*The 28th Annual*

# Symposium

# On

# Chemical Physics

*at the*

*University of Waterloo*

*November 2-4, 2012*

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## Acknowledgements

*We are very grateful to the following sponsors*
*for their generous financial support of this conference.*

Vice President Academic & Provost, University of Waterloo
Faculty of Science, University of Waterloo
Department of Chemistry, University of Waterloo

*The 28th Annual*

# Symposium

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**REGISTRATION** begins at 7:00 p.m. EIT Foyer

**SESSION I**: Friday, November 2, 2012 — P.M. EIT-1015

Chair: **Robert J. Le Roy**

7:30 – 8:15 **Viktor Staroverov**
(University of Western Ontario)
*Recent advances in the theory and application of model Kohn-Sham potentials*

8:15 – 8:30 **Gustavo Avilla Blanco**
(Department of Chemistry Queen's University)
*Pruned-basis variational calculations demonstrate that a four-mode expansion is not good enough for $C_2H_4$*

8:30 – 8:45 **Klaus Bescherer**, Jack Barnes, and Hans-Peter Loock
(Chemistry Department, Queen's University)
*Cavity Ring-Down Spectroscopy using Liquid Core Waveguides*

8:45 – 9:00 **Randall S. Dumont**
(McMaster University)
*Molecular charging and polarization in a molecular electronic device at non-zero bias*

**SESSION II**: Saturday, November 3, 2012 – A.M. EIT-1015

Chair: **Jim Martin**

9:00 – 9:45 **Gabriel Hanna**
(University of Alberta)
*Multidimensional vibrational spectroscopy of mixed quantum-classical systems: From simple models to water*

9:45 – 10:00 **Peter A. Limacher**, Paul W. Ayers, Paul A. Johnson, Stijn De Baerdemacker, Dimitri Van Neck, Patrick Bultinck
(Department of Chemistry & Chemical Biology, McMaster University)
*Nonorthogonal Geminal Product Wavefunctions for Strongly Correlated Electrons: Highly Accurate Bond Dissociation Curves at Modest Computational Cost due to Projection*

10:00 – 10:15 **Hans-Peter Loock**, Jack Barnes, Saverio Avino, Gianluca Gagliardi, Xijia Gu, David Gutstein, James Mester and Costa Nicholaou
(Department of Chemistry Queen's University)
*The Photonic Guitar: Low-Noise Vibration Sensing with Fiber-Optic Cavities*

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 3, 2012 – A.M. EIT-1015
Chair: **Pierre-Nicholas Roy**

10:45 – 11:45 ***The Roger E. Miller Lecture*** : **David Manolopoulos**
(University of Oxford)
*Ring Polymer Molecular Dynamics -- A Review of our last 6 Years Work Including a Wide Variety of Applications*

11:45 – 12:00 **Jeff Crouse**, Stephen Walker, Natalie Cann, Hans-Peter Loock
(Department of Chemistry Queen's University)
*Using Velocity Map Imaging and Molecular Dynamics to Investigate Ice Photochemistry*

12:00 – 12:15 **P. A. Johnson**, P. W. Ayers, P. A. Limacher, S. De Baerdemacker, D. Van Neck, and P. Bultinck
(Department of Chemistry & Chemical Biology, McMaster University)
*Nonorthogonal Geminal Product Wavefunctions for Strongly Correlated Electrons: Polynomial Scaling Variational Approaches for Off-Shell Bethe Vectors*

12:15 – 1:30 **Lunch** – EIT Foyer

**SESSION IV**: Saturday, November 3, 2012 – P.M. EIT-1015
Chair: **Mikko Karttunen**

1:30 – 2:15 **Poul Peterson**
(Cornell University)
*Ultrafast Dynamics at Soft Interfaces*

2:15 – 2:30 **Xiaogang Wang** and Tucker Carrington, Jr
(Department of Chemistry Queen's University)
*Calculating rovibrational levels of polyatomic molecules with internal coordinates and the Eckart frame : application to $CH_4$*

2:30 – 2:45 **Fedor Y. Naumkin**
(University of Ontario Institute of Technology)
*Metal-Organic Molecular Units for Induced Structure Manipulation*

2:45 – 3:00 **Styliani Consta**
(Department of Chemistry, University of Western Ontario)
*The "Phase-diagram" of macroion release from charged nanodroplets*

3:00 – 6:00 **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 3, 2012 from 3:00 P.M. EIT 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 4, 2012 – A.M. EIT 1015
Chair: **Takayoshi Amano**

9:15– 10:00 **Marcos Dantus**
(Michigan State University)
*Coherent Control Principles and Applications Based on Shaped Ultrafast Pulses*

10:00 – 10:15 **John T. Titantah** and Mikko Karttunen
(Department of Applied Mathematics, Western University)
*Fast intermolecular energy transfer in water: a signature of strengthened hydrogen-bond network*

10:15 – 10:30 **Jesse Baldwin** and Robert J. Le Roy
(Department of Chemistry, University of Waterloo)
*Improved Models for the Potential Energy Functions of the* $X\,^1\Sigma_g^+$ *and* $a\,^3\Sigma_u^+$ *states of* $Cs_2$ *from fits to Spectroscopy and Scattering Lengths*

10:30 – 11:00 **Coffee Break**

**SESSION VII**: Sunday, November 4, 2012 – A.M. EIT 1015
Chair: **Scott Hopkins**

11:00 – 11:45 **Nasser Moazzen-Ahmadi**
(University of Calgary)
*Weakly-Bound Molecular Complexes Formed from Three- and Four-Atom Linear molecules*

11:45 – 12:00 **Stephen Constable** and Pierre-Nicholas Roy
(Department of Chemistry, University of Waterloo)
*The LE-PIGS Method for Nuclear Ground States*

12:00 – 12:15 **Hengameh Omrani**, Jack A. Barnes, Alexander E. Dudelzak, Hans-Peter Loock and Helen Waechter
(Queen's University)
*Fiber-Coupled Fluorescence and Absorption Spectroscopy for Machinery Fluids Characterization*

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

**POSTER SESSION** EIT Upstairs Foyer

Chair: **Pierre-Nicholas 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) **Fatemeh R. Rahsepar** and K.T. Leung
(University of Waterloo)
***Quantum Dynamics of Au on Si(111)7x7: Comparison of VASP Trajectory Calculations with STM Observation***

1(b) **W. C. Theodore Chow** and Scott Hopkins
(University of Waterloo)
***Computational Modelling of Carbonyl Sulfide Adsorption on Cationic Rhodium Clusters***

2(a) **N.L.P. Andrews**, D.A. Horke and J.R.R. Verlet
(Durham University)
***Femtosecond Dynamics of Polyanions***

2(b) **Adrian Adamescu**, Marshall Lindner, Ian Hamilton, Hind Al-Abadleh
(Chemistry Department, Wilfrid Laurier University)
***Density Functional Theory Calculations on the Complexation of p-Arsanilic Acid to Iron Oxide Clusters***

3(a) Adam Gribble,[1] **Leila Tamina Schneider**,[1] Jack Barnes,[1] Xijia Gu,[2] Hans-Peter Loock[1]
([1]Queen's University and [2]Ryerson University)
***Cavity-enhanced Photoacoustic Spectroscopy***

3(b) **Farnaz Heidar Zadeh**, Paul W. Ayers
(Department of Chemistry & Chemical Biology, McMaster University)
***Machine Learning Approaches for Molecular Property Prediction***

4(a) **Stephen Walker**, Jeff Crouse, Natalie Cann, Hans-Peter Loock
(Queen's University)
***Developments into Photochemical Interactions of Condensed Phase Materials Using VMI/IRAS Coupled with MD Simulations***

4(b) **Nabil F. Faruk**, Hui Li, Jing Yang, Robert J. Le Roy, Pierre-Nicholas Roy
(Department of Chemistry, University of Waterloo)
***Simulation Studies of the Vibrational Dynamics of para-Hydrogen Clusters***

5(a) N. Kariya, J. Miyawaki, K. Sugawara, I. Arai, J. Vey, and **I. Hamilton**
(Department of Chemistry, Wilfrid Laurier University)
***Reactions of $Au_n^+$ with $SiH_4$: An Experimental and Computational Study***

5(b) **Tao Zeng**, Gr egoire Guillon, Hui Li, and Pierre-Nicholas Roy
(Department of Chemistry, University of Waterloo)
***Asymmetric top rotors in superfluid para-hydrogen nano-clusters: the molecules with three buckets***

6(a) **M. Schmidt**, S. Constable, J. Yang, T. Zeng, and P.-N. Roy
(Department of Chemistry, University of Waterloo)
***Molecular Dynamics simulations on various weakly bound water-parahydrogen systems at low temperature***

6(b) **James Brown**, Xiao-Gang Wang, Tucker Carrington Jr., and Richard Dawes
(Queen's University)
***Computational Study of the Rovibrational Spectrum of $CO_2$-$CS_2$ : Evidence of Internal Rotation***

7(a) **Yalina Tritzant-Martinez**,[1] Toby Zeng,[2] Aron Broom,[1] Robert J. Le Roy,[2] and Pierre-Nicholas Roy[1,2]
([1] University of Alberta and [2] University of Waterloo)
***On the Analytical Representation of Free Energy Profiles with a 00Morse/Long-Range Model: Application to the Water Dimer***

7(b) **W. Chen**, J. Saunders, C. Brauer, J. Barnes, S. Yam, H.-P. Loock , and D.-X. Xu
(Departments of Chemistry and Electrical and Computer Engineering,
Queen's University)
***Real-time Chemical Sensing on Miniaturized Resonators and Interferometers***

8(a) L. A. Jones, J. D. Carter, **J. D. D. Martin**
(Department of Physics and Astronomy, University of Waterloo)
*Rydberg Atom Electric Dipole Nulling using Non-Resonant Microwave Dressing Fields*

8(b) **Frances Mackay**, and Colin Denniston
(Department of Applied Mathematics, University of Western Ontario)
***Colloidal Particles Interacting in the Presence of a Liquid Crystal***

9(a) **Mona Habibi**, Colin Denniston , and Mikko Karttunen
(Department of Applied Mathematics, University of Western Ontario)
***Spherical Micelles Under the Shear Flow***

9(b) **Christopher Ing**, Konrad Hinsen, and Pierre-Nicholas Roy
(Department of Chemistry, University of Waterloo)
***A Modular Framework for Path-Integral Molecular Dynamics Methods Development***

10(a) **Alexander Marshall** and Mikko Karttunen
(Department of Applied Mathematics, University of Western Ontario
***Water Flow in Carbon Nanotubes***

10(b) **Christopher Haddad**, Santa Rabi, Sandra Rabi, Toon Verstraelen and Paul W. Ayers
(Chemistry and Chemical Biology, McMaster University)
*Finding an Initial Guess for a Transition State Using Redundant Internal Coordinates*

11(a) **Kiran Beera**, Weiran Cheng, Inga Haedicke, Xiao-an Zhang and Artur Izmaylov
(Department of Physical and Environmental Sciences, University of Toronto - Scarborough)
***Assessment of Relaxivity Models for Mn(III)-based MRI Contrast Agents***

11(b) **Isabelle Gauthier**, X.Cui, M. MacDonald, and L. Zuin
(Canadian Light Source Inc.)
***The Varied Line Spacing Plane Grating Monochromator Beamline of the Canadian Light Source***

12(a) **Jari Jalkanen**, Jason O'Young, Susanna Hug, Yinyin Liao, Bernd Grohe, Harvey A. Goldberg, Graeme K. Hunter and Mikko Karttunen
(Department of Applied Mathematics, University of Western Ontario)
***Molecular Simulations of Protein-Crystal Interactions in Biomineralization***

12(b) **G. Guillon**, T. Zeng, P.-N. Roy
(Department of Chemistry, University of Waterloo)
***Theoretical Study of a Water Dimer in a Cryogenic Environment***

13(a) **Allan Adam**, Jonathan Daigle, Lyndsay Esson, Aaron Granger, Ashley Smith, Colan Linton and Dennis Tokaryk
(University of New Brunswick, Department of Chemistry and Centre for Laser, Atomic, and Molecular Sciences (CLAMS)
***High Resolution Laser Spectroscopy of Iridium Monoxide***

13(b) Prateek Goel (S), Marcel Nooijen
(Department of Chemistry, University of Waterloo)
***First Principles Simulations of Vibrationally Resolved Photodetachment Spectra of Select Biradicals***

14(a) **M. Hasan**, J. Baldwin, W.S.Hopkins
(Department of Chemistry, University of Waterloo)
***Uranyl Microsolvation to Form Aqueous Nanosolutions***

14(b) M. Turnbull and S. Constas
(University of Western Ontario, Chemistry department)
**Charge-Induced Instability in Droplets with Polyhistidine Complexes**

Invited Speakers for Past **Symposia on Chemical Physics** at the University of Waterloo.

| *Name* | *Affiliation* | *Title of Presentation* |
|---|---|---|
| ***2011*** | | |
| R. McKellar | NRC, Canada | Spectroscopy of Molecular Clusters |
| J. Autschbach | SUNY Buffalo | Spectroscopy 'In Silico' |
| J. Klassen | U. Alberta | Structure and Stability of Protein-Ligand Complexes in the Gas Phase |
| V. Mandelshtam | U. California Irvine | Simulation of Quantum Liquids and Clusters by Thermal Gaussian Molecular Dynamics |
| A. Stolow | NRC Canada | CARS Microscopy Made Simple |
| J. Van Wijngaarden | U. Manitoba | High Resolution Spectroscopy from the Microwave Through the Infrared Region |
| ***2010*** | | |
| T. Ziegler | U. Calgary | The Description of Excited States by Density Functional Theory |
| N. Mosey | Queen's U. | First-Principles Simulations of Tribological Processes |
| Y. Shi | U. Calgary | Catalytic Chemical Vapour Deposition Chemistry in the gas Phase and on Catalytic Surfaces |
| A. Suits | Wayne State U. | Roaming Radicals! Results from High-Resolution Imaging Studies |
| A. Vilesov | U. Southern California | Growing Clusters in He Droplets: From Nano- to Micro-Droplets |
| K. Walker | U. Toronto | Using Spectroscopy to Study Atmospheric Composition |
| ***2009*** | | |
| M. Lester | U. Pennsylvania | Dynamical Outcomes of Quenching: Reflections on a Conical Intersection |
| J. Hutson | U. Durham | Ultracold Molecules and Ultracold Collisions |
| W. Jäger | U. Alberta | Doped Superfluid Clusters |
| R. Krems | U. British Columbia | Ultracold Chemistry |
| K. Lehman | U. Virginia | Cavity Ring-Down Spectroscopy |
| R.J. Le Roy | U. Waterloo | Adventures in 'Potentiology' |
| G. Scoles | Princeton U. & Internat. School Advanced Studies (Trieste) | Nanomedicine: Towards New Definitions, Diagnostics and Cure of Illness in Modern Medicine |
| ***2008*** | | |
| J. Bowman | Emory U. | Reaction and Vibrational Dynamics on Full Dimensional *ab initio*-based Potential Energy Surfaces |
| P. Bernath | U. York | Molecular Astronomy |
| G. Chan | Cornell U. | Strongly Interacting Electrons in Chemistry |
| T. Leung | U. Waterloo | Spintronics: Emerging Nanotechnology or Just Applied Chemical Physics? |
| R. Signorell | U. British Columbia | Vibrational Excitons in Aerosol Spectroscopy |
| D. Tokaryk | U. New Brunswick | Rings and Things at the Ring: FTIR Spectroscopy of Moderately Large Molecules at the Canadian Light Source |

| *Name* | *Affiliation* | *Title of Presentation* |
|---|---|---|
| ***2007*** | | |
| F. Merkt | ETH Zurich | Rydberg Stark Deceleration and Zeeman Deceleration of Atoms and Molecules |
| P. Ayers | McMaster U. | Chemical Reaction Mechanism Prediction and Elucidation with the Fast-Marching Method |
| A. Brown | U. Alberta | Laser Control of Polyatomic Molecules: The Optimal Control Theory Multi-Configuration Time-Dependent Hartree Approach |
| E. Grant | U. British Columbia | Spectroscopic Manifestations of High-Rydberg Dynamics (Intra- and Intermolecular) |
| J. Martin | U. Waterloo | Resonant Electric Dipole-Dipole Interactions Between Ultra-Cold Rydberg Atoms |
| A. Wodtke | U. California Santa Barbara | Do We Have a Theory for Reactions at Metal Interfaces? The Unsolved Problem of Electronic Non-Adiabaticity |
| ***2006*** | | |
| R. Bartlett | University of Florida | Coupled-Cluster Theory for Large Molecules: The Natural Linear Scaled Coupled-Cluster Method |
| A. Dickinson | U. of Newcastle | Transport Properties of Gases: Beyond Linear Molecules |
| T. Momose | U. British Columbia | Spectroscopy and Dynamics in Solid Parahydrogen and in He Droplets |
| A. Ross | Université Lyon I | Cavity-Enhanced Laser-Induced Emission Spectroscopy |
| G. Scoles | Princeton U. & University of Trieste | HENDI Spectroscopy: the Genesis of an Idea and Some Recent Results |
| Y. Xu | U. Alberta | Exploring Chirality and Chiral Recognition Using Spectroscopic and Ab Initio Methods |
| ***2005*** | | |
| S. Leone | California Berkeley | Ultrafast Molecular Dynamics: Rydberg Wave Packets, Coherent Control, and High Harmonic Probing |
| T. Baer | U. of North Carolina | PEPICO Studies of Energy Selected Sequential and Parallel Ionic Dissociation Reactions |
| J. Stanton | U. Texas at Austin | The Unusually Complicated $NO_3$ Molecule |
| R. Laflamme | U. of Waterloo | Quantum Computer and NMR |
| P. Vaccaro | Yale University | Lifting the Veil of Solvation: The Chiral-Optical Response of isolated Molecules |
| P.-N. Roy | U. of Alberta | Molecular Dynamics in Doped Quantum Clusters: Rotation and Superfluid Response |
| ***2004*** | | |
| W.H. Miller | California Berkeley | Some Recent Applications of the Semiclassical Initial Value Representation |
| J.A. Coxon | Dalhousie U. | Some Modern Applications of Numerical Methods in the Interpretation of Rotational Structure in Band Spectra of Diatomic Molecules |
| J. Donaldson | U. of Toronto | Atmospheric Reactions at the Air-Water Interface |
| H.-P. Loock | Queen's University | Fibre-Optic Detectors and Sensors |
| T. Steimle | Arizona State U. | Optical Stark and Zeeman Studies of Metal Containing Molecules |
| B. Winnewisser | Ohio State U. | NCNCS: An Ideal Example of Molecular 'Quantum Monodromy' |

| *Name* | *Affiliation* | *Title of Presentation* |
|---|---|---|
| ***2003*** | | |
| M. Shapiro | U. British Columbia | Quantum Control of Chiral Conversion, Spontaneous Decay and Tunneling |
| W. Balfour | U. Victoria | The Challenging Playground of Transition Metal Diatomic Spectroscopy |
| M.Gerry | U. British Columbia | Microwave Spectroscopy of Noble Gas–Coinage Metal Halide Complexes and the Nature of the Noble Gas–Coinage Metal Bond |
| W.J. Meath | U. Western Ontario | Mechanism for Multiphoton Excitation of Molecules, and On the Enhancement of "Direct" Two- and Three-Photon Excitations |
| K. Szalewicz | U. Delaware | Theoretical Spectroscopy of Van der Waals Molecules |
| T. Zwier | Purdue University | Laser Probes of the Potential Energy Landscapes and Conformational Isomerization Dynamics of Flexible Biopolymers |
| ***2002*** | | |
| J. Maier | U. Basel | Electronic Spectroscopy of Carbon Chains and Their Relevance to Astrophysics |
| N. Bigelow | U. Rochester | Photoassociation of Molecules in Laser-Cooled Atomic Gases: Precision Spectroscopy, Photoionization, Molecule Formation |
| F. De Lucia | Ohio State U. | Spectroscopy, Collisions and Energy in the Submillimeter |
| C. Linton | U. New Brunswick | Laser Spectroscopy of Lanthanide Molecules - Past, Present and Future |
| J. Lisy | U. Illinois at Urbana-Champaign | Competition Between Non-Covalent Interactions: Suprising Size-Selectivity |
| G. Patey | U. British Columbia | Forces Between Immersed Objects: A Discussion of Interactions on Different Length Scales |
| ***2001*** | | |
| W.C. Stwalley | U. Connecticut | Making Molecules at MicroKelvin |
| J. Abbatt | U. Toronto | Interactions of Atmospheric Trace Gases with Ice: Adsorption and Reaction Studies |
| T. McElroy | Meteorological Service of Canada | The MAESTRO Instrument that will fly on SciSat I, the Atmospheric Chemistry Experiment (ACE) |
| G.H. Peslherbe | Concordia U. | Photochemistry in Diverse Environments |
| H. Rabitz | Princeton U. | Teaching Lasers to Control Molecules: The Molecule Knows Best |
| R. Steer | U. Saskatchewan | Explorations of the Photophysics of Higher Electronic Valence States of Large Molecules: From Spectroscopic Curiosity to Photonics Applications |
| ***2000*** | | |
| G. Scoles | Princeton U. | He Atom Reflectivity Studies of Chemical Dynamics on Metal Surfaces |
| U. Buck | M.-P.-I. Strömungsforschung | Photodissociation and Caging in Different Cluster Environments |
| M. Klein | U. Pennsylvania | Computer Simulation Studies of Biophysical Systems: From Micelles to Model Membranes and Membrane Proteins |
| L. Mattera | U. Genova | Correlation Between Growth and Magnetic Behaviour at the Surface of Ultrathin Films |
| R.E. Miller | U. North Carolina | Exploring Potential Energy Landscapes: Cluster Growth in He Nanodroplets |
| P. Rowntree | U. Sherbrooke | Electron-Induced Processes In (and ON) Self-Assembled Organic Monolayers |

| *Name* | *Affiliation* | *Title of Presentation* |
|---|---|---|
| ***1999*** | | |
| P. Corkum | S.I.M.S., NRC | Strong Fields Molecular Optics |
| K. Chance | Harvard U. | Fitting Atmospheric Spectra in the Infrared Through Ultraviolet: Exercises in Spectroscopy and Radiative Transfer |
| J. Farrar | U. Rochester | Electronic Spectroscopy of Mass-Selected Clusters: Probes of Ion Solvation |
| W. Jäger | U. Alberta | Spectra of van der Waals Complexes: Fingerprints of Intermolecular Interactions |
| D. Pratt | U. Pittsburgh | Static and Dynamic Properties of Molecular Assemblies in the Gas Phase |
| J. Tennyson | U. London | Assigning the Spectrum of Water on the Sun and Elsewhere |
| ***1998*** | | |
| J. Jortner | U. Tev Aviv | On Dynamics. From Isolated Molecules to Biomolecules |
| A. Adam | U. New Brunswick | High Resolution Laser Spectroscopy of Diatomic Molecules Containing Cobalt |
| F. Davis | Cornell U. | Transition Metal Chemistry in a Crossed Molecular Beam |
| M. Johnson | Yale U. | Making and Breaking Water Networks Around Halide Ions: Ions vs. Interwater Hydrogen Bonding |
| R.J.D. Miller | U. Toronto | Femtosecond Surface reaction Dynamics: Mapping the "Electron Trajectory" |
| N. Westwood | U. Guelph | Ground, Excited and Ionic States of Unstable Molecules: Experiment and Theory |
| ***1997*** | | |
| T. Oka | U. Chicago | Detection of Interstellar $H_3^+$ Molecules in Astronomy |
| Y. Endo | U. Tokyo | Laser-Induced Fluorescence Spectroscopy of Carbon Chain Free Radicals |
| M. Okumura | Cal. Tech. | Solvation and State-Mixing in Clusters |
| R. Saykally | U.C. Berkeley | Infrared Cavity Ring-Down Laser Absorption Spectroscopy |
| T. Sears | Brookhaven | Transient Frequency Modulation Spectroscopy of Simple Carbenes |
| J.K.G. Watson | S.I.M.S., NRC | The Diffuse Interstellar Band Problem |
| ***1996*** | | |
| A.D. Buckingham | Cambridge U. | Molecules in Optical, Electric and Magnetic Fields |
| M. Alexander | U. Maryland | Weakly Bound Complexes of Atomic Boron with Argon and Hydrogen |
| R. Curl | Rice U. | Infrared Laser Spectroscopy, and Comments on the Discovery of $C_{60}$ |
| M.A. Duncan | U. Georgia | Electrostatic Bonding in Gas Phase Metal Atom Complexes |
| A. Stolow | S.I.M.S., NRC | Time Resolved Photoelectron/Photoion Spectroscopy: Towards Wavepacket Technology |
| D. Wardlaw | Queen's U. | Molecular Surface Hopping in Intense Laser Fields |

| *Name* | *Affiliation* | *Title of Presentation* |
|---|---|---|
| ***1995*** | | |
| W. Klemperer | Harvard U. | Spectroscopy, Structure and Dynamics of Molecular Complexes |
| T. Carrington | U. Montréal | A Time Dependent Multi-Surface Calculation of the Orientation of Photofragments: The Photodissociation of ICN |
| T.A. Miller | Ohio State U. | Laser Spectroscopy of Cold Methoxy Radicals and Its Derivatives: Molecules that Sometimes Fluoresce and Sometimes Don't |
| M. Moskovits | U. Toronto | Thinking Small – Megascience with Nanostructures |
| B. Simard | S.I.M.S, NRC | Experimental and Theoretical Studues of Cu-group 13 and Al-group 14 Diatomics |
| W. Weisshaar | U. Wisconsin | Understanding Methyl Rotor Barriers |
| ***1994*** | | |
| G. Scoles | Princeton U. | Clusters Within Clusters: Matrix Isolation Spectroscopy in Condensed Helium Beams |
| M.S. Child | Oxford U. | Inversion of Spectroscopic Data |
| T.E. Gough | U. Victoria | Infrared Spectroscopy of Molecular Microcrystallites |
| J.M. Hutson | U. Durham | Additive and Non-Additive Intermolecular Forces from the Spectroscopy of Van der Waals Complexes |
| A.R.W. McKellar | H.I.A., NRC | Long-Path Infrared Spectra of Weakly-Bound Complexes |
| R.E. Miller | U. North Carolina | Photofragmentation of Oriented Molecules: New Insights into Photodissociation Dynamics from Pendular States |
| ***1993*** | | |
| A. Zewail | Cal. Tech. | Recent Advances in Femtochemistry |
| P. Hackett | NRC | Studies of the Structure and Reactivity of Small Clusters |
| R. Kapral | U. Toronto | The Structure and Dynamics of Binary Clusters |
| E.C. Lim | U. Akron | Excited-State Dynamics and Photochemistry of Van der Waals Dimers and Clusters of Aromatic Molecules |
| A. Myers | U. Rochester | Dissecting the Ensemble Average: Spectroscopy and Dynamics of Individual Molecules |
| P. Schultz | U. Western Ontario | Probing Defects in Semiconductors with Slow Positrons |
| ***1992*** | | |
| W.C. Lineberger | U. Colorado | Time-Resolved Cage Recombination Dynamics in Large Molecular Cluster Ions |
| P.R. Bunker | H.I.A., NRC | The Infrared Spectrum, Tortional Barrier and Vibrational Motions in Dimethylacetylene |
| J.B. McConkey | U. Windsor | Use of Laser-Induced Fluorescence Techniqures to Probe the Breakup of Simple Molecules Under Electron Impact |
| D. Perry | U. Akron | Infrared Molecular Eigenstate Spectroscopy: A Probe for the Rate and Mechanism of Intramolecular Relaxation |
| L. Sanche | U. de Sherbrooke | Surface Reactions and Desorption Induced by Electron Attachment |
| A.J. Thakkar | U. New Brunswick | Van der Waals Coefficients, Polarizabilities and Hyperpolarizabilities: Current Calculational Possibilities |

| *Name* | *Affiliation* | *Title of Presentation* |
|---|---|---|
| ***1991*** | | |
| R.Z. Zare | Stanford U. | State-Selected and State-Detected Reaction Dynamics |
| T. Amano | H.I.A., NRC | The Dissociative Recombination Rate of $H_3^+$ |
| P. Houston | Cornell U. | The HCO Potential Energy Surface: Probes Using Molecular Scattering and Photodissociation |
| W.J. Meath | U. Western Ontario | Effects of Permanent Dipoles on the Resonance Profiles and Dynamics Associated with Single- and Multi-Photon Laser-Molecule Interactions |
| T. Rizzo | U. Rochester | Multiple Laser Probes of Intramolecular Dynamics |
| D. Roy | Université Laval | The Surface Chemistry of Silicon Investigated by Electron Spectroscopy: Some New Results |
| ***1990*** | | |
| D.G. Truhlar | U. Minnesota | Calculation of Quantum Effects in Chemical Reaction Dynamics |
| D.J. Donaldson | U. Toronto | Predissociation Dynamics of $CS_2$ |
| K.C. Janda | U. Pittsburgh | Pump-Probe Studies of the Structure and Dynamics of Van der Waals Molecules |
| J. Barker | U. Michigan | Collisional Deactivation of Highly Excited Polyatomic Molecules |
| B. Henry | U. Guelph | Sources of Intensity for Local Mode Overtones |
| D. Salahub | U. Montréal | Density Functional Theory and the Quantum Chemistry of Transition Metal Systems |
| ***1989*** | | |
| J.P. Toennies | MPI, Göttingen | Hot Molecules and Cold Clusters |
| P. Corkum | NRC | Femtosecond Lasers for Chemical Physics |
| A.P. Hitchcock | McMaster U. | Inner-Shell Excitation Spectroscopy of Molecules |
| S. Mukamel | U. Rochester | Solvation Dynamics in Electron Transfer and Non-Linear Optical Susceptibilities: A Unified Description |
| R. Lipson | U. Western Ontario | VUV Laser Spectroscopy of Reactive States: Valence to Ion-Pair Transitions of Halogens |
| V.H. Smith | Queen's U. | Adventures in the 3-Body Problem: Exotic Molecules |
| ***1988*** | | |
| R.S. Berry | U. Chicago | How Good is Neil Bohr's Model of the Atom? |
| D. Rosner | U. Western Ontario | Testing Quantum Electrodynamics with Lasers and Simple Atoms |
| R.F.W. Bader | McMaster U. | A Quantum Theory of Molecular Structure |
| M.J. Dignam | U. Toronto | Spectroscopy of Ordered Molecular Assemblies |
| W. Siebrand | NRC | Tunneling of Hydrogen and Heavier Atoms |
| S. Filseth | York University | Energy Disposal in CN Produced by Photodissociation and Reactions |
| ***1987*** | | |
| D.R. Herschbach | Harvard U. | Electronic Structure in Strange Dimensions |
| P. Norton | U. Western Ontario | Phase Transitions and Surface Reactivity |
| R.J.D. Miller | U. Rochester | Picosecond Dynamics of Surface Mediated Electron Transfer Processes at Single Crystal Semiconductor Interfaces |
| B. Schlegel | Wayne State U. | Spin Pojection and Moller-Plessit Perturbation Theory |
| J. Reid | McMaster U. | Optically Pumped $NH_3$ Laser: A New Approach to Stable Lasers |
| P. Brumer | U. Toronto | Chaotic Intramolecular Energy Transfer |

| *Name* | *Affiliation* | *Title of Presentation* |
|---|---|---|
| ***1986*** | | |
| Y.T. Lee | U.C.-Berkeley | Dynamics and Spectroscopy by Lasers and Molecular Beams |
| A. Bandrauk | U. Sherbrooke | Non-Adiabatic Effects in Multiphoton Transitions |
| T.H. Ellis | U. Montréal | Direct Measurements of Surface Kinetics by Time Resolved EELS |
| W.L. Hase | Wayne State U. | Potential Energy Surface Properties and Dynamics of $H + CH_3$ Recombination and IVR in Benzene |
| G. Scoles | U. Waterloo | Atomic Beam Scattering Studies of Intermolecular Forces at the Gas-Solid Interface |
| S.C. Wallace | U. Toronto | Excited State Dynamics of Van der Waals Clusters |
| ***1985*** | | |
| R.B. Gerber | Hebrew U. | Molecular Dissociation in Impacts on Crystal Surfaces |
| J.C. Polanyi | U. Toronto | Photodissociation and Photodesorption of Adsorbed Species |
| T.F. George | SUNY-Buffalo | Molecular Dynamics and Spectroscopy at Gas-Solid Interfaces |
| J. Hepburn | U. Waterloo | State-to-State Photofragmentation of Small Molecules and Molecular Clusters |
| C.M. Sadowski | York University | Energy Disposal in the Photodissociation of Triatomic Cyanides |
| M. Moskovitz | U. Toronto | Photochemistry at Metal Surfaces |

# 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 |
| ***Courtyard Waterloo***: | 519-884-9295 | 50 Benjamin Road E., Waterloo |
| ***Airways Transit***: | 519-886-2121 | https://secure.airwaystransit.com |
| ***Waterloo Taxi***: | 519-886-1200 | |
| ***United Taxi***: | 519-888-0400 | |
| ***City Cab***: | 519-747-7777 | |
| **P.-N. Roy:** | 519-498-6723 | (mobile) |