The 35th Annual

Symposium

On

Chemical Physics

at the

University of Waterloo

In honour of Robert J. Le Roy

November 1-3, 2019

Acknowledgements

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

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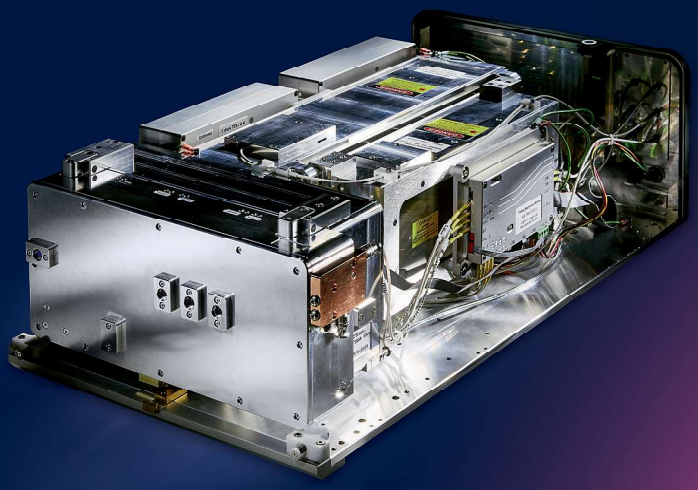

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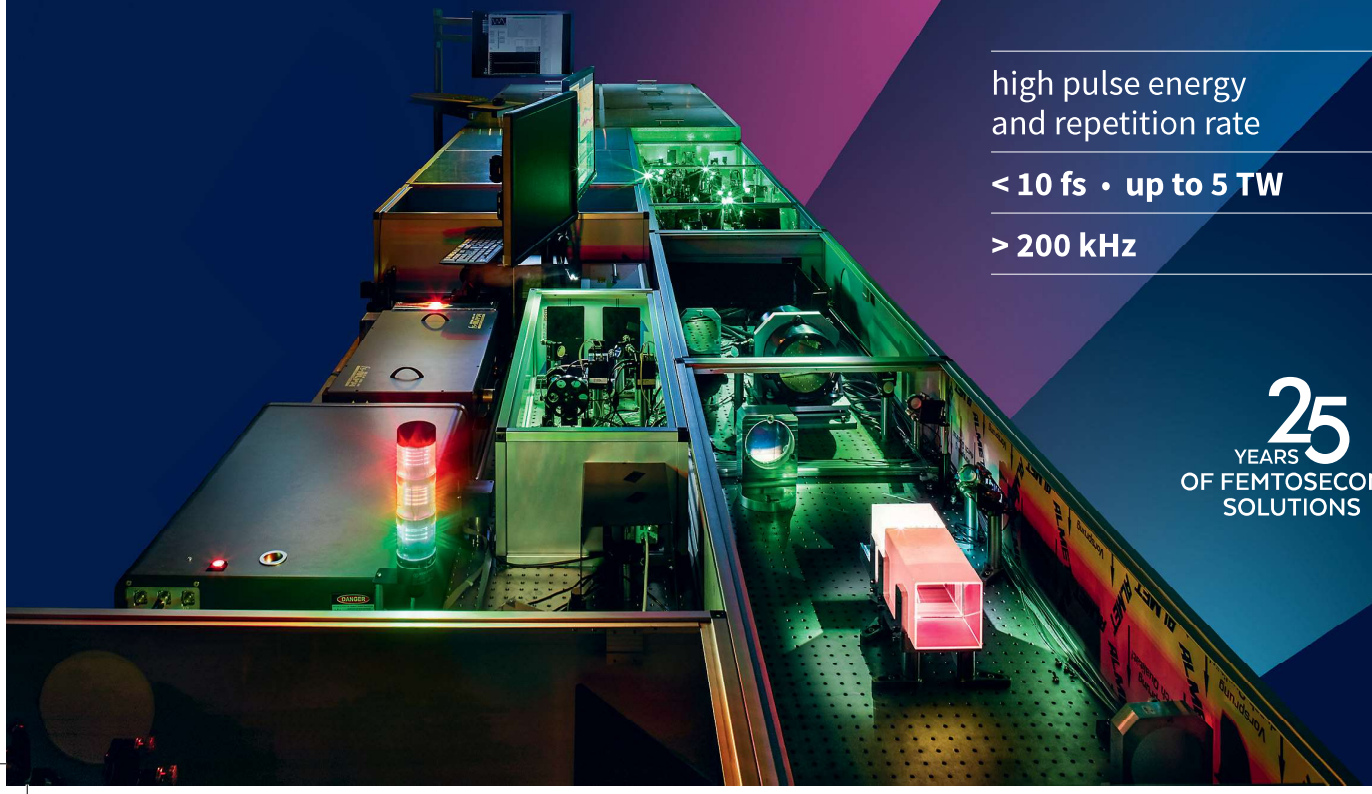

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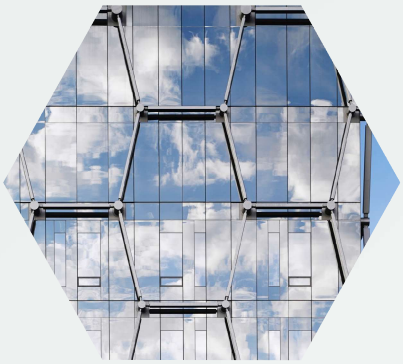

IN A NEW PLACE

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Symposium on Chemical Physics
at the University of Waterloo
November 1-3, 2019

IMPORTANT NOTE FOR SCP2019 TALK FORMATS

The **Roger E. Miller Lecture** is 60 min, including 15 min for discussion and introduction.
The **Robert J. Le Roy Lecture** this year is 75 min, including 15 min for discussion and introduction.
Invited talks are 45 min, including 5 min for discussion
Contributed talks are 15 min, including 3min for discussion

REGISTRATION begins at 6:00 P.M. EIT Foyer

SESSION I: Friday, November 1, 2019 – P.M. EIT-1015
Chair: **Marcel Nooijen**

7:30 – 8:15 **Toby Zeng**
(Carleton University)
Our recent studies in vibronic coupling: simulation of optoelectronic materials, derivation of Jahn-Teller formalisms, and interpretation of photoelectron spectrum

8:15 – 8:30 **Philippe B. Green,** P. Sohn, C. J. Imperiale, M. W. B. Wilson
(University of Toronto)
Cluster intermediates control the growth of PbS nanocrystals

8:30 – 8:45 **Alexander Haack,** F-J. Schlüter, T. Benter
(University of Wuppertal)
and J. Crouse, W. S. Hopkins
(University of Waterloo)
A first principles model of differential ion mobility: the effect of ion-solvent clustering

8:45 – 9:00 **Anja Röder,** R. J. MacDonell, A. B. Skov, A. E. Boguslavskiy, A. Stolow and M. S. Schuurman
(University of Ottawa)
Following the excited-state isomerization of 2,3-dihydrofuran to cyclopropanecarboxaldehyde

9:00 – 11:59 **WELCOME RECEPTION –** GradHouse (GH). *Check your badge, there should be a drink ticket* for the welcome reception. There is also a map of UW campus on the last page of the program; everything is within walking distance.*

***DRINK TICKETS:** You should find a total of **two drink tickets** in your badge. One drink ticket is for the **WELCOME RECEPTION (Friday night – GradHouse)** and another drink ticket is for the **REFRESHMENTS AND POSTER SESSION (Saturday evening – EIT Upstairs Foyer).**

SESSION II: Saturday, November 2, 2019 – A.M. EIT-1015
Chair: **Pierre-Nicholas Roy**

9:00 – 9:45 **Amanda Ross**
(Université Claude Bernard Lyon 1)
Laser-induced fluorescence measurements to feed dParFit and dPotFit

9:45 – 10:00 **Randall Dumont**
(McMaster University)
Dirac Tunneling: Superluminal velocities and Closed Time-like Curves?

10:00 – 10:15 **Fariha Mahmood,** A. D. Hudson, M. R. Ponte, T. P. Ventura, A. Narvali, K. Saravanamuttu
(McMaster University)
A Soft Polymer Cuboid that Computes with Binary Strings of White Light

10:15 – 10:45 **COFFEE BREAK**

SESSION III: Saturday, November 2, 2019 – A.M. EIT-1015
Chair: **Scott Hopkins**

10:45 – 11:45 ***The Roger E. Miller Lecture***: **Jeremy Hutson**
(Durham University)
Controlling ultracold molecules with magnetic and laser fields

11:45 – 12:00 **Ronald Lees,** C. Beaman, L-H. Xu
(University of New Brunswick)
and B. E. Billinghurst
(Canadian Light Source)
FTIR Synchrotron Spectroscopy of CD_3SH - the Vanishing C-S Stretch

12:00 – 12:15 **Saber Naserifar,** W. A. Goddard III
(California Institute of Technology)
New Description of 'Mysterious' Water and Phenomena Underlying Supercooled Critical Point

12:15 – 1:30 **LUNCH** – EIT Foyer

SESSION IV: Saturday, November 2, 2019 – P.M. EIT-1015
Chair: **Germán Sciaini**

1:30 – 2:45 ***The Robert J. Le Roy Lecture:*** **Donna Strickland**
(University of Waterloo)
From nonlinear optics to high-intensity laser physics

2:45 – 3:00 **Joel Tellinghuisen**
(Vanderbilt University)
Reminiscences, and New Directions for a Spectroscopic Data Analyst

3:00 – 3:15 **Guojie Li,** J. Cheramy, Y. Xu
(University of Alberta)
Plasmons in the few-atom limit: chirality transfer and amplification in resonant Raman optical activity

3:15 – 3:30 **Fedor Naumkin**
(Ontario Tech)
Dipole-inside-dipole supramolecular complexes - very polar, very bright

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

***DRINK TICKETS:** You should have **one drink ticket** left in your badge for the **REFRESHMENTS AND POSTER SESSION (EIT Upstairs Foyer).**

SESSION V: Saturday, November 2, 2019 from 3:30 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)**

SESSION VI: Sunday, November 3, 2019 – A.M. EIT 1015

Chair: **Pierre-Nicholas Roy**

9:15 – 10:00 Philip Bunker
(National Research Council Canada)
The Planck constant and its units

10:00 – 10:15 **Dennis Tokaryk,** N. Caron, B. G. Guislain, R. A. R. Harvey, A. G. Adam, C. Linton
(University of New Brunswick)
Laser excitation and dispersed fluorescence spectroscopy of MgS

10:15 – 10:30 **Robert Lang,** A. F. Izmaylov
(University of Toronto)
Towards cost-efficient quantum computing algorithms for quantum chemistry

10:30 – 11:00 **COFFEE BREAK**

SESSION VII: Sunday, November 3, 2019 – A.M. EIT 1015
Chair: **Scott Hopkins**

11:00 – 11:45 Terry McMahon
(University of Waterloo)
Novel binding modes in gas phase ion molecule complexes

11:45 – 12:00 **Robert Izsak**
(Max Planck Institute – KOFO)
Domain-based pair natural orbitals for excited states using the similarity transformed equation of motion formalism

12:00 – 12:15 **Robert Wodraszka,** T. Carrington Jr.
(Queen's University)
A collocation-based multi-configuration time-dependent Hartree approach using mode combination and improved relaxation to calculate accurate vibrational spectra of complex molecular systems

12:15 – 1:30 Light **LUNCH & COFFEE –** EIT Foyer

POSTER SESSION: Saturday, November 2, 2019 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) Ilvie Havalyova, A. Pashov, A. Adam, D. Tokaryk, P. Crozet and A. J. Ross.
(Université Claude Bernard Lyon 1)
Electronic structure of low-lying states of NiD and NiH

1(b) Eduardo Castro-Juarez, X-G. Wang, T. Carrington Jr., (Queen's University)
Ernesto Quintas-Sánchez, Richard Dawes.
(Missouri University of Science and Technology)
Using theory to understand the ro-vibrational spectrum of CO–CO_2

2(a) Tzu-ChingYen, R. Lang, A. Izmaylov
(University of Toronto)
Vladyslav Verteletskyi
(Taras Shevchenko National University of Kyiv)
Addressing the measurement problem in Variational Quantum Eigensolver

2(b) Kathryn Benincasa, H. Lin, A. D. Hudson, I. D. Hosein, K. Saravanamuttu
(McMaster University)
Bio-inspired waveguide encoded lattices (WELS): from slim polymer films with wide fields of view to dynamic lenses

3(a) Hang Hu, G. H. Peslherbe
(Concordia University)
Quantum chemical simulation of thermal-mechanical coupling in high pressure and temperature materials synthesis

3(b) Cailum M. Stienstra, N. Coughlan, J. Crouse, P. Carr, W. S. Hopkins
(University of Waterloo)
Preliminary velocity map imaging experiments for the photodissociation of Xenon dimer

4(b) Gary Douberly
(University of Georgia)
Infrared spectra of alkyl radicals in Helium droplets

5(a) Christian Ieritano, J. Featherstone, W. S. Hopkins,
(University of Waterloo)
J. L. Campbell
(SCIEX)
How hot are your ions in Differential Mobility Spectrometry?

5(b) Dmitri Iouchtchenko, K. Bishop, P-N. Roy
(University of Waterloo)
Constrained path integral Langevin equation integrators

6(a) Feng Li, E. Khairullina, X. Medvedeva, A. Klinkova
(University of Waterloo)
Structural stability of nanostructured cathode materials for CO_2 electroreduction

6(b) Yuting Li, N. Coughlan, C. Zhou, W. Scott Hopkins
(University of Waterloo)
J. L. Campbell
(SCIEX)
Photodissociation and electronic spectroscopy of DMS-selected amino acids

7(a) Ignacio Loaiza, A. Izmaylov, P. Brumer
(University of Toronto)
Radiationless transitions induced by natural incoherent light

7(b) Stephanie Schaertel, G. C. McBane, T Schultz
(Grand Valley State University)
Toward predictive chemical kinetics: pressure broadening of spectral lines in carbon monoxide

8(a) Ted Schultz, S. Schaertel, G. McBane
(Grand Valley State University)
Pressure broadening in the 3←0 band of carbon monoxide

8(b) Florian Stappert, D. Erdogdu, W. Wißdorf, H. Kersten, T. Benter
(University of Wuppertal)
Maria Allers, Ansgar T. Kirk, Stefan Zimmermann
(Leibniz University Hannover)
Investigations on the field dependency of cluster dynamics using High Kinetic Energy IMS (HiKE-IMS)

9(a) Kun Wang, Tao Zeng
(York University)
Hamiltonian formalism of spin–orbit Jahn–Teller and pseudo-Jahn–Teller problems in trigonal and tetragonal symmetries

9(b) Allan Adam, R. A. R. Harvey, D. W. Tokaryk
(University of New Brunswick)
Observation of several transitions involving the g6F state of FeD using laser spectroscopy

10(a) Alex Brown, M. Mondrusova, M. Rossano-Tapia
(University of Alberta)
Evaluation of multi photon absorption properties in canonical and non-canonical amino acid-based fluorescent protein chromophores

10(b) Jeffrey Crouse, W. S. Hopkins,
(University of Waterloo)
Alexander Haack, Thorsten Benter
(University of Wuppertal)
Understanding non-traditional differential mobility behavior: a case study of the tricarbastannatrane cation, $N(CH_2CH_2CH_2)_3Sn^+$

11(a) Mike Lecours, M. Zanon, Q. Sun, M. Nooijen
(University of Waterloo)
Fast and compact Coulomb Integrals using short-range real-space and long-range Fourier representations

11(b) Neville Coughlan, P. J. J. Carr, S. C. Walker, C. Zhou, W. S. Hopkins,
(University of Waterloo)
M. Guna, J. L. Campbell
(SCIEX)
Electronic spectra of mobility-selected ions in the gas phase

12(a) Mark Zanon, M. Lecours, M. Nooijen
(University of Waterloo)
Benchmark study of regularized coulomb interactions and an extension on the cluster-in-molecule method

12(b) Fiorella Villanueva, N. Coughlan, W. S. Hopkins,
(University of Waterloo)
J. L. Campbell
(SCIEX)
Exploring the UV-PD action spectra of cationic adenine protomers

13(a) Weiqiang Fu, C. Zhou, P. Carr, M. Lecours, M. Burt, E. Fillion, E. Loire, T. McMahon, W. S. Hopkins
(University of Waterloo)
The structures of homodimers of phenylalanine derivatives

13(b) Nour Mashmoushi, W. S. Hopkins,
(University of Waterloo)
J. L. Campbell
(SCIEX)
Characterizing PFOS Solvent Interactions using Differential Mobility Spectrometry

14(a) Jennifer van Wijngaarden, K. Bergmann
(University of Manitoba)
Microwave spectroscopic and ab initio study of 2- and 3-fluoroanisole

14(b) Mohamed Aboelnga, S. W. Wetmore
(University of Lethbridge)
Unveiling a single-metal-mediated phosphodiester bond cleavage mechanism for nucleic acids

15(a) Tyler Lott, A. A. Petruk, X. Medvedeva, A. Klinkova, T. Prozorov, G. Sciaini
(University of Waterloo)
Liquid Cell Electron Microscopy of Nanomaterials and Biospecimens

15(b) Meixin Cheng, N. Rivas, S. J Lim, K. Pichugin, A. A. Petruk, A. Klinkova, R. D. L. Smith, W. S. Hopkins, G. Sciaini
(University of Waterloo)
Trapping a photoelectron behind a repulsive coulomb barrier in solution

16(a) Patrick Gicala, N. Rivas, S. Zhong, T. Dekker, A. A. Petruk, M. Cheng, F. Chen, X. Luo, Y. Sun, K. Pichugin, A. Tsen, G. Sciaini.
(University of Waterloo)
Generation and detection of acoustic waves in ultrathin 1T'-$MoTe_2$ flakes

16(b) Fabian Thiemann, M. Cheng, T. Lott, P. Gicala, E. Kjell, S. Oliphant, N. Rivas, A. A. Petruk, K. Pichugin, G. Sciaini
(University of Waterloo)
Femtosecond spectroscopic and structural techniques at the Ultrafast electron Imaging Lab

17(a) William Adams,
(McMaster University)
Rob Paton
(Colorado State University)
Automated and Accessible Computational Chemistry Benchmarking

17(b) Christian Imperiale, M. W. B. Wilson
(University of Toronto)
Kinetic simulations of triplet-fusion: evidence of quintet exciton pair dynamics in a tetracene dimer

18(a) Adam Marr, T. Halverson, A. Tripp, P-N. Roy
(University of Waterloo)
Prediction of Raman vibrational shifts for Hydrogen spin isomers and isotopologues

18(b) Neil Raymond, D. Iouchtchenko, P-N. Roy, M. Nooijen
(University of Waterloo)
Free energies of nonadiabatic systems using MCTDH and PIGS

19(a) Samuel Cloutier, P. Johnson, C-É. Fecteau
(Université Laval)
Strong correlation: Two projected quartet-inspired methods to resolve Schrödinger's equation.

19(b) Charles-Émile Fecteau, P. Johnson, L. Carrier, S. Cloutier, F. Berthiaume, M. Gratton, (Université Laval)
Patrick Bultinck, Dimitri Van Neck,
(Ghent University)
S. de Baerdemacker
(University of New Brunswick)
Variational mean-field treatment of strong correlation with Richardson-Gaudin wavefunctions

20(a) Laurie Carrier, C-É. Fecteau, P. A. Johnson
(Université Laval)
Treatment of Hartree-Fock with Bethe Ansatz

20(b) Matthias Heger, J. Cheramy, W. Jäger, Y. Xu
(University of Alberta)
How to train your SCORPION: Progress of the IRMPD-HENDI Instrument

21(a) Arsh Hazrah, W. Jäger
(University of Alberta)
Broadband rotational spectroscopy of α-pinene and its photooxidation product pinonic acid

21(b) Mohamad Al-Jabiri, W. Jäger
(University of Alberta)
Structural analysis of vanillic acid using broadband microwave spectroscopy

22(a) Edward Goudreau, E. S. Goudreau, A. Stolow, A. Roder, A. Boguslavskiy, D. Moffatt, V. Makhija, R. Lausten
(University of Ottawa)
Progress toward 3D velocity map imaging

22(b) Songhao Bao, S. Bao, M. Nooijen
(University of Waterloo)
Numerically exact results for (up to) quadratic non-adiabatic vibronic Hamiltonians from a time-dependent coupled cluster approach

23(a) Steven Gravelsins, A-A. Dhirani
(University of Toronto)
A rapid method for size-selective precipitation of Au nanoparticles in organic solvents

23(b) Zahra Alinia, M. Tafazzoli
(Concordia University)
Dynamic NMR study of thiobencarb (S-4-chlorobenzyl N,N-diethylcarbamothioate)

24(a) Takamasa Momose, M. Vashishta, K. Enomoto, P. Djuricanin, T. Momose
(University of British Columbia)
AC Stark shift of NH_3 in strong MW fields

24(b) Sangeeth Das Kallullathil, T. Carrington Jr.
(Queen's University)
Calculation of vibrational energy levels of molecules using a tensor method that avoids storing large matrices or vectors

25(a) Ritu Arora, V. Parmar, G. H. Peslherbe, A. M. English
(Concordia University)
Structure of the death complex between glyceraldehyde-3-phosphate dehydrogenase and seven-in-absentia homolog 1 (GAPDH-Siah1)

25(b) Philippe Archambault, H. M. Muchall, G. H. Peslherbe
(Concordia University)
Electronic structure analysis on the effects of purine Hoogsteen edge hydration on sugar edge H-bonding

26(a) Alexander Ibrahim, L. Wang, T. Halverson, R. J. Le Roy, P-N. Roy
(University of Waterloo)
Equation of state and vibrational matrix shift of solid parahydrogen

26(b) Joshua Featherstone, T. McMahon
(University of Waterloo)
Solving a problem of cluster geometries using systematic solvation

27(a) Leanne Chen
(University of Guelph)
Atomic-Scale Computational Insight into Electrochemical Reactions: from Mechanistic Understanding to Materials Engineering

27(b) Jesse Simmons, X. Wang, T. Carrington Jr.
(Queen's University)
Computational study of the ro-vibrational spectra of CH_2D^+ and CHD_2^+ using a Lanczos method

28(a) Nazli Jodaeeasl, R. Majidi
(Concordia University)
Molecular dynamics simulation of noble gases adsorption on homogeneous and heterogeneous carbon nanotube bundles

28(b) Tapas Sahoo, D. Iouchtchenko, C. M. Herdman, P-N. Roy
(University of Waterloo)
Estimation of ground state entanglement entropy for continuous rotational degrees of freedom: a path integral replica trick approach

29(a) Bae-Yeun Ha
(University of Waterloo)
A soft mater approach to bacterial chromosome organization

29(b) Denis J. Gendron
(Claire Lasers Corporation)
Reinventing the crude oil refinery for global leadership in cleantech.

30(a) Xichen Lou, P-N. Roy
(University of Waterloo)
Path integral simulation of water chain and new algorithm

30(b) Spencer Yim, P-N. Roy
(University of Waterloo)
Thermodynamic properties of $H_2O@C_{60}$ via exact diagonalization

31(a) Xiaolong Zhang, P-N. Roy,
(University of Waterloo)
H. Li
(Jilin University)
Path integral Monte Carlo simulations of confined molecules

31(b) Jianying Sheng, J. G. Rau, S. Yim, M. Nooijen, P-N. Roy, M. J. P. Gingras
(University of Waterloo)
Symmetry breaking effects in endofullerenes: anisotropic interactions versus cage distortions

32(a) Adeniyi Olajide, Soran Jahangiri, Gilles H. Peslherbe
(Concordia University; Centre for Research in Molecular Modeling and Department of Chemistry and Biochemistry)
First-Principles Simulations of Environmentally-Relevant Halides and Oxyhalides Hydration

32(b) Paul Johnson, Marianne Gratton
(Université Laval)
Stijn De Baerdemacker
(University of New Brunswick)
Open-Shell Geminal Wavefunctions

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 your 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.

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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 walking distance.