The 32nd Annual

Symposium

On

Chemical Physics

at the

University of Waterloo

November 4-6, 2016

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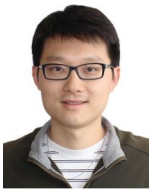
Adam Wei Tsen


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Michael Tam


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nano-instrumentation


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NEW FACULTY MEMBERS

Na Young Kim	Solid-state quantum simulators
Kevin Musselman	Functional nanomaterials
Germán Sciaini	Time-resolved electron diffraction and microscopy
Adam Wei Tsen	Low-dimensional quantum materials and devices
Alfred Yu	Biomedical ultrasound

82 Faculty Members

19 Research Chairholders

Symposium on Chemical Physics
at the University of Waterloo
November 4-6, 2016

REGISTRATION begins at 7:00 p.m. EIT Foyer
SESSION I: Friday, November 4, 2016 — P.M. EIT-1015
Chair: **Scott Hopkins**

7:30 – 8:15 **Paul Mayer**
(University of Ottawa)
Reaction Dynamics of PAH ions: overview and challenges

8:15 – 8:30 **Tuan K. A. Hoang** and P. Chen
(University of Waterloo)
Gel electrolyte for secondary zinc batteries

8:30 – 8:45 **Ryan MacDonell** and Michael S. Schuurman
(University of Ottawa / NRC)
Directing nonadiabatic dynamics via chemical substitution: Ab initio molecular dynamics simulation of cyano-substituted alkenes

8:45 – 9:00 **Paul Godin**, K. Le Bris (St. Francis Xavier University), and K. Strong
(University of Toronto)
Conformational analysis and global warming potential of 1,1,1,3,3,3-hexafluoro-2-propanol using absorption spectroscopy

SESSION II: Saturday, November 5, 2016 – A.M. EIT-1015
Chair: **Pierre-Nicholas Roy**

9:00 – 9:45 **Zlatko Bačić**
(New York University)
Coupled translation-rotation dynamics of H_2 and H_2O inside C_{60}: Rigorous quantum treatment

9:45 – 10:00 **Javix Thomas**, Eric Mariona, and Yunjie Xu
(University of Alberta)
Rotational Spectra of Two Six-Membered Heterocyclic N-Methyl-Piperdinol Compounds

10:00 – 10:15 **Nathan Seifert**, and Wolfgang Jaeger
(University of Alberta)
Current Developments Towards a New 2.0-6.0 GHz Chirped-Pulse Fourier Transform Microwave Spectrometer

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 5, 2016 – A.M. EIT-1015
Chair: **Marcel Nooijen**

10:45 – 11:45 ***The Roger E. Miller Lecture***: **Frank Neese**
(Max Planck Institute, Mülheim)
Coupled Cluster Theory for systems with hundreds of atoms

11:45 – 12:00 **Amin Moazeni**, and Yunjie Xu
(University of Alberta)
Interactions of Iodine with Carbonyl and Thiocarbonyl Functionalities in Solution: Competition Between Halogen- and Hydrogen-Bonding and New Halogen-Bonding Motif

12:00 – 12:15 **Ebenezer Owusu-Ansah**, and Yujun J. Shi
(University of Calgary)
Characterization of Si Atomic Electronic Transitions Using Pulsed Electric Discharge and Resonance-enhanced Multiphoton Ionization

12:15 – 1:30 **Lunch** – EIT Foyer

SESSION IV: Saturday, November 5, 2016 – P.M. EIT-1015
Chair: **German Sciaini**

1:30 – 2:15 Ralph Ernstorfer
(Fritz-Haber Institute, Berlin)
Ultrafast Electronic and Structural Dynamics on the Nanoscale

2:15 – 2:30 **Prasanta Das**, Chrissy J. Knapp, and Wolfgang Jaeger
(University of Alberta)
Formation of the Cyclic Formic Acid Dimer in Helium Nanodroplets

2:30 – 2:50 ***The 2015 'D.J. Le Roy Prize' Lecture***: **Amro Dodin**, Paul Brumer, and Timur Tscherbul (University of Nevada)
(University of Toronto / MIT)
In the Blink of an Eye - Incoherent Excitation of Molecular Systems by Time-Varying Incoherent Light

2:50 – 3:05 **James Anderson**, P.W. Ayers, H. Nakatsuji, and H. Nakashima
(RIKEN, Kobe)
Boys'Collocation Approach to Solve the Electronic Schrödinger Equation

3:05 – 3:20 **Valerie Gabelica**
(University of Bordeaux)
What happens to DNA duplexes upon electrospray ionization?

3:25 – 6:00 **Refreshments and Poster Session**

The Roger E. Miller Lecture is 60 min. including 10 min for discussion.
The D.J. Le Roy Prize Lecture is 20 min including 5 min for discussion
Contributed talks are 15 min. including 3min. for discussion
Invited talks are 45 min. including 5 min. for discussion

SESSION V: Saturday, November 5, 2016 from 3:25 P.M. EIT Upstairs Foyer
POSTER SESSION
Chair: **Marcel Nooijen**

6:00 P.M.	Poster sessions ends Depart for Large Conference Room, ***Federation Hall*** (*check your maps!*)
6:30 P.M.	Cash Bar: Large Conference Room, ***Federation Hall***
7:00 P.M.	**DINNER:** Large Conference Room, ***Federation Hall***
8:30 P.M. - …	Informal Discussions: Large Conference Room, ***Federation Hall***

SESSION VI: Sunday, November 6, 2016– A.M. EIT 1015
Chair: **Wei Tsen**

9:15– 10:00 **Dominika Zgid**
(University of Michigan)
Rigorous quantum embedding using Green's functions

10:00 – 10:15 **Mark Wilson**
(University of Toronto)
Solid-state organic/nanocrystal films for infrared↔visible photon conversion via excitonics

10:15 – 10:30 **Issaka Seidu**, Mykhaylo Krykunov (University of Ottawa), and Tom Ziegler
(University of Calgary)
(Carleton University)
Time-Independent approach for excited-state studies

10:30 – 11:00 **Coffee Break**

SESSION VII: Sunday, November 6, 2016– A.M. EIT 1015
Chair: **Jim Martin**

11:00 – 11:45 **Patrick Ayotte**
(Université de Sherbrooke)
Nuclear spin isomers of H_2O and their interconversion: implication for their separation, storage, and applications

11:45 – 12:00 **Myong In Oh**, and Styliani Consta
(University of Western Ontario)
How does the droplet environment affect the stability of a noncovalent protein complex?

12:00 – 12:15 **Jiwen Guan**, and Yang Song
(University of Western Ontario)
Pressure Effects on Non-Adiabatic Photochemistry: Frozen Pedal Motion versus Photocycloaddition of Stilbene

12:15 – 1:30 Light **Lunch & Coffee** – EIT Foyer

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

POSTER SESSION: Saturday, November 5, 2016 EIT Upstairs Foyer

Chair: **Marcel Nooijen**

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) **Allan Adam,** Colan Linton, Nicole Nickerson, and Dennis Tokaryk
(University of New Brunswick)
The Electronic Spectrum of Ruthenium Monohydride: Recent Results

1(b) **Nicholas Andrews**, Kh. M. Bahmanpour, R. Ross, D. Munzke, C. van-Hoorn, A. Brzezinski, J. A. Barnes, O. Reich, and H-P. Loock
(Queen's University)
In-fibre Interferometer Using a Hollow-core Photonic Crystal Fibre

2(a) **Angelo Perera**, Javix Thomas, Christian Merten (Ruhr-Universität Bochum), and Yunjie Xu
(University of Alberta)
Vibrational Circular Dichroism Spectral Features of Methyl Glycidate in Carbon Tetrachloride and Water: Implicit and Explicit Solvation Models

2(b) **Gustavo Avila,** and Tucker Carrington Jr.
(Queen's University)
A comparison of sparse-grid quadrature and collocation for the calculation of vibrational levels of methane

3(a) **Jack Barnes**, and Hans-Peter Loock
(Queen's University)
Application of coupled mode theory to phase-shift and intensity measurements in optical microresonators

3(b) **Kevin Bishop**, and P.-N. Roy
(University of Waterloo)
Quantum mechanical free energy profiles of the water dimer

4(a) Hao Chen, John Saunders, **Sogol Borjian Borojeni**, Xiaowei Wu, Connor Saunders, Jack Barnes, Cathleen M. Crudden, Hans-Peter Loock
(Queen's University)
Detection of aqueous Pb(II) and Hg(II) using periodic mesoporous organo-silica coated ring resonators

4(b) **Li-Hong Xu**, Elias M. Reid, Bradley Guislain and Jon T. Hougen
(University of New Brunswick)
Torsionally Mediated Spin-Rotation Hyperfine Splittings in Acetaldehyde

5(a) **Patrick Carr**, M. J. Lecours, E. Fillion, T.B. McMahon, R. Marta, V. Steinmetz, and W. S. Hopkins
(University of Waterloo)
Exploring Mode-Selective Ligand Scrambling of Palladium Catalysts

5(b) **Xiaotian Chen**, Prateek Goel, and Marcel Nooijen
(University of Waterloo)
Examples of Potential Energy Surfaces for Chemical Reaction using Vibronic Models

6(a) **Prateek Goel**, Xiaotian Chen, and Marcel Nooijen
(University of Waterloo)
Modelling of Potential Energy Surfaces for Chemical Reactions using Vibronic Models

6(b) **Isaac De Vlugt**, Michael Lecours, Ahdia Anwar, Rick Marta, Vincent Steinmetz (CLIO / LCP), Terry McMahon, Eric Fillion, and W. Scott Hopkins
(University of Waterloo)
Infrared-Driven Charge Transer in Cu, Ag and Cd $B_{12}H_{12}$ (2-) Clusters

7(a) **Gary Douberly**
(University of Georgia)
Infrared Zeeman Spectroscopy of Radicals in Helium Droplets

7(b) **Travis Ferguson**, N.L.P. Andrews, A.R.Bernicky, A.M.M. Rangaswamy, N. Henning, A. Dudelzak, O. Reich, J.A. Barnes, and H-P. Loock
(Queen's University)
A Multiplex Approach in Fluorescence Excitation Emission Matrix Spectroscopy

8(a) **Stijn Fias**, Farnaz Heidar-Zadeh, Paul Geerlings, and Paul W. Ayers
(Free University Brussels (VUB))
Chemical Transferability of Functional Groups Follows From the Nearsightedness of Electronic Matter

8(b) **Weiqiang Fu**, Patrick Carr, Mike Lecours, Michael Burt, Rick A. Marta, Eric Fillion, Vincent Steinmetz, Terry McMahon, and W. Scott Hopkins
(University of Waterloo)
The Structures and Properties of Protonated Phenylalanine Derivatives

9(a) **Hao Chen**, John Saunders, Sogol Borjian, Xiaowei Wu, Connor Saunders, Jack Barnes, Cathleen M. Crudden, and Hans-Peter Loock
(Queen's University)
Detection of aqueous Pb(II) and Hg(II) using periodic mesoporous organo-silica coated ring resonators

9(b) **Cristina E. Gonzalez Espinoza**, Paul W. Ayers, Jacek Karwowski (Nicolaus Copernicus University), and Andreas Savin (Laboratoire de Chimie Théorique)
(McMaster University)
Smooth models for the Coulomb Potential

10(a) **Chris Herdman**
(University of Waterloo - IQC)
Entanglement Area Law in Superfluid ^4He

10(b) **Piaoyu Hu**, Siyuan Wu, and Marcel Nooijen
(University of Waterloo)
Multireference Benchmark Calculations for Prototype Magnetic Systems

11(a) **Siyuan Wu**, and Marcel Nooijen
(University of Waterloo)
Magnetic Coupled Cluster

11(b) **Jiao Gao**, Javix Thomas, Yunjie Xu, and Wolfgang Jaeger
(University of Alberta)
Non-equivalent Methyl Internal Rotations in the Acetone—H_2O Complex Studied by Microwave Spectroscopy and Ab Initio Calculations

12(a) **Loic Joubert-Doriol**, Ilya G. Ryabinkin, and Artur F. Izmaylov
(University of Toronto Scarborough)
Generalized Schrödinger equation for open system simulations

12(b) **Anna B. Krin**, Xiaoli Cai (Wuhan Research & Development Center of Pfizer, Wuhan), Mohammad Reza Poopari, Yuefei Zhang (Wuhan Institute of Technology, Wuhan),Amin Moazeni, and Yunjie Xu
(University of Alberta)
Chiral Analysis of Steroid Hormones: IR and Vibrational Circular Dichroism Spectroscopy

13(a) **Mike Lecours**, Rick A. Marta, Vincent Strinmetz (CLIO, Orsay), Peter Liuni (York University), Derek J. Wilson (York University), Terrance B. McMahon, Eric Fillion, and W. Scott Hopkins
(University of Waterloo)
Coupling Ultrafast ESI with Trapped Ion Spectroscopy

13(b) **Ronald Lees**, B.G. Guislain, E.M. Reid, R.M. Lees and Li-Hong X, S. Twagirayezu (Lamar University, Beaumont), D.S. Perry (University of Akron), B. Thapaliya (University of Akron), and M.B. Dawadi (University of Akron, Ohio)
(University of New Brunswick)
Shining Light on the Methyl-Bending Spectrum of CH_3SH at the Canadian Light Source

14(a) **Kristina Lekin**, Kazuma Ogata, Stephen M. Winter, Adrian Maclean, Aaron Mailman, Abdeljalil Assoud, Masaki Mito, John S. Tse, Serge Desgreniers, Paul A. Dube, and Richard T. Oakley
(University of Waterloo)
Performance under Pressure; Pushing TC to 27 K in a Heavy Atom Radical Ferromagnet

14(b) **Jiaru Li**, Loic Joubert-Doriol, and Artur F. Izmaylov
(University of Toronto Scarborough)
Geometric phase effects in the excited state dynamics of N-dimensional linear vibronic coupling mode

15(a) **Amy MacLean**, Nadia Bragagnolo, Michaela Thomas, Sophie Lehnert, Jack Barnes, Carlos Escobedo, Cathy Crudden, Hugh Horton, and Hans-Peter Loock
(Queen's University)
Will it stick? The binding kinetics of N-heterocyclic carbenes to plasmonic biosensors

15(b) **Philip Myatt**, Justin Burgess, Michael Sadkowski, Ariel Petruk, Nicolás Rivas, Kristina Lekin, and German Sciaini
(University of Waterloo)
Current 494 student projects at the Ultrafast Electron Imaging Lab

16(a) **Anand H.G. Patel**, Ahmed A. K. Mohammed, and Paul W. Ayers
(McMaster University)
Calculation of nonlinear optical properties using a rational function model

16(b) **Ariel Petruk**, Caroline Allen, Nicolas Castro-Folker, Nicolas Rivas, Kostyantyn Pichugin, and German Sciaini
(University of Waterloo)
Accessories for electron microscopy: nanofluidics, and detection systems

17(a) **Kostyantyn Pichugin**, Ariel Petruk, and German Sciaini
(University of Waterloo)
Ultrafast electron diffraction and microscopy: breaking time-resolution limits

17(b) **Jarrod Psutka**, Ahdia Anwar, Steve Walker, Scott Hopkins, and Larry Campbell
(SCIEX)
(University of Waterloo)
Separation of Tautomers of Protonated Nucleobases

18(a) **Neil Raymond**, Marcel Nooijen, and Pierre-Nicholas Roy
(University of Waterloo)
Thermodynamic Properties of Nonadiabatic Systems

18(b) **Michael Richer**, and Paul Ayers
(McMaster University)
Tractable Geminal-Product Wavefunctions for Treating Open-Shell and Dynamically-Correlated Systems

19(a) **Matthew Schmidt**, N. Faruk, K. Bishop, D. Iouchtchenko, and Pierre-Nicholas Roy
(University of Waterloo)
Methodological Advances in Low (and Zero) Temperature Path Integral Molecular Dynamics

19(b) **Michael Schuurman**, and Simon Neville (University of Ottawa)
(National Research Council of Canada)
Time-Resolved Core Spectroscopies as Probes of Nonadiabatic Dynamics

20(a) **Yujun Shi**, G. T. Huo, J. Y. Yuan, and Y. J. Shi
(University of Calgary)
Study of decomposition of BTBAS on a heated W or Ta metal surface

20(b) **Phillip Thomas**, and Tucker Carrington, Jr.
(Queen's University)
Using iterative tensor methods to compute vibrational spectra of molecules with more than 10 atoms

21(a) **Jonathan Vermette**, Pierre-Alexandre Turgeon, Patrick Ayotte, Gil Alexandrowicz, and Xavier Michaut
(Université de Sherbrooke)
Study of H_2O magnetic nuclear spin conversion and its separation from Stern-Gerlach like experiment in molecular beam

21(b) **Stephen Walker**, B. Verbuyst, A. Mark, J. L Campbell (SCIEX) B. Bogdanov, and W.S. Hopkins.
(University of Waterloo)
Inverstigating Tautomers of Anilinium with Differential Ion Mobility Spectrometry

22(a) **Alicia Welden**, Alexander A. Rusakov, and Dominika Zgid
(University of Michigan)
Temperature Dependent Thermodynamics from a Second-Order Green's Function

22(b) **Blair Winograd**, Dominika Zgid, and Emanuel Gull
(University of Michigan)
A Stochastic Implementation of the Second-order Green's Function

23(a) **Robert Wodraszka**, and Tucker Carrington Jr.
(Queen's University)
Using a systematically expanding nondirect product basis in conjunction with the multi-configuration time-dependent Hartree (MCTDH) approach

23(b) **Jason (Wenyuan) Huang**, Javix Thomas, Wolfgang Jaeger, and Yunjie Xu
(University of Alberta)
Rotational Spectrum of the 2-Fluoroethanol—Water Complex: Water Tunneling Dynamics and Structure

24(a) **Xiaowei Wu**, John Saunders, Sogol Borjian, Hao Chen, Cathleen M. Crudden, and Hans-Peter Loock
(Queen's University)
Trace Dihydrogen Phosphate Sensing Using Silicon-on-Insulator Ring Resonators

24(b) **Javix Thomas,** Michael J. Carrillo (University of Texas Rio Grande Valley), Agapito Serrato III (University of Texas Rio Grande Valley), Wei Lin (University of Texas Rio Grande Valley), Wolfgang Jäger, and Yunjie Xu
(University of Alberta)
Rotational Spectroscopic and Theoretical Studies of the Perfluorobutyric acid—Formic Acid Complex

25(a) **Xiaotian Yang**, and Paul W. Ayers
(McMaster University)
Two Types of Flat-Planes Conditions in Density Functional Theory

25(b) **Jingfei Yao**, Robert Le Roy, Marcel Nooijen, and W. Scott Hopkins
(University of Waterloo)
The Electronic Structure of Co^{+}•RG (RG = Ar, Kr): A Theoretical MR-EOM Study

26(a) **Tao Zeng**
(Carleton University)
A new diabatization protocol including spin-orbit coupling

26(b) **Qiuying Zhang**, Stephen Walker, Steve Innocente, and W. Scott Hopkins
(University of Waterloo)
Characterizing Humulone Content in Beer

27(a) **Ce Zhou**, Amy Yang, Mike Lecours, Stephen Walker, Rick A. Marta, Eric Fillion, Terry McMahon, and W. Scott Hopkins
(University of Waterloo)
Structures and Properties of Serine Clusters

27(b) **Alex Brown,** M. Alaraby Salem, and I. Twelves
(University of Alberta)
Fluorescent protein chromophores with large two-photon absorption

28(a) **Jeff Crouse**
(Queen's University)
Investigating Ice Photolysis Using Classical Molecular Dynamics Simulations

28(b) **Randy Dumont**
(McMaster University)
Modeling Molecular Electronic Devices - Molecular Rectifying and Light Emitting Diodes

29(a) **Denis J. Gendron**, and Roydon A. Fraser (University of Waterloo)
(Claire Lasers Corp.)
Exotic flames: Observation and correlation between spectral emission of flames in their wild natural habitat and in captivity

29(b) **Gabriel Hanna**, and Farnaz Shakib
(University of Alberta)
Nonadiabatic Dynamics of Condensed Phase Proton-Coupled Electron Transfer Reactions

30(a) **Ilya Ryabinkin**, and Artur F. Izmaylov
(University of Toronto)
Collective electronic mode approach to non-adiabatic dynamics at metallic surfaces

30(b) **Thomas Halverson**, and Pierre-Nicholas Roy
(University of Waterloo)
Quantum dynamics calculations of coupled molecular rotor systems using adiabatic approximations

31(a) **James Keller**, Markus Schulz-Weiling, Hossein Sadeghi, and Edward Grant (Univ British Columbia)
(Kenyon College)
Mapping the evolution of Rydberg gas to plasma via selective field ionization

31(b) **Taewon Kim**, Michael Richer, Kumru A. Dikmenli, and Paul W. Ayers
(McMaster University)
Generalized Multideterminant Wavefunction Structure

32(a) **Dmitri Iouchtchenko**, and Pierre-Nicholas Roy
(University of Waterloo)
Estimating ground state entanglement entropy using path integral molecular dynamics

32(b) **Yulia Kalugina**, Francois Lique (University of Le Havre), and Jacek Klos (University of Maryland)
(University of Waterloo)
Inelastic scattering of CN radical with para- and ortho-H_2

33(a) **Aly Hassan**, Ariel Petruk, and German Sciaini
(University of Waterloo)
Accessories for electron microscopy: cryo-holders

Notes

SUPPLEMENTARY INFORMATION

- **Poster Preservation**
  In past years, posters left up after the poster session have sometimes 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**:
  Airways Transit: 519-886-2121 https://secure.airwaystransit.com
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  United Taxi: 519-888-0400
  City Cab: 519-747-7777

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

Name	*Affiliation*	*Title of Presentation*
2015		
R.J.D. Miller	Max Planck	Mapping Atomic Motions with Ultrabright Electrons: The Chemists' Gedanken Experiment Enters the Lab Frame
R. Jockush	U. Toronto	Combined Mass Spectrometry and Fluorescence Studies to Separate Intrinsic Behavior from Environmental Effects: from Fundamental Investigations of Fluorescent Probes to FRET for Gas-phase Protein Conformation
V. Molinero	U. Utah	Crystallization of water: a molecular perspective
G. Douberly	U. Georgia	Laser Spectroscopy of Reactive Intermediates in Superfluid Helium Droplets
A. Izmaylov	U. Toronto	Role of Topology in Chemical Dynamics Beyond Born-Oppenheimer Approximation
E. Johnson	Dalhousie U.	Properties of molecular crystals from density-functional theory
2014		
D. Ceperley	U. Illinois	Dense hydrogen: What we can calculate, Implications for density functionals, and Multi-scale approaches
D. Cory	U. Waterloo	Quantum Sensors and Computers
G. Lamoreux	Concordia U.	Molecular modeling of proton cotransport in proteins
A. Mullen	U. Maryland	Dynamics of Molecular Gyroscopes
A. Krylov	U.S.C.	A Fresh Look at Resonances: An Equation-of-Motion Coupled-Cluster Based Approach
L.-S. Wang	Brown. U.	Electrospray Photoelectron Spectroscopy: From Multiply Charged Anions to Ultracold Anions
2013		
M. Ashfold	U. Bristol	Molecular Photofragmentation Dynamics in the Gas and Liquid Phase: Parallels and Differences
N. Blinov	U. Alberta	Bridging the gap between Explicit and Implicit Solvation: Perspective of the Molecular Theory of Solvation
M. Ernzerhof	U. Montral	Kekul formulae, Hckel theory, and Dirac's Equation: Combining Various Concepts to better Understand Electron Transport in Conjugated systems
T. Fridgen	Memorial U.	Experimental and Computational Studies of Gas Phase Structures and Energetics of Non-Covalent Complexes of DNA Bases
K. Madison	U.B.C.	Production and Study of Ultra-Cold Molecules from Laser-Cooled Atoms: A New Regime for Ultracold Chemistry and Physics
W. Poirier	Texas Tech. U.	Ten Thousand Quantum States of Acetonitrile
2012		
D. Manolopoulos	U. Oxford	Ring Polymer Molecular Dynamics – A Review of 6 Years Work Including a Wide Variety of Applications
M. Dantus	Michigan State U.	Coherent Control Principles and Applications Based on Shaped Ultrafast Pulses
G. Hanna	U. Alberta	Multidimensional vibrational spectroscopy of mixed quantum-classical systems: From simple models to water
N. Moazzen-Ahmadi	U. Calgary	Weakly-Bound Molecular Complexes Formed from Three- and Four-Atom Linear molecules
P. Peterson	Cornell U.	Ultrafast Dynamics at Soft Interfaces
V. Staroverov	U. Western Ontario	Recent advances in the theory and application of model Kohn-Sham potentials

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
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

Name	*Affiliation*	*Title of Presentation*
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'
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

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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
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

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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
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

Name	*Affiliation*	*Title of Presentation*
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
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

Name	*Affiliation*	*Title of Presentation*
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
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