ZnD*
- 9a) Rudolf Polak and Jiri Cizek (University of Waterloo)  
*On the Interpretation of Binding Properties in Molecular Dications*
- 9b) Jaroslav Zamastil, Jiri Cizek, Lubomir Skala and Vladimir Spirko (University of Waterloo)  
*Multidimensional WKB Approximation for Henon-Heiles Potentials*
- 10a) Gang Li, Tsuyoshi Hirao, Jackie Lievin, Ram S. Ram and Peter F. Bernath (University of Waterloo)  
*Electronic Transitions of Tungsten Monoxide*
- 10b) N. Siddique, N.S-K. Sze, I.M. Borrero and J.J. Sloan (University of Waterloo)  
*Chemical Speciation of Urban Particulate Matter by Raman Spectroscopy*
- 11a) Michelle Leslie and Bob Berno (Saint Mary's University)  
*The Study of a Potential Abiotic Receptor Molecule at the Air-Water Interface*
- 11b) Anthony Lee, J.P. Shaffer, C.C. Hayden, M. Spanner and Albert Stolow (Queen's University) (NRC of Canada)  
*New Approaches to the Onset of Statistical Dynamics in Unimolecular Reactions*
- 12a) Tsuyoshi Hirao, Keith Tereszchuk and Peter F. Bernath (University of Waterloo)  
*Fourier Transform Emission Spectroscopy of Zinc Hydride*



- 12b) I. Calugareanu and N.M. Cann (Queen's University)  
*The Impact of Molecular Shape and Polarity on Chiral Discrimination*
- 13a) Xiaowei Fan and K.T. Leung (University of Waterloo)  
*Absolute Generalized-Oscillator-Strength Measurement of Ar and SiF<sub>4</sub> by Angle-Resolved Electron Energy Loss Spectroscopy*
- 13b) Tanya Kikteva, Dmitry Star and Gary W. Leach (Simon Fraser University)  
*Interface Structure and Dynamics Probed by Nonlinear Optical Spectroscopy*
- 14a) A.G. Brolo, M. Musa, J.W. Hepburn (University of Waterloo), P.R. Norton and K. Griffiths (University of Western Ontario)  
*Quantum-Specific Determination of Hydrogen Formed from the Decomposition of Water on Zr Surfaces*
- 14b) S. Dobrin, J. B. Giorgi, T.G. Lee, F.Y. Naumkin, J.C. Polanyi, S.A. Raspopov and J. Wang (University of Toronto)  
*Dynamics of Photoreactions on Surfaces: HCℓ..Na and HF..Na Complexes*
- 15a) Richard Dawes and Kathleen M. Gough (University of Manitoba)  
*Theoretical and Spectroscopic Investigation of Raman Scattering Intensities in Bicyclo[1.1.1]Pentane*
- 15b) Qadir K. Timerghazin and Gilles H. Peslherbe (Concordia University)  
*A Theoretical Study of Charge Transfer to Solvent in Photoexcited Iodide-Acetonitrile Clusters*
- 16a) Carlo Callegari, André Conjusteau, Franco Dalfovo, Kevin K. Lehmann, Irene Reinhard, Roman Schmied and Giacinto Scoles (Princeton University) (Universite a Cattolica Brescia, Italy) (Ecole Polytechnique, Lausanne, Switzerland) (Gesellschaft Schwerionenforschung, Darmstadt, Germany)

*Hydrodynamic Theory for the Motion of Dopant Molecules In Superfluid  $^4\text{He}$*

- 16b) Tao-Nhan V. Nguyen and Gilles H. Peslherbe (Concordia University)  
*Theoretical Studies of Alkali and Halide Ions in Acetonitrile Clusters*
- 17a) P.M. Brodersen, T. Tyliczszak, A.P. Hitchcock (McMaster University) and Z.H. Lu (University of Toronto)  
*Surface Structure of  $(\text{NH}_4)_2\text{S}_x$ -treated GaAs(111): An XAFS Investigation*
- 17b) Ao Lin, Antonis Tsakotellis, Tai Sang Ahn and George C. McBane (Ohio State University)  
*Dynamical Constraints in Rotationally Inelastic Scattering of NO*
- 18a) Nicholas Blinov and Pierre-Nicholas Roy (University of Alberta)  
*A Quantum Molecular Dynamics Approach for the Study of Doped Helium Clusters*
- 18b) R.R. Toczyłowski, F. Doloresco and S.M. Cybulski (Miami University)  
*Theoretical Study of the He-HCN, Ne-HCN, Ar-HCN, and Kr-HCN Complexes*
- 19a) Robert J. Doerksen, Ralf I. Kaiser, Yuan T. Lee and Martin Head-Gordon (University of California, Berkeley) (Academia Sinica, Taipei, Taiwan) (University of York, UK)  
*Theoretical Studies on the Crossed-Beam Reaction of  $\text{C}(^3\text{P}_j)$  with Acetylene*
- 19b) R. Escibano, R. Mosteo, L.F. Pacios and P.C. Gomez (Inst. De Estructura de la Materia, CSIC, Madrid) (Escuela U. Politecnica, Teruel) (ETSI MontesU. Politecnica, Madrid) (F. Quimicas, U. Complutense, Madrid)  
*The Cl-O Bond in Chlorine Oxides: Electronic Structure and Empirical Force Constants*
- 20a) Sergei Manzhos, Hans-Peter Looock, Bernard L.G. Bakker and David H. Parker (Queens

- University) (University of Nijmegen, The Netherlands)
- Photodissociation of Hydrogen Iodide in the A-band Region: Branching Ratios and Potential Energy Curves*
- 20b) Chris Boone, Sean McLeod, Randall Skelton and Peter F. Bernath (University of Waterloo)
- The Atmospheric Chemistry Experiment (ACE)*
- 21a) A. Gil, J. Colchero, J. Gomez-Herrero and A.M. Baro (Princeton University) (Universidad Autonoma de Madrid, Spain)
- Different Stages of Water Absorption on Au Studied by Dynamic and Jumping Mode Scanning Force Microscopy*
- 21b) F. Temme (Queen's University)
- On Uniform Identical  $n$ -fold ( $1 \leq I_i \leq 3$ ) Dual Tensorial Bases, from the  $SU(3 \leq m \leq 7)$  Weight Sets, and the  $S_n$  Scalar Invariants Underlying Such Bases: A Direct Partitional Set-Based Combinatorial Approach.*
- 22a) Jason R. Dwyer, Bradley J. Siwick, R.E. Jordan, R.J. Dwayne Miller (University of Toronto)
- Ultrafast Electron Diffraction: Reaction Dynamics at the Atomic Level*
- 22b) Denise M. Koch, Gilles H. Peslherbe and Holger Vach (Concordia University)
- Mechanisms of Translational and Rotational Energy Transfer in ( $N_{2n}$ ) Cluster Surface Scattering*
- 23a) Changhong Xia, Kaley A. Walker and A.R.W. McKellar (S.I.M.S., NRC of Canada)
- The Weakly Bound Complex  $NH_3 - CO$ : Observation and Analysis of Spectra in the Infrared (C - O Stretching) and Millimeter Wave (76 - 106 GHz) Regions*
- 23b) Yaqian Liu and Wolfgang Jaeger (University of Alberta)

*Experimental and Theoretical Studies of the Ar-C<sub>2</sub>H<sub>4</sub> and Ne-C<sub>2</sub>H<sub>4</sub> van der Waals Complexes*

24a) Robert J. Le Roy and Yiye Huang (University of Waterloo)

*Representing Born-Oppenheimer Breakdown Radial Correction Functions for Diatomic Molecules*

24b) David Cramb, Zoya Leonenko, Anna Carnini and Thao Kha (University of Calgary)

*Real Time Dynamics of Self Assembled Phospholipid Bilayers using Atomic Force Microscopy*

25a) K.J. Higgins, H.J. Jung, D.B. Kittelson, J.T. Roberts and M.R. Zachariah (University of Minnesota)

*Kinetics of Soot Nanoparticle Oxidation*

25b) Christelle Hauchard, Christian Pepin and Paul Rowntree (Université de Sherbrooke)

*Structure and Physical Transformation of Fe(CO)<sub>5</sub> Thin Films Cryodeposited on Au(111) and on Highly Structured Organic Layers*

26a) Zhenhua He and K.T. Leung (University of Waterloo)

*Surface Processes on Si(111)7x7 and SiO<sub>2</sub> Mediated by Low-Energy Ion Irradiation in CF<sub>4</sub> and CH<sub>2</sub>F<sub>2</sub>*

26b) Qiang Li and K.T. Leung (University of Waterloo)

*Pyridine Interactions with the 2x1 and Modified Si(100) Surfaces*

27a) K.J. Kubarych, S. Lin, C.J. Milne, V. Astinov and R.J.D. Miller (University of Toronto)

*Diffraction Optics Based Two-Color Six-Wave Mixing: Phase Contrast Heterodyne Detection of the Fifth Order Raman Response of Liquids*

27b) Q. J. Hu, X. K. Hu, R. C. Shiell and J. W. Hepburn (University of Waterloo)

*Threshold Ion Pair Production Spectroscopy of H<sub>2</sub>S*

28a) F. Stienkemeier, D. Schumacher, P. Claas and C.P. Schulz (Universität Bielefeld)

*Femtosecond Spectroscopy of Potassium Clusters on the Surface of Superfluid Helium Nanodroplets*