The 37th Annual

Symposium on

Chemical Physics

at the

University of Waterloo

November 3-5, 2023

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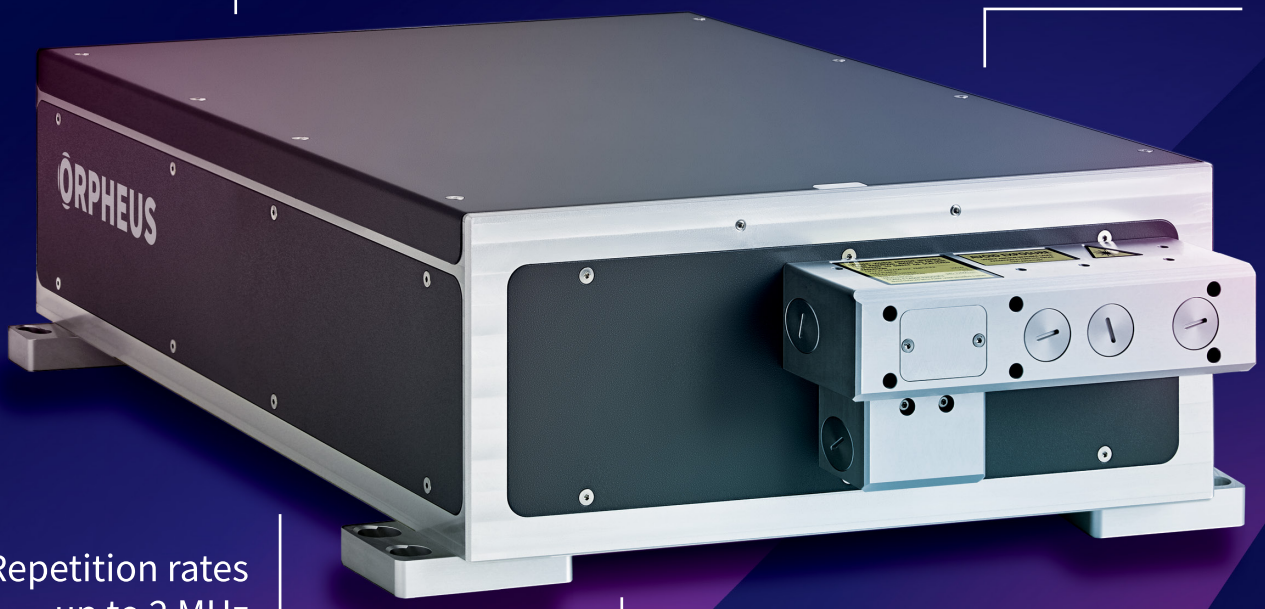

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Symposium on Chemical Physics
at the University of Waterloo
November 3-5, 2023

IMPORTANT NOTE FOR SCP 2023 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 as **T#** are oral presentations delivered by students/postdocs, who participate in the CJC 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 3, 2023 – P.M. EIT-1015
Chair: **Rodney Smith**

7:30 – 8:15 **Leanne D. Chen**
(University of Guelph)
Scaling Relations for the Electrocatalytic Ammonia Oxidation Reaction

8:15 – 8:30 (**T1**) **Christian Ieritano,** J. Bissonnette, A. Haack, Y. Le Blanc, B. Schneider, W. S. Hopkins
(University of Waterloo)
Protonation-Induced Chirality Drives Separation by Differential Mobility Spectrometry

8:30 – 8:45 (**T2**) **Songhao Bao,** N. Raymond, M. Nooijen
(University of Waterloo)
Direct Calculation of Time Dependent and Stat Mech Properties Applying Thermal Normal Ordering Exponential (TNOE) Ansatz and Thermal Field Dynamics

8:45 – 9:00 **(T3) Rees Hughes,** M. Hasham, M. W. B. Wilson
(University of Toronto)
Probing the Pervasive, Dynamic, Emissive Trap States in Individual Colloidal Quantum Dots

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: Saturday, November 4, 2023 – A.M. EIT-1015
Chair: **Conrard Tetsassi**

9:00 – 9:45 **Brian Clowers**
(Washington State University)
Manipulating Molecular Ion Trains: Selective Ion-Neutral Clustering, HDX, and Cryogenic IR Spectroscopy

9:45 – 10:00 **Stella Consta,** Victor Kwan
(Western University)
Direct Observation of the Rayleigh Jet Links the Chemistry Between Microscopic and Nanoscopic Charged Droplets Used in Ionization Methods Coupled to Mass Spectrometry

10:00 – 10:15 **Juan Carlos Castro-Palacio[1],** B. Khammar[1], O. Peña-Rodríguez[2], P. Fernández de Córdoba[1], J. A. Monsoriu[1]
([1]Universitat Politècnica de València, [2]Universidad Politécnica de Madrid)
(Invited) Shape Dynamics of Plasmonic Gold Nanoparticles Upon Ultrashort Laser Irradiation

10:15 – 10:45 **COFFEE BREAK**

SESSION III: Saturday, November 4, 2023 – A.M. EIT-1015
Chair: **Marcel Nooijen**

10:45 – 11:45 **Piotr Piecuch**
(Michigan State University)
Recent Progress in Externally Corrected Coupled-Cluster Methods: Following the Footsteps of a Legend
Lecture in Memory of Professor Josef Paldus

11:45 – 12:00 **(T4) Jiarui Ma[1],** A. Insausti[1,2], W. Jäger[1], Y. Xu[1]
([1]University of Alberta, [2]University of the Basque Country)
Gas Phase Detection of a Mutarotation Intermediate: A Rotational Spectroscopic Study

12:00 – 12:15 **(T5) Praveen Jayakumar,** S. Choi, A. Izmaylov
(University of Toronto)
Error Mitigation via Measurement Grouping: Making Noisy Quantum Computers to Do Some Quantum Chemistry

12:15 – 1:30 **LUNCH** – EIT Foyer

SESSION IV: Saturday, November 4, 2023 – P.M. EIT-1015
Chair: **W. Scott Hopkins**

1:30 – 2:30 **The Robert J. Le Roy Plenary: Pierre-Nicholas Roy**
(University of Waterloo)
Quantum Molecular Dynamics Simulations of Confined Molecules

2:30 – 2:45 **(T6) Martha Yaghoubi Jouybari,** S. P. Neville, M. S. Schuurman
(University of Ottawa)
The Effect of Vibronic Coupling on X-ray Absorption Spectra

2:45 – 3:00 **H. Floyd Davis,** Sagnik Datta
(Cornell University)
Casting Light on Alkylcarbene Formation and Unimolecular Reactions

3:00 – 3:15 **(T7) Shyam Parshotam,** W. Zhang, B. Rehl, A. Darlington, Md. D. Sikder, A. Brown, J. M. Gibbs
(University of Alberta)
Revealing Silica's pH-Dependent Second Harmonic Generation Response with Overcharging

3:15 – 3:30 **(T8) Guoying Yao,** L. Zhao, T. Zeng, Z. Yang
(York University, Sun-Yat Sen University)
0D/2D Mixed-Dimensional Perovskite Constructed by Thiol- and Disulfide-Containing Ligands

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 4, 2023 from 3:30 P.M. EIT Upstairs Foyer
POSTER SESSION
Chair: **W. Scott Hopkins**

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 5, 2023 – A.M. EIT 1015
Chair: **Marcel Nooijen**

This year our Sunday session (first talk) will start at 10:15 due to a talk cancellation.

10:15 – 10:30 **(T9) Nita Ghosh,** R. J. D. Miller
(University of Toronto)
Probing Spin-Vibronic Coherence Driven Intersystem Crossing in Pt(II) Dimer

10:30 – 11:00 **COFFEE BREAK**

SESSION VII: Sunday, November 5, 2023 – A.M. EIT 1015
Chair: **Germán Sciaini**

11:00 – 11:45 Daniel Kuroda
(Louisiana State University)
Unraveling the Complex Structure and Dynamics of Lithium Ions in Organic Solvents Using IR Spectroscopy

11:45 – 12:00 **(T8) Robert Wodraszka,** T. Carrington
(Queen's University)
Using More Points than Basis Functions When Using Collocation with MCTDH to Do Quantum Dynamics Calculations on a General PES

12:00 – 12:15 **Jianbo Gao**
(Brock University)
Ultrafast Carrier Dynamics in Emerging Perovskites

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

SESSION VIII: Sunday, November 5, 2023 – A.M. EIT 1015
Chair: **W. Scott Hopkins**

ADDITIONAL WORKSHOP ON THE FUTURE OF IR-FEL CAPABILITIES

Speakers:

(1:30 – 1:50) **W. Scott Hopkins**
(University of Waterloo)
Towards Establishing Free Electron Laser Technology in Canada

(1:50 – 2:10) **Takamasa Momose**
(University of British Columbia)
Application of THz/FIR light to basic science

(2:10 – 2:30) **Scott Rosendahl**
(The Canadian Light Source)
CLS Infrared Program - Current Status and Future Directions

(2:30 – 2:50) **Victor Verzilov**
(TRIUMF)
Prospects for an accelerator based THz photon source at TRIUMF

(2:50 – 3:10) **Germán Sciaini**
(University of Waterloo)
A Canadian Ultrafast Electron Diffraction Facility: Accessing Molecular Structure and Dynamics with Atomic Spatial & Temporal Resolutions

POSTER SESSION: Saturday, November 4, 2023 – 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: Most posters below are delivered by students/postdocs, who participate in the Robert Le Roy award. Those marked with ****** at the end of the list are delivered by faculty members who do not participate in this award. Use these codes when selecting the best poster from a uWaterloo-student/postdoc and the best poster from a non-uWaterloo-student/postdoc.

P1(a) **William Francis,** R. J. D. Miller
(University of Toronto)
Resonant Multiphoton Processes and Fluence Limits to Structural Dynamics

P1(b) **Muhammad Amjad,** R. Dumont
(McMaster University)
Understanding the Influence of Proton Tunnelling on Protein Dynamical Activity and Nucleic Acid Mutations

P2(a) **Conrad Moore,** V. N. Staroverov
(The University of Western Ontario)
Discontinuities in Density Functional Ingredients Constructed Using Slater-Type Orbitals

P2(b) **Jiayang Jiang,** M. Zhang, A. Gu, Z. Li, R. R. J. D. Miller
(University of Toronto)
Quantum Tomography of Electronic States of Molecules Using Ultrafast Electron Diffraction

P3(a) **Benny Chen[1],** T. Zeng[2], M. Nooijen[1]
([1]University of Waterloo, [2]York University)
Exploration of Vibronic Model Diabatization Protocols and VECC Approaches

P3(b) **Colton Carlson[1],** J. Ma[1], M. Al-Jabiri[1], A. Insausti[2], Y. Xu[1]
([1]University of Alberta, [2]University of the Basque Country)
Large Amplitude Motions in Ternary Aggregates of 1-Phenyl-2,2,2-Trifluroethanol with Two Water Molecules

P4(a) **Chen Liang,** F. Naumkin
(Ontario Tech University)
A MP2 Study of Counterion Trapped Norcaradiene and Cycloheptatriene

P4(b) **Miguel Lara,** T. Carrington
(Queen's University)
Inelastic Cross Sections: A Time-Dependent Wavepacket Approach

P5(a) **Jibrael Rolston,** M. Schuurman
(University of Ottawa)
Observing Charge Transfer Dynamics in Molecules: First Principles Simulation of Valence and Core Spectroscopies of DMABN and its Derivatives

P5(b) **Teagan Costain,** S. Neville, M. Schuurman
(University of Ottawa)
A purely ab initio DFT/MRCI Parameterization for the Determination of Core-Excited Electronic States

P6(a) **Ruofei Zheng[1],** A. A. Petruk[1], K. Pichugin[1], M. Fleischauer[2], D. Homeniuk[2], T. Lott[1], M. Salomons[2], G. Sciaini[1]
([1]University of Waterloo, [2]NRC)
Atomic-Resolution Hyperspectral Cathodoluminescence Imaging

P6(b) **Tyler Lott,** N. A. Shaw, A.A. Petruk, K. Pichugin, K. Barber-Ormerod, G. Sciaini
(University of Waterloo)
High-Resolution Bio-Imaging via Liquid Phase-Electron Microscopy

P7(a) **Stephen Tatarchuk[1],** A. J. MacKay[1], R. M. Choueiri[1], S. J. Johnston[1], W. M. Cooper[1], K. Snyder[1], J. J. Medvedev[2], A. Klinkova[2], L. D. Chen[1]
(University of Guelph, University of Waterloo)
Understanding the Bifurcation of Pathways toward N2 and NOx Formation in Urea Oxidation with a First-Principles Approach

P7(b) **Muna Abdulaziz[1], A. A. Petruk[2], G. Sciaini[2], L. Trevani[1]**
([1]Ontario Tech University, [2]University of Waterloo)
Novel High T,P Channel Flow Cell Design and Thin-Film Electrodes for Electrochemical Studies Under Hydrothermal Conditions

P8(a) **Ivan Bosko,** V. N. Staroverov
(The University of Western Ontario)
Exchange Functionals for Fermions of Arbitrary Spin

P8(b) **Georgii Sizov,** V. N. Staroverov
(The University of Western Ontario)
Faithful Reconstruction of Potentials from their Matrix Representations

P9(a) **Gwonhak Lee[1],** Artur Izmaylov[2]
([1]Sungkyunkwan University, [2]University of Toronto)
Reduction of Sampling Error in Quantum Krylov Subspace Diagonalization

P9(b) **Amir Hemmati,** A. Klinkova
(University of Waterloo)
The Modulation of Electrochemical Activity Inside the Nanoconfined Space

P10(a) Shuoyang Wang, G. Sanchez-Diaz, M. Martinez Gonzalez, P. W. Ayers
(McMaster University)
Gradient-based Mean-field Optimization Algorithm

P10(b) Brendan Laframboise, S. J. Johnston, R. M. Choueiri, X. Liu, S. W. Tatarchuk, L. D. Chen
(University of Guelph)
Ammonia Oxidation Thermodynamic Investigation on the M-doped ß-Ni(OH)$_2$ (M = Cr, Co, Cu, Fe) Surface using Density Functional Theory

P11(a) Jixi Zhang, R. Smith
(University of Waterloo)
Developing Reaction Models for Complex Solid State Phase Transitions

P11(b) Joaquin Carlos Chu, F. Y. Villanueva, M. W. B. Wilson
(University of Toronto)
Lead-Free Quaternary Ag_2ZnSnS_4 Quantum Dots

P12(a) Samihat Rahman, K-M. Yokuda, F. Y. Villanueva, M. W. B. Wilson
(University of Toronto)
Exploring Carrier Transport in Quantum Dots to Achieve Sub-Solar, Solid-State Photon Upconversion

P12(b) Adrien Bathellier, S.Chen, D. Schipper, C. Tetsassi Feugmo
(University of Waterloo)
Aqueous CO_2 Capture Through Electrochemical Mechanisms: A Bond Evolution Theory Perspective

P13(a) Tobias Serwatka, P-N. Roy
(University of Waterloo)
Quantum Phase Transitions in Confined Systems

P13(b) Han Ngo Gia Nguyen, V. Kwan, S. Constas
(University of Western Ontario)
Toward Computational Prediction of the Charge State Distribution of a Protein in ESI-MS Experiments

P14(a) Tzu Yu Wang, M. Schuurman
(University of Ottawa)
Machine Learning Seams of Conical Intersection: A Characteristic Polynomial Approach

P14(b) Aliaksandra Radchanka, X. Medvedeva, A. Klinkova
(University of Waterloo)
Exploring Ruthenium Nanoparticles Geometric Complexity to Boost Kellogg Advanced Ammonia Process Through Confinement Effect

P15(a) Soumyajit Mitra, R. J. D. Miller
(University of Toronto)
Elucidating the Reaction Kernel : Holy Grail of Chemical Reaction

P15(b) Sam Netzke[1], C. Viernes[1], A. A. Petruk[1], S. Early[1], J. Jiang[2], R. J. D.Miller[2], B. Siwick[3], K. Pichugin[1], G. Sciaini[1]
(1University of Waterloo, 2University of Toronto, 3McGill University)
Design and Operation of a Compact, 100 kV Ultrafast Electron Diffraction Instrument

P16(a) Cat-Tuong Huynh, M. Schuurman
(University of Ottawa)
Multi-configuration time-dependent Hartree investigation on cis- and trans-stilbene

P16(b) Megan Dawson, P-N Roy
(University of Waterloo)
Path Integral Simulations of Confined Molecules Using Post-Quantization Constrained Propagators

P17(a) Alexander Ibrahim, P-N Roy
(University of Waterloo)
Creating a Four-Body Potential Energy Surface for Parahydrogen

P17(b) Simon Chen, M. Dawson, P-N Roy
(University of Waterloo)
Implementation of The Langevin Equation Path Integral Ground State Method in OpenMM

P18(a) Shaeer Moeed, P-N Roy
(University of Waterloo)
Simulating Planar Rotor Chains with the Pair Product Approximation

P18(b) Estevao de Oliveira, P-N Roy
(University of Waterloo)
Stochastic Series Expansion Quantum Monte Carlo for a System of N Planar Rotors in Linear Chain

P19(a) Jonathon Kambulow, P-N Roy
(University of Waterloo)
Simulating Chains of Entangled Molecules with Tensor Networks

P19(b) Wenxue Zhang, P-N Roy
(University of Waterloo)
Simulating Confined Molecules Using Path Integral Monte Carlo with Gibbs Sampling and a Discrete Variable Representation

P20(a) Nithin Aaron, P-N Roy
(University of Waterloo)
Path Integral Monte Carlo in a Discrete Variable Representation: Vibrational Coordinates

P20(b) Cailum Stienstra, L. Hebert, P. Thomas, J. Guo, W. S. Hopkins
(University of Waterloo)
Graphormer-IR: Graph Transformers Can Predict Anharmonic IR Spectra Using Highly Specialized Attention

P21(a) Christopher Ryan, E. Nazdrajic E., W. S. Hopkins
(University of Waterloo)
Novel Separation Method of PFAS via 2-Dimensional LCxDMS

P21(b) Arthur Lee[1], J. Featherstone[1], Jon Martens[2], T. McMahon[1], S. W. Hopkins[1]
([1]University of Waterloo, [2]Radboud University)
Fragmentation of Deprotonated Fluorinated Propionic

P22(a) Shannon Lemmens, E. Nazdrajic, A. Lee, S. W. Hopkins
(University of Waterloo)
Qualitative Analysis of Per- and Polyfluoroalkyl Substances in Contact Lenses and Brita Filters

P22(b) Gilles A. Dessap Pefete, P. Ayotte
(Sherbrooke University)
Spectroscopic Investigations of Mining Residues Drying Kinetics to Predict and Prevent Fugitive Dust Emissions

P23(a) Azharuddin (Oz) Mohammed, M. Nooijen
(University of Waterloo)
G.U.T. General Unitary Transformation

P23(b) Nyhenflore Delva, J. Medvedev, A. Klinkova
(University of Waterloo)
Treatment of Contaminants of Emerging Concern: Electrochemically Meditated Oxidation of 1,4-Dioxane

P24(a) Ben DeVries, C. G. Tetsassi Feugmo
(University of Waterloo)
Automated Workflow for Catalyst Discovery

P24(b) Pedro J. Castro Pelaez, T. S. Dibble
(SUNY Environmental Science and Forestry)
Exploring Atmospheric Redox Chemistry of Mercury: Insights from Quantum Chemistry and Computational Kinetics

P25(a) Justin Laroche[1], T. Putaud, S. Tousignant, C. Wespiser, Y. Kalugina, P-A Turgeon, P-N Roy[2], P. Ayotte[1]
([1]Université de Sherbrooke, [2]University of Waterloo)
NSI Conversion Rates of Water Isotopologs in Rare Gas Matrix

P25(b) Thomas Putaud[1,2], P-A. Turgeon[1], C. Wespiser[1], J-C. Chartrand[1], J. Vermette[1], Y. Kalugina[1,3], T. Serwatka[3], P-N. Roy[3], X. Michaud[2], P. Ayotte[1]
([1]Université de Sherbrooke, [2]Sorbonne Université, [3]University of Waterloo)
Confinement Effects on Nuclear Spin Isomers Interconversion Mechanism and Rates of H_2O

++++++++++ **Student's and PDF's Posters for Award Selection End Here** ++++++++++

P26(a) Jennifer van Wijngaarden[1],** T. Poonia[2], D. James[1]
([1]York University, [2]University of Manitoba)
Conformational Stability in Organic Ethers Versus Sulfides via Microwave Spectroscopy

P26(b) Toby Zeng**
(York University)
The Absence of Thermodynamically Favourable Triplet Fusion and a Reconciliation of an Intrinsic Incompatibility of Intramolecular Singlet Fission Chromophores

P27(a) Rodney Smith**
(University of Waterloo)
Identifying Spectroscopic Fingerprints for Defects in Heterogeneous Electrocatalysts

P27(b) James Brown[1],** A. Fleury[1], E. Lloyd[1], I. Kim[2]
([1]Good Chemistry Company, [2]UC Davis)
Using Non-Unitary CCSD for Both Near-Term And Fault-Tolerant Quantum Algorithms

P28(a) Patrick Ayotte,** J. Maurais, C. Wespiser
(Université de Sherbrooke)
Trapping Heterogeneous NO_2 Hydrolysis Reaction Intermediates on Ice

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.

- **Phone Numbers**:

Airways Transit:	519-886-2121	https://secure.airwaystransit.com
Waterloo Taxi:	519-747-7777	https://unitedtaxi.ca/contact-us.html
United Taxi:	519-888-9999	https://waterlootaxi.ca/

Please note that Waterloo Taxi and United Taxi offer flat rates to airport locations, which are usually cheaper than Airways Transit!

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 **<u>you should be able to pay with credit card.</u>** Parking lots M and N are the closest to EIT. The cost per day is $5 – $6.
Everything is within walking distance.