The 34th Annual

Symposium

On

Chemical Physics

at the

University of Waterloo

November 2-4, 2018

Acknowledgements

We are very grateful to the following sponsors
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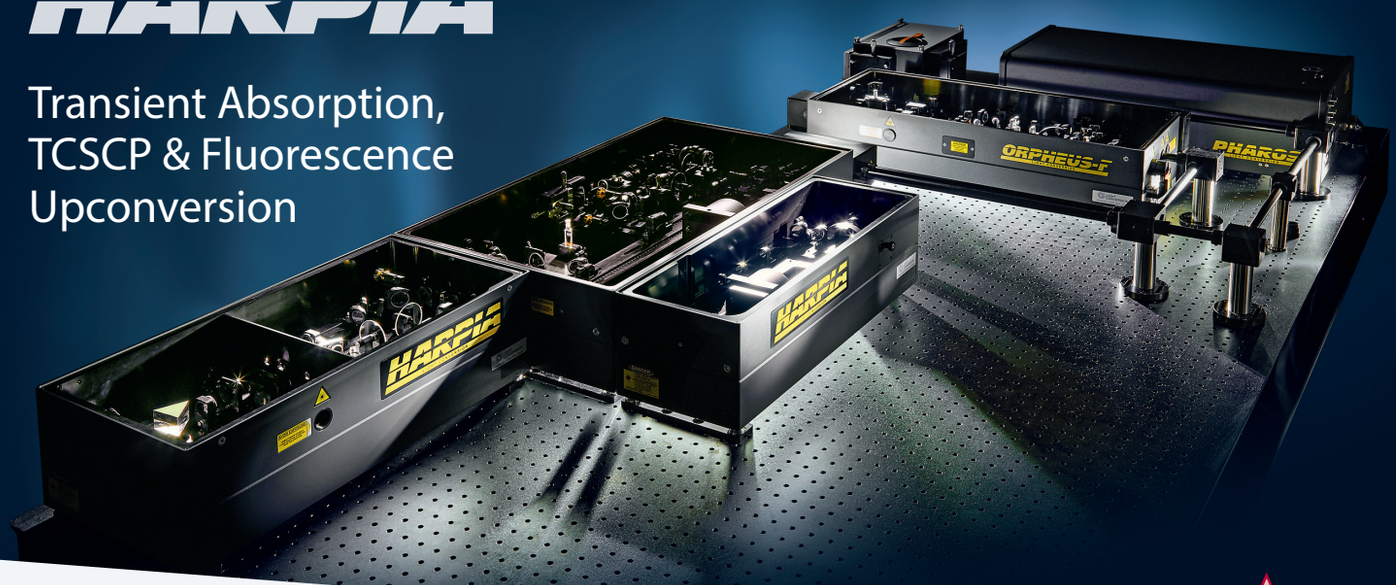

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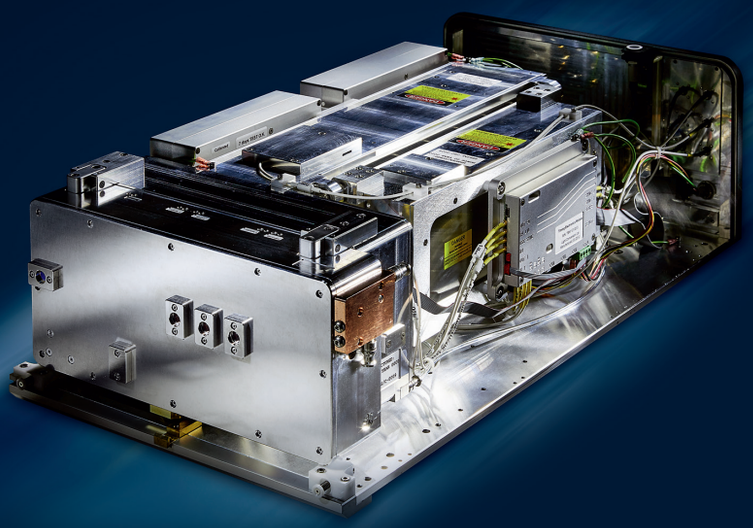

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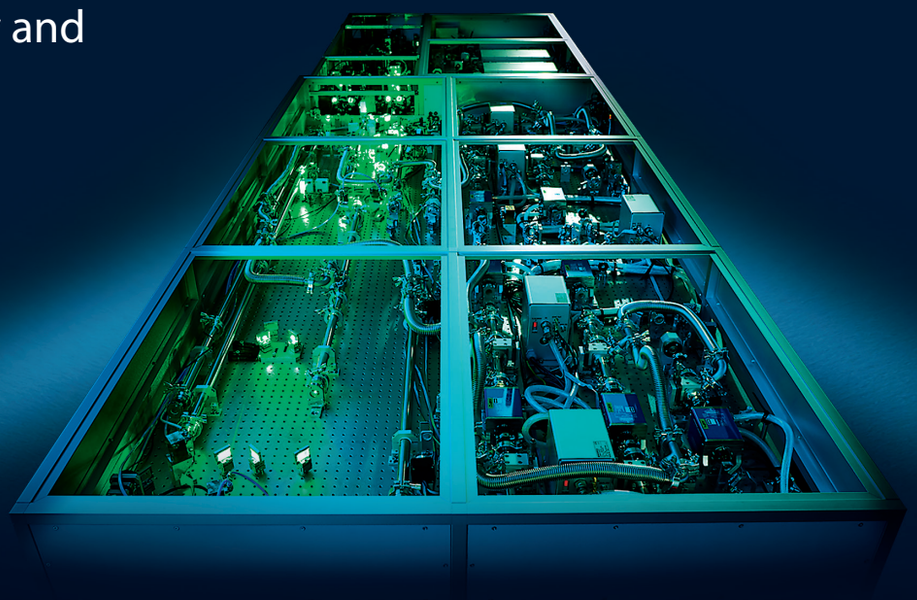

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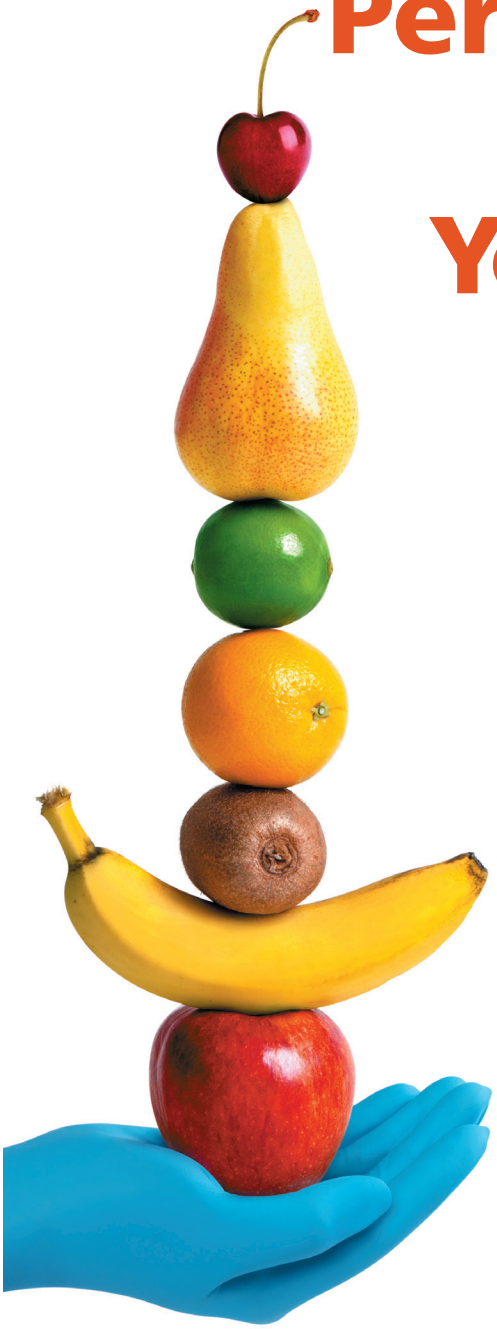

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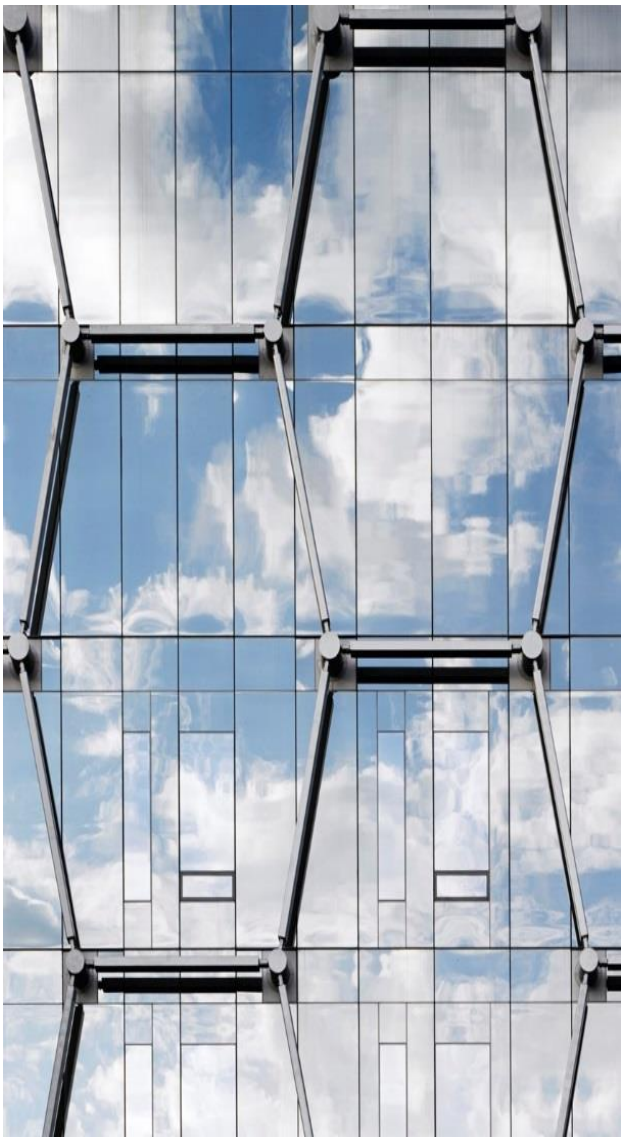

Photo: Quantum-Nano Centre modeled after hexagonal structure of graphene

THEME RESEARCH AREAS

93 faculty researchers

20 research chairs

500 nanotechnology undergraduate and 180 graduate students

UW Recognized excellence as Canada's most innovative university for 25 years *-Maclean's Magazine*

WIN has the largest number of researchers & infrastructure in Canada for nanoscience & nanotechnology

9 DEPARTMENTS

Engineering
- **Chemical**
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Mathematics
- **Applied Mathematics**

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WATERLOO INSTITUTE FOR NANOTECHNOLOGY

nanofellowships

The Waterloo Institute for Nanotechnology Nanofellowships are awarded to top graduate students pursuing nanotechnology research at the University of Waterloo.

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nano.uwaterloo.ca/nanofellowships

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Assistant Director, Research Programs
Waterloo Institute for Nanotechnology

UNIVERSITY OF WATERLOO

WATERLOO INSTITUTE FOR nanotechnology

Symposium on Chemical Physics
at the University of Waterloo
November 2-4, 2018

REGISTRATION begins at 6:30 p.m. EIT Foyer

SESSION I: Friday, November 2, 2018 — P.M. EIT-1015
Chair: **Marcel Nooijen**

7:30 – 8:15 **Paul Zimmerman**
(University of Michigan)
Breaking Up Scaling Limits with the Many-Body Expansion

8:15 – 8:30 Christian Imperiale, Philippe Green, Niels H. Damrauer (Colorado Boulder) and Mark W. B. Wilson
(University of Toronto)
Enabling low-threshold photon upconversion using electronically decoupled acene dimers

8:30 – 8:45 Ilya Ryabinkin, Scott N. Genin and Artur F. Izmaylov (Toronto)
(OTI Lumionics Inc.)
Qubit coupled clusters: A systematic approach to quantum chemistry on a quantum computer

8:45 – 9:00 John E. Saunders, Mark Panas, William Knee-Walden, Alexander Fogal, Noah Cassidy, Young-Min Cho, Pierre Fogal, Jennifer Murphy, Wolfgang Jaeger (Alberta) and Kaley Walker.
(University of Toronto)
The Canadian Atmospheric Laser Absorption Spectrometer Experiment Test-bed (CALASET) Stratospheric Balloon Campaign: Timmins, ON, 2018

9:00 – 11:59 **WELCOME RECEPTION – Grad House (GH)**. *Check your badge, there should be a drink ticket for Friday at Grad House (GH). Please note that there should be also a second drink ticket for Saturday to be used during the poster session or during our banquet at Federation Hall (FED) cash bar.*

There is a map of UW campus on the last page of the program; everything is within walking distance (look for EIT, GH, and FED).

SESSION II: Saturday, November 3, 2018 – A.M. EIT-1015
Chair: **Pierre-Nicholas Roy**

9:00 – 9:45 **François Lagugné-Labarthet**
(University of Western Ontario)
Infrared Plasmonics with Fractal Metastructures

9:45 – 10:00 Jesse Simmons, Xiaogang Wang and Tucker Carrington
(Queen's University)
Comparing Experimental Results with Rovibrational Levels of CH_3^+ Isotopologues Computed with a Lanczos Eigensolver

10:00 – 10:15 Weslley G. Dias de Paiva Silva and Jennifer van Wijngaarden
(University of Manitoba)
Rotational spectroscopic and theoretical investigation of the conformational preferences of methyl-3-mercaptopropionate

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, 2018 – A.M. EIT-1015
Chair: **Scott Hopkins**

10:45 – 11:45 ***The Roger E. Miller Lecture***: **Tucker Carrington Jr.**
(Queen's University)
Solving the Schrödinger equation without the variational method: no integrals

11:45 – 12:00 Matthias Heger, Joseph Cheramy, Wolfgang Jaeger, Yunjie Xu
(University of Alberta)
The SCORPION: A New Instrument for Hot and Cold Ion Spectroscopy

12:00 – 12:15 Jaroslav Zamastil
(Charles University)
Multi-dimensional WKB approximation for particle tunneling

12:15 – 1:30 **LUNCH** – EIT Foyer

SESSION IV: Saturday, November 3, 2018 – P.M. EIT-1015
Chair: **Fred McCourt**

1:30 – 2:30 ***The Robert J. Le Roy Lecture:*** **Peter Bernath**
(Old Dominion University)
Molecular Opacities and Other Applications of Bob LeRoy's Theoretical Spectroscopy

2:30 – 2:45 Hui Li, Yu Zhai and Robert J. Le Roy (Waterloo)
(Jilin University)
Constructing sub-spectroscopic accuracy intermolecular potential energy surface with multi-dimension Morse Long-Range model

2:45 – 3:30 Anne McCoy
(University of Washington)
Spectral Signatures of Large Amplitude Motions in Protonated Water Clusters and Other Charged Systems

3:30 – 6:00 **REFRESHMENTS AND POSTER SESSION** EIT Upstairs Foyer

The Roger E. Miller Lecture is 60 min. including 10 min for discussion.
The Robert J. Le Roy 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, 2018 from 3:25 P.M. EIT Upstairs Foyer
POSTER SESSION
Chair: **Marcel Nooijen**

6:00 P.M. **POSTER SESSION ENDS**
Depart for Large Conference Room, ***Federation Hall*** **(FED)**; *check your maps!*

6:30 P.M. **CASH BAR:** Large Conference Room, ***Federation Hall*** **(FED)**

7:00 P.M. **DINNER:** Large Conference Room, ***Federation Hall*** **(FED)**

9:00 P.M. **AFTERHOURS:** Our band plays at ***Federation Hall*** **(FED)** *... Informal Discussion. Check your badge, there should be a drink for Saturday to be used during the poster session or during our banquet at Federation Hall (FED) cash bar.*

SESSION VI: Sunday, November 4, 2018– A.M. EIT 1015

Chair: **Pierre-Nicholas Roy**

9:15– 10:00 Julia Laskin
(Purdue University)
Rational Design of Solid Interfaces Using Soft-landing of Mass-Selected Ions

10:00 – 10:15 James Brown and James D. Whitfield
(Dartmouth College)
The Wilson basis applied to electronic structure

10:15 – 10:30 Jonas Warneke
(Purdue University)
Boron based electrophilic anions

10:30 – 11:00 **COFFEE BREAK**

SESSION VII: Sunday, November 4, 2018– A.M. EIT 1015
Chair: **Germán Sciaini**

11:00 – 11:45 Pat Kambhampati
(McGill University)
Surface Science on the Nanoscale and Optical Analogs of 2D-NMR

11:45 – 12:00 Nike Dattani, Zhedong Li (Caltech), Junhao Li (Cornell), Cyrus Umrigar (Cornell), Garnet Chan (Caltech)
(National Research Council)
Computer Spectroscopy with Classical and Quantum Computers

12:00 – 12:15 James Keller and E.R. Grant (British Columbia)
(Kenyon College)
Molecular ultracold plasma: evolution from a Rydberg gas and arrested relaxation

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 3, 2018 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, Jacob Dore, Colan Linton, Dennis Tokaryk
(University of New Brunswick)
High resolution visible spectroscopy of ruthenium monoboride

1(b) Cody Aldaz
(University of Michigan)
High-Fidelity Computational Screening of Arene-Alkene Photochemistry

2(a) Fernanda B.V. Martins, J.S. Keller and E.R. Grant (UBC)
(Kenyon College)
Ultracold Plasma Dynamics in a Radio Frequency Field

2(b) Songhao Bao and Marcel Nooijen
(University of Waterloo)
Develop Periodic Localized Orbitals (PLOs) for Solid State Systems

3(a) Mahdi Beedel, Md. Anisur Rahman, J. P. Thomas, Nina F. Heinig and K. T. Leung
(University of Waterloo)
VLS Growth of Single Crystalline HfO_2 Nanowires Using Pulse laser Deposition

3(b) Adam Bernicky and Travis Ferguson
(Queen's University)
Hadamard-Transform Fluorescence Excitation-Emission-Matrix Spectroscopy

4(a) Zack Bowman, Jeff Crouse, Adam Scenna, Christian Ieritano, Josh Featherstone, J. Larry Campbell (SCIEX), and W. Scott Hopkins
(University of Waterloo)
Machine Learning Collision Cross Sections using Differential Mobility Spectrometry

4(b) Patrick Carr, Jonas Warneke (Purdue), Josh Featherstone, Carsten Jenne (Bergische Universitat Wuppertal), Estelle Loire (CLIO), and W. Scott Hopkins
(University of Waterloo)
The Structures of Proton-bound Triethylammonium $[B_{12}X_{12}]^{2-}$ (X = F, Cl) Clusters

5(a) Eduardo Castro-Juarez, Tucker Carrington Jr., Xiao-gang Wang and Richard Dawes
(Missouri S&T)
(Queen's University)
Computational Study of the Rovibrational Spectra of CO-CO_2

5(b) Jean-Claude Chartrand
(Université de Sherbrooke)
Water-endofullerene Nano-laboratory: A New Way to Study the Nuclear Spin Conversion of H_2O.

6(a) Meixin Cheng, Nicolas Rivas, Eric Haugen, Steven Ngo, Kostyantyn Pichugin and German Sciaini
(University of Waterloo)
Femtosecond transient absorption spectroscopy at UeIL

6(b) Michael Coates and Michael Schuurman
(University of Ottawa/NRC)
VUV excited state dynamics of cyclopropane: time-resolved photoelectron spectroscopy and ab initio dynamics

7(a) Jeff Crouse, Steve Walker, Ahdia Anwar, Jarrod Psutka, J. Larry Campbell (SCIEX), and W. Scott Hopkins
(University of Waterloo)
Determining Molecular Properties using Machine Learning and Differential Mobility Spectrometry

7(b) Hanieh Farkhondeh, F. R. Rahsepar, L. Zhang and K. T. Leung
(University of Waterloo)
Step Edges of Si(111)-v3×v3-Ag, a Combined STM and DFT study

8(a) Travis Ferguson, A. R. Bernicky, N. L. P. Andrews, A. M. M. Rangaswamy, N. Henning, A. Dudelzak (GasTOPS Ltd), O. Reich (Potsdam), J. A. Barnes, and H.-P. Loock
(Queen's University)
Hadamard-Transform Fluorescence Excitation-Emission-Matrix Spectroscopy

8(b) Alexandre Fleury and Yves L. Dory
(Université de Sherbrooke)
Dimerisation of delta and mu opioid receptors

9(a) Weiqiang Fu, Patrick Carr, Mike Lecours, Michael Burt, Eric Fillion, Estelle Loire (CLIO), Terry McMahon, and W. Scott Hopkins.
(University of Waterloo)
The Structures and Properties of the Homodimers of Protonated Phenylalanine Derivatives

9(b) Patrick Gicala, Nicolas Rivas, Ariel Alcides Petruk, Kostyantyn Pichugin and German Sciaini
(University of Waterloo)
Final steps in the Development of the 300 kV Femtosecond Electron Diffractometer at UeIL

10(a) Xiaoyi (Frank) Guan, Joseph Thomas, Saurabh Srivastava, Jung-Soo Kang and Anisur Rahman and K. T. Leung
(University of Waterloo)
Defect-rich Size-Selected ZrO_2 Nanoclusters with Diluted Magnetic Semiconductor Properties

10(b) Emily Groper, Hans-Peter Loock, and Kyle Bachus
(Queen's University)
Development of Photo-Enhanced Electrospray Emitters for Nano-ESI Mass Spectrometry

11(a) Minhal Hasham
(University of Toronto)
Two-Colour Fluorescence Intermittency Spectroscopy

11(b) Christian Ieritano, Jeff Crouse, J. Larry Campbell (SCIEX), and W. Scott Hopkins
(University of Waterloo)
A parallelized molecular collision cross section package with optimized accuracy and efficiency for trajectory method calculations

12(a) Paul Johnson
(Université Laval)
Open-Shell Geminal Wavefunctions

12(b) Sangeeth Das Kallullathil, and Tucker Carrington Jr.
(Queen's University)
Calculation of vibrational spectra of molecules using approximate fekete points

13(a) Su Ji Lim, J. Larry Campbell (SCIEX), and W. Scott Hopkins.
(University of Waterloo)
Investigations of $B_{12}X_{12}$ (X=H, F, Cl, Br, I) Using Differential Mobility Spectrometry

13(b) Tyler Lott, Nicolas Rivas, Kostyantyn Pichugin, and German Sciaini
(University of Waterloo)
Ultrafast Dynamical Studies on Molecular Systems

14(a) Xichen Lou
(University of Waterloo)
Path Integral Methods Development

14(b) Ariel Petruk, Christine Johnston, and German Sciaini
(University of Waterloo)
Nanofluidics for electron microscopy and femtosecond electron diffraction measurements in liquids

15(a) Michael Lecours, Mark Zanon, Songhao Bao, W. Scott Hopkins, and Marcel Nooijen
(University of Waterloo)
Compact Regularized AO Integrals for Molecules and Solids

15(b) Ryan J. MacDonell, K. Veyrinas (Bordeaux), R. Forbes (University College London), M. A. Larsen (Copenhagen), V. Makhija, A. Boguslavskiy, and M. S. Schuurman (NRC) and Albert Stolow (NRC)
(University of Ottawa)
Time-resolved photoelectron spectroscopy of cis-stilbene: Theory and experiment

16(a) Amy MacLean, Annica Freytag, Mahtab Abtahi, Jack Barnes, and Hans-Peter Loock
(Queen's University)
All-optical measurements of viscosity and density using a vibrating cantilever

16(b) Nour Mashmoushi, J. Larry Campbell (SCIEX), and W. Scott Hopkins
(University of Waterloo)
Characterizing Lipid Isomers Using Differential Mobility Spectrometry

17(a) Yujun Shi, I. Badran, L. Tong, S. Mulmi and Y. J. Shi
(University of Calgary)
Characterization of thin film deposits on W and Ta filaments in Catalytic CVD using four-membered-ring organosilicon molecules

17(b) Francis Temme
(Queen's University)
Democratic -recoupling-defined "indistinguishable point-sets": a reduced-Littlewood view of "set-theoretic" S_n invariant modelling

18(a) B. G. Guislain, R. A. R. Harvey, Dennis W. Tokaryk and A. G. Adam, Amanda J. Ross and Patrick Crozet (Université Lyon)
(University of New Brunswick)
Giving a BOMEM DA3 interferometer a new lease of life: spectra of laser-excited NiD taken in dispersed fluorescence

18(b) Olamide P. Sogeke, Wenhao Sun, Weslley G. D. P. Silva and Jennifer van Wijngaarden
(University of Manitoba)
The conformational landscape of allyl isocyanate

19(a) Fiorella Villanueva Heldmaier, Qiuying Zhang, Cailum Stienstra, J. Larry Campbell (SCIEX), and W. Scott Hopkins
(University of Waterloo)
Differential Mobility Spectrometry Studies of Hop Extracts

19(b) Clément Wespiser, Pierre-Alexandre Turgeon, Jonathan Vermette, Yulia Kalugina (Waterloo), Pierre-Nicholas Roy (Waterloo), and Patrick Ayotte
(Université de Sherbrooke)
Confinement Effects on Water's Nuclear Spin Isomer Conversion

20(a) Tokio Yukiya, Shinji Kobayashi, Kanta Mikawa, Nobuo Nishimiya and Masao Suzuki
(Tokyo Polytechnic University)
Wavenumber measurement for the wide tuning range in the near infrared region by using the spectral atlas of the A-X band system of IBr

20(b) Mark Zanon and Marcel Nooijen
(University of Waterloo)
Regularised Coulomb Interactions for Efficient Computation of the Electronic Hamiltonian

21(a) Emil Zak and Tucker Carrington Jr.
(Queen's University)
A hierarchical discrete variable representation-like method for solving the vibrational Schroedinger equation

21(b) Simon Neville and Michael Schuurman (NRC)
(University of Ottawa)
Chebyshev-Slepian Filter Diagonalisation: An Efficient Route to Calculating X-Ray Absorption Spectra

22(a) Issaka Seidu, Simon Neville, Michael Schuurman (NRC)
(University of Ottawa)
DFT/MRCI for Core Spectroscopies

22(b) Nathan A. Seifert, Arsh Hazrah, Issac J. Miller (James Madison), Paul L. Raston (James Madison), and Wolfgang Jaeger
(University of Alberta)
Probing Solvation of Asymmetric Rotors with Helium Atoms Using Broadband Rotational Spectroscopy

23(a) Robert Wodraszka and Tucker Carrington Jr.
(Queen's University)
A pruned, collocation-based multi-configuration time-dependent Hartree approach using nondirect product bases and Smolyak grids to efficiently solve the Schroedinger equation with general potential energy functions

23(b) Francis Lajoie-Leroux, Jonathan Vermette, Isabelle Braud, Pierre-Alexandre Turgeon and Patrick Ayotte
(Université de Sherbrooke)
Study of heterogeneous nuclear spin conversion with ortho-H_2O supersonic beam

24(a) Ce Zhou, Estelle Loire (CLIO), Terry McMahon, Eric Fillion, and W. Scott Hopkins
(University of Waterloo)
Mapping Complex Potential Energy Landscapes

24(b) Neville Coughlan, Michael Lecours, J. Larry Campbell, and W. Scott Hopkins
(University of Waterloo)
Modifier gases in DMS show preferential solvation behaviour

25(a) Arsh Hazrah, Nathan A. Seifert, and Wolfgang Jaeger
(University of Alberta)
Intermolecular Interplay within 1-Naphthol Dimers Studied using Broadband Rotational Spectroscopy

25(b) Charles-Émile Fecteau
(Université Laval)
Projected quartet wavefunction ansatz for strong electron correlation

26(a) Fan Xie, Nathan A. Seifert, Xiaoqian Ng, Javix Thomas, Matthias Heger, Wolfgang Jäger, Yunjie Xu
(University of Alberta)
The complicated conformational landscapes of tetrahydro-2-furoic acid in its monomer, dimer, and monohydrate: broadband rotational spectra and comprehensive conformational searches

26(b) Angelo S. Perera, Joseph Cheramy, Yunjie Xu
(University of Alberta)
Vibrational Optical Activity Spectra of Methyl-β-D-glucopyranose in Water: The Application of the Clusters-in-a-Liquid Solvation and GFN-xTB Models

27(a) Yanqing Yang, Joseph Cheramy, Fan Xie, Yunjie Xu
(University of Alberta)
Vibrational optical activity studies of conformers and non-covalent interactions of tetrahydro-2-furoic acid in liquid and in aqueous solution.

27(b) Reynolds Dziobek-Garrett
(University of Toronto)
Quantum Dot Layer Thickness in Upconversion Devices

28(a) Adam Pejic
(Queen's University)
Flow-through plasmonic sensing based on Polymer-coated nanohole arrays

28(b) Philippe Green
(University of Toronto)
TBA

29(a) Olivia Fandiño, S. Sasidharanpillai, D.V.Soldatov and P. R. Tremaine
(University of Guelph)
Proof of the Stability of 2-Methylpiperidine-N-Carboxylate Ion by Raman Spectroscopy and X-Ray Diffraction

29(b) Hang Hu and Gilles H. Peslherbe
(Concordia University)
Electronic Structure and Properties of Zinc Oxide Crystals and Nanotubes

30 (a) Dmitri Iouchtchenko, Neil Raymond, Pierre-Nicholas Roy, Marcel Nooijen
(University of Waterloo)
Ground state energy and entanglement entropy of vibronic models using path integral Monte Carlo

30 (b) Dmitri Iouchtchenko, Neil Raymond, Pierre-Nicholas Roy, Marcel Nooijen
(University of Waterloo)
Thermodynamic Properties of Nonadiabatic Systems using Gaussian mixture distributions

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.

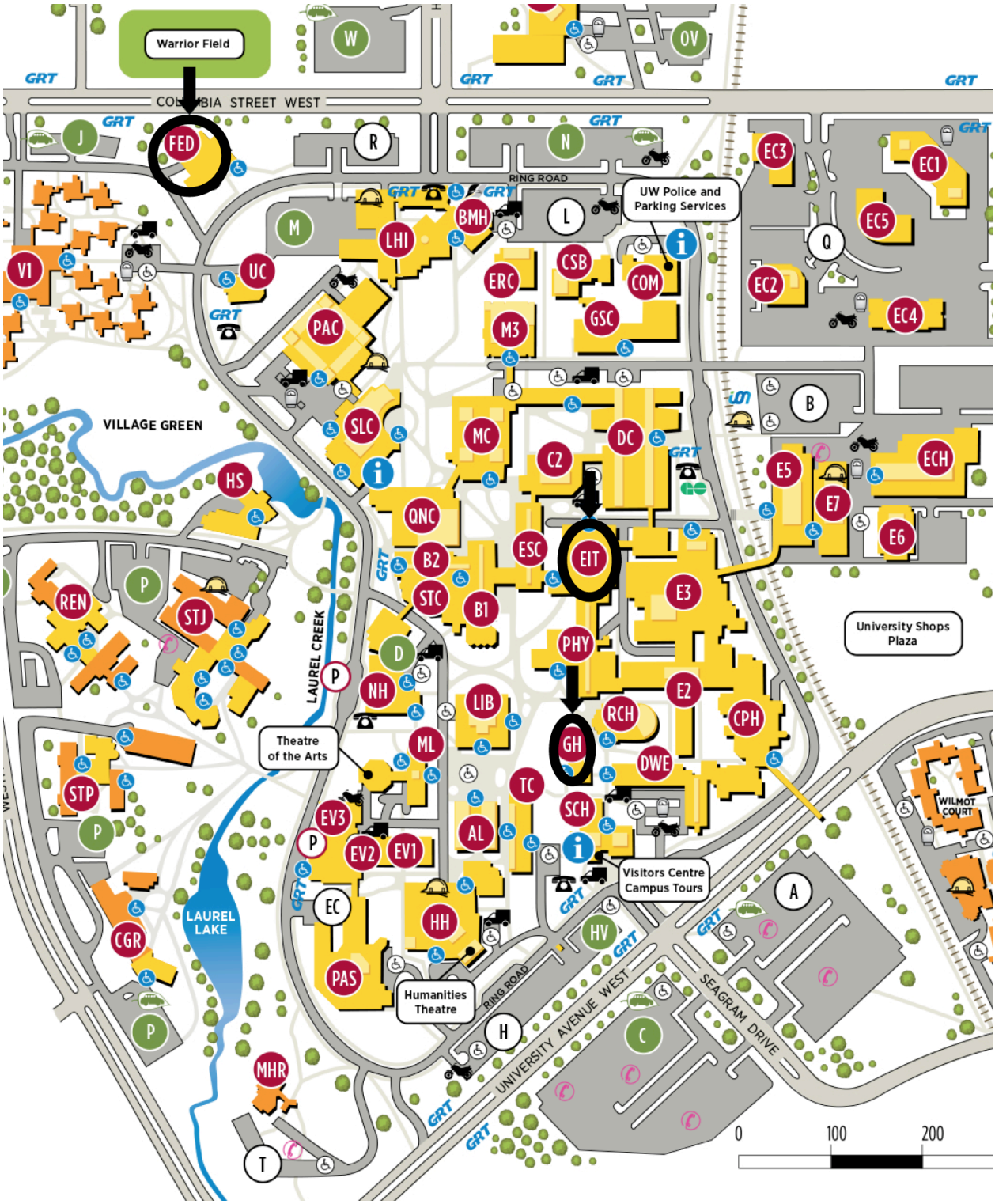
- **Recycling**
  Before leaving on Sunday, please drop you plastic name-tag holder into the cardboard box by the entrance to the Registration area. This will allow recycling and reduced our costs for next year.

- **Phone Numbers**:
  Airways Transit: 519-886-2121 https://secure.airwaystransit.com
  Waterloo Taxi: 519-886-1200
  United Taxi: 519-888-0400
  City Cab: 519-747-7777

Arrows indicate the most important locations for our symposium

EIT = Centre for Environmental and Information Technology. Here we host our conference.
FED = Federation Hall. Here we have our dinner on Saturday starting at 7 pm.
GH = Grad House. Here we have our mixer on Friday starting at 9 pm.

PARKING LOTS FOR VISITORS are marked with green letters and you should be able to pay with credit card. Parking lots M and N are the closest to EIT. Everything is within waking



distance.