

The 38th Annual

Symposium on

Chemical Physics

at the

University of Waterloo

November 8-10, 2024

Acknowledgements

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

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Symposium on Chemical Physics
at the University of Waterloo
November 8-10, 2024

IMPORTANT NOTE FOR SCP 2024 TALK FORMATS

The **Roger E. Miller Lecture** is 60 min, including 10-15 min for discussion and introduction.
The **Robert J. Le Roy Lecture** is 60 min, including 10-15 min for discussion and introduction.
Invited talks are 45 min, including 5-10 min for discussion
Contributed talks are 15 min, including 3 min for discussion

IMPORTANT: Talks listed below as T# are oral presentations delivered by students/postdocs, who participate in the Canadian Journal of Chemistry award. Use these codes when selecting the best two oral presentations at the end of the symposium.

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

SESSION I: Friday, November 8, 2024 – P.M. EIT-1015
Chair: **Christian Ieritano**

- 7:30 – 8:15** **Mark Wilson**
(University of Toronto)
Advancing solid-state triplet-fusion upconversion
- 8:15 – 8:30 **(T1) Shreyas Malpathak, S. Das Kallullathil, and A. F. Izmaylov**
(University of Toronto)
Simulating Anharmonic Vibrational Dynamics using Continuous Variable Quantum Computing
- 8:30 – 8:45 **(T2) Alexandre De Camargo** and R. A. Vargas-Hernandez
(McMaster University)
Leveraging Normalizing Flows for Orbital-Free Density Functional Theory
- 8:45 – 9:00 **(T3) Christian Viernes,¹ S. Netzke,¹ R. Zheng,¹ D. Sutarma,² P. Kratzer,² K. Pichugin,¹ and G. Sciaini¹**
(¹University of Waterloo, ²Universität Duisburg-Essen)
Monitoring Ultrafast Structural Dynamics in NbTe₂ by Femtosecond Electron Diffraction
- 9:00 – 11:30** **WELCOME RECEPTION – Grad-House (GH in map).** *Check your badge, there is one drink ticket*. 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 – GH) and another drink ticket is for the Refreshments & Poster Session (Saturday evening – EIT Upstairs Foyer).

SESSION II:
Chair: **Conrard Tetsassi**

Saturday, November 9, 2024 – A.M.

EIT-1015

9:00 – 9:45 Farnaz Heidar-Zadeh
(Queen's University)

Dipole Constrained Additive Variational Hirshfeld Partitioning Method

9:45 – 10:00 **(T4) Christian Ieritano**, M. Abaeva, A. Haack, D. Schipper, and W. S. Hopkins
(University of Waterloo)
Symmetry (in)action: How protonation can induce pseudochirality within achiral molecules

10:00 – 10:15 **(T5) Luca Corneo**, and T. Carrington
(Queen's University)
An Algorithm to Compute Vibrational Spectra That Obviates Integrals but Uses a Symmetric-Matrix Eigensolver

10:15 – 10:45 **COFFEE BREAK**

SESSION III:
Chair: **W. Scott Hopkins**

Saturday, November 9, 2024 – A.M.

EIT-1015

10:45 – 11:45 The Plenary Roger E. Miller Lecturer: Vicki H. Wysocki
(Ohio State University)

Electrons and/or a surface: characterization of capsids, glycoproteins, and nucleoproteins

11:45 – 12:00 **(T6) Smik Patel**,¹ A. S. Brahmachari,² J. T. Cantin,¹ L. Wang,¹ and A. F. Izmaylov¹
(¹University of Toronto, ²Indian Institute of Science Education and Research)
Block Invariant Symmetry Shift: Reducing molecular Hamiltonian 1-norm via linear programming

12:00 – 12:15 **(T7) Gabriela Sanchez-Diaz**, P. W. Ayers, and D. Salahub
(University of Calgary)
Correlation energy from extended random phase approximations

12:15 – 1:30 **LUNCH** – EIT Foyer

SESSION IV: Saturday, November 9, 2024 – P.M.
Chair: **Pierre-Nicholas Roy**

EIT-1015

- 1:30 – 2:30 The Robert J. Le Roy Plenary: Victor Batista**
(Yale University)
Simulating Chemistry on Bosonic Quantum Devices
- 2:30 – 2:45 **(T8) Muna Abdulaziz,¹ K. Pichugin,² G. Sciaini,² and Liliana Trevani¹**
(¹Ontario Tech University, ²University of Waterloo)
Numerical Modelling and Experimental Validation of a New Channel Flow Cell for High Temperature Electrochemistry
- 2:45 – 3:00 **(T9) Tomislav Begusic,** and Garnet Kin-Lic Chan
(California Institute of Technology)
Operator Time Evolution via Sparse Pauli Dynamics
- 3:00 – 3:15 **(T10) Fanwang Meng,^{1,2,3} J. Huang,² V. Chuiko,² G. Melacini,² P. W. Ayers², F. Heidar-Zadeh,¹**
(¹Queen's University, ²McMaster University, ³Massachusetts Institute of Technology)
Predicting Protein Allostery with Incomplete NMR Data
- 3:15 – 3:30 **Tao (Toby) Zeng,¹ and G. Yao²**
(¹York University, ²Sun-Yat Sen University)
A computational tool for analyzing excitons in solids
- 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 9, 2024, from 3:30 P.M. EIT Upstairs Foyer
POSTER SESSION
Chair: **Pierre-Nicholas Roy**

- 6:00 P.M. **POSTER SESSION ENDS**
Depart for Main Hall, *Federation Hall (FED)*; *check your maps!*
- 6:30 P.M. **CASH BAR:** Main Hall, *Federation Hall (FED)*
- 7:00 P.M. **DINNER:** Main Hall, *Federation Hall (FED)*

SESSION VI:

Sunday, November 10, 2024 – A.M.

EIT 1015

Chair: **W. Scott Hopkins****9:30 – 10:15 Brenda Rubenstein**

(Brown University)

*Modeling Biology on a Quantum Computer*10:15 – 10:30 **Wolfgang Jäger,² A. S. Hazrah,¹ C. D. Carlson,² M. H. Al-Jabiri,³ Y. Xu²**⁽¹Max Planck Institute for Polymer Research, ²University of Alberta, ³University of Toronto)*Conformers of the α -Pinene - Water Complex and their Atmospheric Impacts*10:15 – 10:30 **(T11) Shuoyang Wang, M. Martinez Gonzalez, P. W. Ayers**

(McMaster University)

*Quadratically Convergent Self-Consistent Field (QC-SCF) Orbital Optimization*10:30 – 11:00 **COFFEE BREAK****SESSION VII:**

Sunday, November 10, 2024 – A.M.

EIT 1015

Chair: **Conrard Tetsassi**11:00 – 11:15 **Ryan MacDonell, Jong-Kwon Ha, and E. Leal-Sánchez**

(Dalhousie University)

*Quantum Computing Approaches for Photochemistry Without The Born-Oppenheimer Approximation*11:15 – 11:30 **(T12) Conrad Moore, and V. N. Staroverov**

(University of Western Ontario)

*Are Exact Exchange-Correlation Potentials Continuous at Atomic Nuclei in Molecules?*11:30 – 11:45 **(T13) Valerii Chuiko, and P. W. Ayers**

(McMaster University)

*Leveraging Unitary Invariance of the Wavefunction for Energy Prediction in Strongly Correlated Systems*11:45 – 12:00 **(T14) Ruofei Zheng,¹ L. Daniel,² Y. Ding,³ O. Kharsah,² Y. Liebsch,² T.****Fabunmi,² G. Bacher,² A. Vescan,³ M. Schleberger², and G. Sciaini¹**⁽¹University of Waterloo, ²Universität Duisburg-Essen, ³RWTH Aachen University)*Defect-Induced Modulation of Ultrafast Exciton Decay Pathways in MOCVD Monolayer WS₂*12:00 – 1:30 Light **LUNCH & COFFEE** – EIT Foyer

POSTER SESSION:

Saturday, November 9, 2024 – P.M.

EIT Upstairs Foyer

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.

IMPORTANT: *The posters listed below are delivered by students/postdocs, who participate in the Robert Le Roy award.*

Please do not forget to evaluate and select the best two talks and the best two posters delivered by students or postdocs. Use the talk and poster codes for your selection. There is space on the back of your name badge to fill these in. Leave your badge in the collection box before leaving the conference.

+++++ POSTER PRESENTATIONS START HERE +++++

P1(a) Xander Gouws, and C. Tetsassi Feugmo

(University of Waterloo)

Improving the Speed of Reverse Monte Carlo with a New Measure for Goodness-of-Fit

P1(b) Shuotong Du, J. Ortlieb, V. Nalewajko, R. Woods, T. S. Lott, K. Pichugin, D.

Schipper, G. Sciaini

(University of Waterloo)

Microcrystal Electron Diffraction Studies in the Transmission Electron Microscope

P2(a) Agnes Katai, and C. Tetsassi Feugmo

(University of Waterloo)

Molten Salt Corrosion of High Entropy Alloys

P2(b) Robert Wodraszka, and T. Carrington

(Queen's University)

Calculating vibrational eigenpairs by relaxing wavefunctions using the CP format and variationally optimised basis functions

- P3(a) Xinning Wang**, and J. Baugh
(University of Waterloo)
Impact of Noise on a Variational Quantum Eigensolver Implemented with Spin Qubits
- P3(b) Georgii Sizov**, and V. N. Staroverov
(University of Western Ontario)
Reduced Density Matrices from Electron Densities within Finite Basis Sets
- P4(a) Han Nguyen**, and S. Constat
(University of Western Ontario)
Treatment of Electrostatic Interactions in Non-periodic Simulations with Application to Biological Macromolecules
- P4(b) Jacob Chausse**, and P-N. Roy
(University of Waterloo)
Observing the Quasiphase Transition of the Water-filled Carbon Nanotube with Quantum Simulations
- P5(a) Joy Andrianasolo**, T. S. Lott, A. A. Petruk, and G. Sciaini
(University of Waterloo)
A Joule-Thomson Refrigerated Specimen Holder for Cryo-Electron Microscopy
- P5(b) Tyler Lott**, N. A. Shaw, A. A. Petruk, T. Maksyuta, K. Pichugin, and G. Sciaini
(University of Waterloo)
High-Resolution Bio-Imaging via Liquid Phase-Electron Microscopy
- P6(a) Patrick Thomas**, and W. S. Hopkins
(University of Waterloo)
Prediction of Collision Cross Sections from Learned Conformer Ensembles
- P6(b) Michael McCarvell**,¹ N. King,² X. Liu,¹ and R. Smith¹
(¹University of Waterloo, ²University of Guelph)
Using Spinel to Determine the Components of XANES Spectra
- P7(a) Katherine Tschirhart**, and W. S. Hopkins
(University of Waterloo)
Comparing Novel Wastewater Disinfection Methods
- P7(b) Daniel Fernando Calero Osorio**, and P. W. Ayers
(McMaster University)
Canonical Transformation Zero with Seniority-Zero Reference
- P8(a) Jiayang Jiang**, S. Keramati, and R. J. D. Miller
(University of Toronto)
Ultrafast Electron Diffraction of Tungsten Disulfide Monolayer in a Compact Gun Chamber

- P8(b) Shayne Johnston, B. Paget, D. Quintal and L. Chen**
(University of Guelph)
Surface Doping Nickel Hydroxide to Improve Ammonia Oxidation Activity
- P9(a) Estevao de Oliveira, and P.-N. Roy**
(University of Waterloo)
Path Integral Quantum Monte Carlo? for a System of N Planar Rotors in Linear Chain
- P9(b) Linjun Wang, I. Loaizam, S. Patel, A. F. Izmaylov**
(University of Toronto)
Engineering Fermionic Hamiltonians with “Planted Solutions”
- P10(a) Justin Laroche,¹ T. Serwatka,² P.-N. Roy,² and P. Ayotte¹**
(¹Université de Sherbrooke, ²University of Waterloo)
Water inside C₆₀. How Extreme Confinement Affect Nuclear Spin Isomers Intersystem Crossing.
- P10(b) Alexander Ibrahim, and P.-N. Roy**
(University of Waterloo)
Path Integral Monte Carlo Simulations of Solid Parahydrogen Using Many-Body Interaction Potentials
- P11(a) Azharuddin Mohammed, and M. Nooijen**
(University of Waterloo)
Time Dependent Couple Cluster
- P11(b) Nithin Aaron, and P.-N. Roy**
(University of Waterloo)
Simulating Water Clusters using Path Integral Monte Carlo with Normal-Mode Sampling
- P12(a) Man Sze Cheng, S. P. Vadhyar, E. Nikbin, H. Grewal, Y. Suzuki, M. L. da Silva-Neto, and R. J. D. Miller**
(University of Toronto)
Development of Femtosecond Laser-Induced Crystallization for Serial Nano Electron Diffraction Studies
- P12(b) Shaer Moeed, S.Moeed, and P.-N. Roy**
(University of Waterloo)
Pair Approximating The PIMC Action For Molecular Rotations
- P13(a) Brendan Paget, Shayne Johnston, and L. Chen**
(University of Guelph)
Density Functional Theory Exploration of Ammonia Oxidation on a Nickel Oxide Surface

- P13(b) Lorena Veliz**, and F. Lagugné-Labarthe
(University of Western Ontario)
Elucidation of Extracellular Vesicles Profile Using MoS₂-Flakes Platforms in Combination with Advanced Raman Spectroscopy Techniques
- P14(a) Cédric Lambin**, and F. Lagugné-Labarthe
(University of Western Ontario)
Tuning of the Excitonic Response in Ultra-Fine Layer MoS₂ Flakes via Diazonium Salts Functionalization
- P14(b) Úna Hogan**, H. B. Voss, B. Lei, and R. Smith
(University of Waterloo)
Integrating C-H Information to Improve Machine Learning Classification Models for Microplastic Identification from Raman Spectra
- P15(a) Megan Dawson**, and P.-N. Roy
(University of Waterloo)
Analyzing the Conformational Properties of Furanosides with Path Integral Molecular Dynamics
- P15(b) Margaret Petrova**, and S. Constat
(University of Western Ontario)
Molecular Simulation of Sodium Chloride in Solvent
- P16(a) Miguel Albaladejo**, and M. W. B. Wilson
(University of Toronto)
Synthesis of PbS Quantum Dots for Photovoltaics with Air-Stable Sulfur Precursors
- P16(b) Samihat Rahman**, K. M. Yokuda, F. Y. Villanueva, and M. W. B. Wilson
(University of Toronto)
Exploring Carrier Transport in Quantum Dots to Achieve Sub-Solar, Solid-State Photon Upconversion
- P17(a) Ayan Amjad**, and H. Zaidi
(University of Toronto)
An Accurate Ground State Energy Calculation of the FeMo-cofactor in Nitrogenase Enzyme
- P17(b) Jasper Lincoln**, A. Benali, K. Gasperich, and B. Rubenstein
(Brown University)
Impact of Finite Cell Size and k-Point Sampling on Electron Correlation in Periodic Systems
- P18(a) Mike Lecours**, C. Boone, M. Schmidt, J. Steffen, N. Raymond, P. Bernath
(Atmospheric Chemistry Experiment)
Atmospheric Chemistry Experiment

P18(b) Sam Netzke,¹ C. Viernes,¹ W. He,¹ J. Jiang,² R. J. D. Miller,² B. Siwick,³ K. Pichugin,¹ and G. Sciaini¹
(¹University of Waterloo, ²University of Toronto, ³McGill University)
An Ultra-Compact and 100-keV Upgradable Femtosecond Electron Diffractometer

P19(a) Shashank Mehendale, and A. F. Izmaylov
(University of Toronto)
Suppressing Trotter Error with Partial Order Trotter

P19(b) Xiaoyue Liu, A. Schaefer, B. Siebeneichler, G. Del Mistro, E. M. Meiering
(University of Waterloo)
Proteolysis and Mass Spectrometry for Structural Characterization of Adnectin Inclusion Bodies

+++++ POSTER PRESENTATIONS END HERE +++++

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.

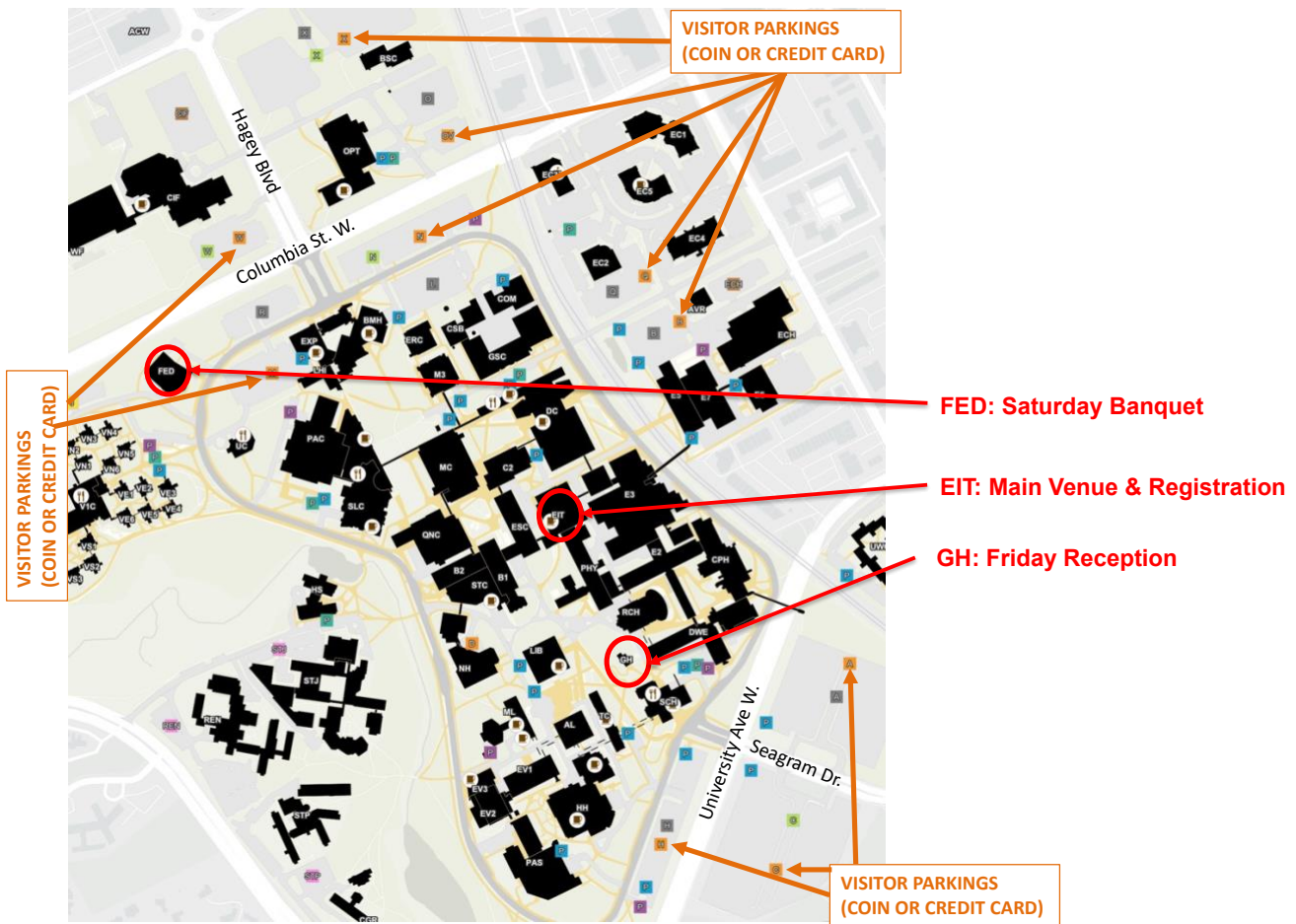
How to commute to and from Pearson Airport.

- **Phone Numbers and Websites:**

- **Waterloo Taxi: 519-747-7777** | <https://waterlootaxi.ca/>
- **United Taxi: 519-888-9999** | <https://unitedtaxi.ca/contact-us.html>

Please note that Waterloo Taxi and United Taxi offer flat rates to and from airport locations, which are usually the most convenient option! Reserve in advance online to receive detailed information about the pick-up location at Pearson.

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 Reception/Mixer on Friday starting at 9 pm.

PARKING LOTS FOR VISITORS are highlighted and you should be able to pay with credit card. Parking lots M and N are the closest to EIT. The cost per day is \$7 – \$9. Everything is within walking distance.