

The 36th Annual

Symposium on

Chemical Physics

at the

University of Waterloo

November 4-6, 2022

Acknowledgements

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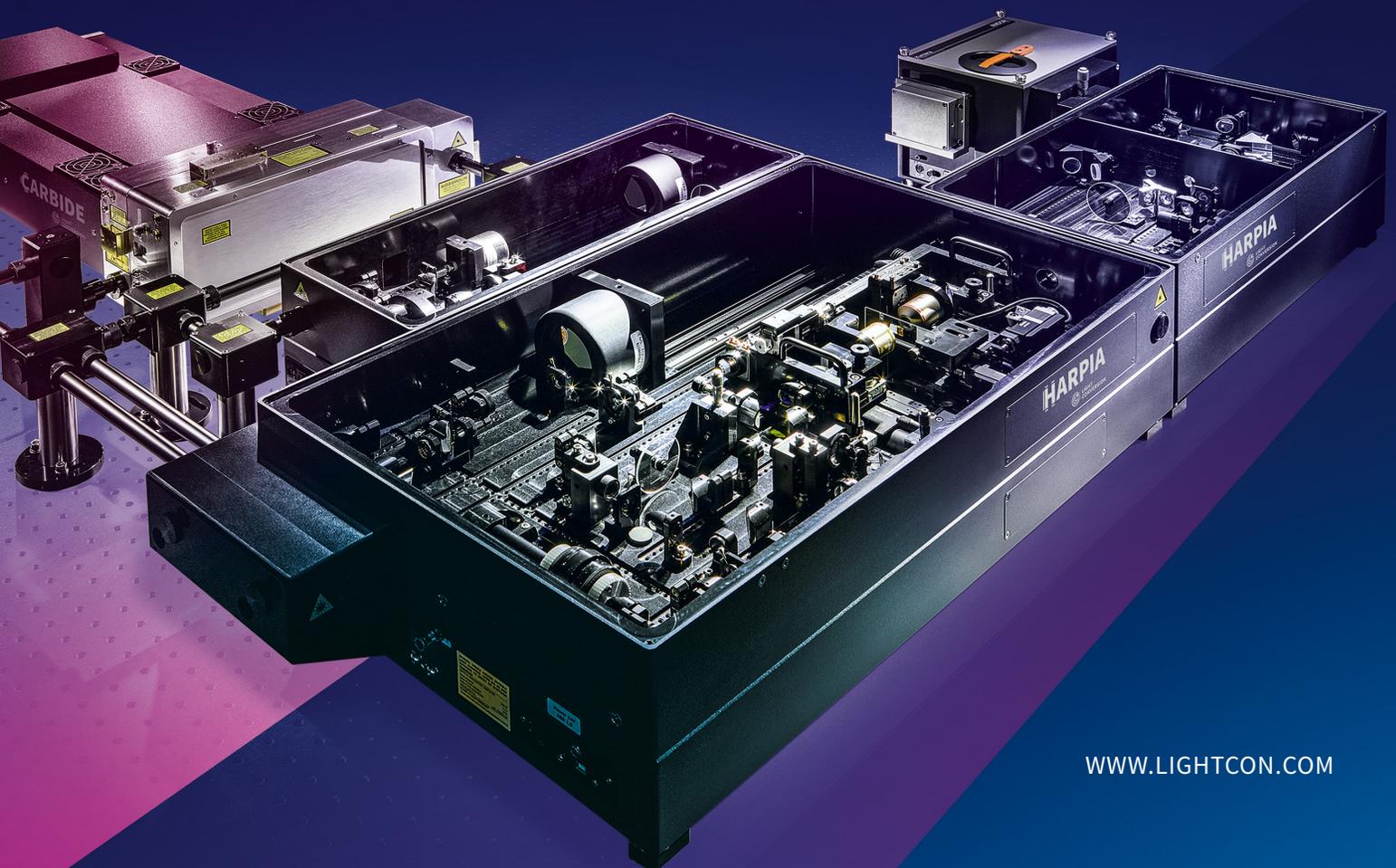
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Symposium on Chemical Physics
at the University of Waterloo
November 4-6, 2022

IMPORTANT NOTE FOR SCP2022 TALK FORMATS

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

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

SESSION I: Friday, November 4, 2022 – P.M. EIT-1015
Chair: **Marcel Nooijen**

7:30 – 8:30 *The Robert J. Le Roy Lecture: Alán Aspuru-Guzik*
(University of Toronto)
Inverted Singlet-Triplet Gap (INVEST) Emitters: A Potential Fifth Generation of Organic Light Emitting Materials

8:30 – 8:45 **Alan Jamison**¹, Juliana Park², Hyungmok Son³, Yukun Lu², Tijs Karman⁴, Timur Tscherbul⁵, Wolfgang Ketterle²
(¹University of Waterloo, ²MIT, ³Harvard, ⁴Radboud University, ⁵UNR)
Quantum Coherent Chemistry with Ultracold Atoms and Molecules

8:45 – 9:00 (T1) **Alastair Price**¹, Alberto Otero de la Roza², Erin R. Johnson¹
(¹Dalhousie University, ²Universidad de Oviedo)
XDM Dispersion with Local Orbitals: Implementation in The Fhaims Package

9:00 – 11:59 WELCOME RECEPTION – IQC Foyer (second floor of QNC). *Check your badge, there should be a 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 – IQC Foyer)** and another drink ticket is for the **REFRESHMENTS AND POSTER SESSION (Saturday evening – EIT Upstairs Foyer)**.

SESSION II: Saturday, November 5, 2022 – A.M.
Chair: **Subha Kalyaanamoorthy**

EIT-1015

9:00 – 9:45 Jean-Christophe Tremblay
(Laboratoire de Physique et Chimie Théoriques UMR)
Ultrafast Charge Migration Driven by Light: Mechanistic Insights from Many-Electron Dynamics Simulations

9:45 – 10:00 (T2) Josée Maurais, Patrick Ayotte
(Université de Sherbrooke)
Tayloring electric field standing waves to probe reactions of trace atmospheric pollutants at ice interfaces

10:00 – 10:15 (T3) Phil LeMaitre, Russell Thompson
(University of Waterloo)
Spontaneous Atomic Shell Structure and Symmetry-Breaking in a Classical Ring Polymer Formulation of Orbital-Free Density Functional Theory

10:15 – 10:45 COFFEE BREAK

SESSION III: Saturday, November 5, 2022 – A.M.
Chair: **W. Scott Hopkins**

EIT-1015

10:45 – 11:45 The Roger E. Miller Lecture: Yunjie Xu
(University of Alberta)
Molecular Spectroscopy of Chirality Recognition/Transfer/Amplification: Fundamental and Practical Advances

11:45 – 12:00 (T4) Jesse Simmons, Tucker Carrington Jr.
(Queen's University)
Computing Vibrational Spectra Using a Pruned Rectangular Collocation Method and an Iterative EigenSolver

12:00 – 12:15 (T5) Tyler Lott, Nicki Shaw, Ariel Petruk, Germán Sciaini
(University of Waterloo)
A New Approach for High Throughput Liquid-Cell TEM with Atomic Resolution

12:15 – 1:30 LUNCH – EIT Foyer

SESSION IV:
Chair: **Germán Sciaini**

Saturday, November 5, 2022 – P.M.

EIT-1015

- 1:30 – 2:15 Gonzalo Cosa**
(McGill University)
Thiol Induced Photo-Switching/Stability of Cyanine Dyes Used in Single Molecule Fluorescence
- 2:15 – 2:30 (T6) Ekadashi Pradhan, Toby Zeng**
(York University)
Design of the smallest intramolecular singlet fission chromophore with the fastest singlet fission
- 2:30 – 2:45 Simon Trudel**
(University of Calgary)
Amorphous Photodeposited Semiconductors in Optoelectronic Devices
- 2:45 – 3:00 (T7) Rachelle Choueiri, Leanne Chen**
(University of Guelph)
Ammonia Oxidation on β -Ni(OH)₂/NiOOH Surfaces from First Principles
- 3:00 – 3:15 (T8) Tamanna Poonia¹, Jennifer van Wijngaarden²**
(¹University of Manitoba, ²York University)
Conformational Equilibrium of The Chalcogen-Bridged Compounds Allyl Ethyl Ether and Allyl Ethyl Sulfide Revealed by Microwave Spectroscopy and Computational Chemistry
- 3:15 – 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:
POSTER SESSION
Chair:

Saturday, November 5, 2022 from 3:30 P.M.

EIT Upstairs Foyer

- 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 6, 2022 – A.M.

EIT 1015

Chair: **Rodney Smith**

9:15– 10:00 Oliviero Andreussi

(Boise State University)

Multiscale Modeling of the Stability and Catalytic Activity of Materials in Electrochemical Environments

10:00 – 10:15 **Patrick Ayotte¹**, Clément Wespiser¹, Jean-Claude Chartrand¹, Pierre-Alexandre Turgeon¹, Jonathan Vermette¹, Thomas Putaud², Xavier Michaut², Yulia Kalugina³ and Pierre-Nicholas Roy³

(¹Université de Sherbrooke, ²Paris Sorbonne, ³University of Waterloo)

Confinement Effect on The H O Nuclear Spin Isomer Interconversion Mechanism and Rate

10:15 – 10:30 **(T9) Seonghoon Choi¹**, Tzu-Ching Yen², Artur Izmaylov¹

(¹University of Toronto Scarborough, ²University of Toronto)

Improving Quantum Measurements by Introducing "Ghost" Pauli Products

10:30 – 11:00 **COFFEE BREAK**

SESSION VII:

Sunday, November 6, 2022 – A.M.

EIT 1015

Chair: **Conrard Tetsassi**

11:00 – 11:45 Lars Konermann

(University of Western Ontario)

Proteins in Solution and in the Gas Phase: MD Simulations Uncover Electrospray Ionization Mechanisms

11:45 – 12:00 **Rebecca Jockusch**, Iden Djavani-Tabrizi, Ioana Clotea.

(University of Toronto)

Dual Fluorescence and Spectral Switching of Acridine Dyes in Highly-Controlled Environments

12:00 – 12:15 **Randall Dumont**

(McMaster University)

Relativistic tunneling and attempts at superluminal signaling

12:15 – 1:30 Light **LUNCH & COFFEE** – EIT 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) Shawn Reeves, Subha Kalyaanamoorthy

(University of Waterloo)

Benchmarking Zero-Shot Ensembles for Predicting Protein Thermostability

P1(b) Miguel Lara Moreno, Tucker Carrington

(Queen's University)

Time-Independent Wavepacket Inelastic Scattering Calculations

P2(a) Shayne Johnston, Leanne D. Chen

(University of Guelph)

How Surface-Doped Cu in β -Ni(OH)₂ Influences the Mechanism for the Ammonia Electrooxidation Reaction

P2(b) Muna Abdulaziz¹, Ariel Petruk², Germán Sciaini², Liliana Trevani¹

(¹Ontario Tech University, ²University of Waterloo)

Development of Thin Film Electrodes for High Temperature and Pressure Electrochemical Studies

P3(a) Ignacio Loaiza, Alireza M. Khah, Nathan Wiebe, Artur F. Izmaylov

(University of Toronto Scarborough)

Reducing Molecular Electronic Hamiltonian Simulation Cost for Linear Combination of Unitaries Approaches

P3(b) Nicki Shaw, Tyler Lott, Ariel Petruk, Germán Sciaini

(University of Waterloo)

Liquid Cell Transmission Electron Microscopy

P4(a) Meixin Cheng¹, Shazhou Zhong¹, Nicolas Rivas¹, Tina Dekker¹, Ariel Alcides Petruk¹, Patrick Gicala¹, Kostyantyn Pichugin¹, Fangchu Chen¹, Xuan Luo², Yuping Sun², Adam W. Tsen¹ and Germán Sciaini¹

(¹University of Waterloo, ²HFIPS, Chinese Academy of Sciences)

Photoninduced Interlayer Phenomena in MoTe₂

- P4(b) Songhao Bao**, Neil Raymond, Marcel Nooijen
(University of Waterloo)
Time dependent Vibrational Electronic Coupled Cluster (VECC) theory
- P5(a) Sam Netzke**¹, Ariel Petruk¹, Sara Early¹, Kostyantyn Pichugin¹, Jiayang Jiang², R. J. Dwayne Miller², Bradley Siwick³, Germán Sciaini¹
(¹University of Waterloo, ²University of Toronto, ³McGill University)
Design and Operation of a Compact 100 kV Ultrafast Electron Diffraction Instrument
- P5(b) Wenxue Zhang**, Pierre-Nicholas Roy
(University of Waterloo)
PIMC Simulation of Entangled Confined Molecules with Discrete Variable Representation
- P6(a) Cailum Stienstra**, Liam Hebert, Patrick Thomas, W. Scott Hopkins
(University of Waterloo)
Prediction of Infrared Spectra using Graph Neural Networks/Transformer Hybrid Models
- P6(b) Christopher Ryan**, Alexander Haack, W. Scott Hopkins
(University of Waterloo)
Does Anharmonic Treatment of Ion-Solvent Cluster Thermochemistry Increase Accuracy of Dispersion Plot Models?
- P7(a) Benny Chen**, Marcel Nooijen
(University of Waterloo)
Exploration of Diabatization Protocols and VECC Approaches
- P7(b) Alexander Ibrahim**, Pierre-Nicholas Roy
(University of Waterloo)
Equation of State of Solid Parahydrogen Using Ab Initio Many-Body Interaction Potentials
- P8(a) Stephen W. Tatarchuk**¹, Rachelle M. Choueiri¹, Jury J. Medvedev², Anna Klinkova², Leanne D. Chen¹
(¹University of Guelph, ²University of Waterloo)
Thermodynamics Of Elementary Reaction Steps in Urea Oxidation Reaction on Nickel Hydroxide Electrodes
- P8(b) Steven Ong**, Subha Kalyaanamoorthy
(University of Waterloo)
Comparing Between Different Cutinase to Better Understand Thermostable Factors
- P9(a) Ruofei Zheng**, Meixin Cheng, Kostyantyn Pichugin, Derek Schipper, Germán Sciaini
(University of Waterloo)
Solvent Effects Unveiled via Cyclic Intramolecular Electron Transfer in 3CzClIPN
- P9(b) Neil Raymond**, Pierre-Nicholas Roy
(University of Waterloo)
Circumventing The Sign Problem In Path Integral Simulations Of Non-Stoquastic Vibronic Models

- P10(a) Megan Dawson, Pierre-Nicholas Roy**
(University of Waterloo)
Effects of a Post-Quantization Constrained Propagator on Path Integral Simulations of Water
- P10(b) Estevao de Oliveira, Pierre-Nicholas Roy**
(University of Waterloo)
Stochastic Series Expansion (SSE) Quantum Monte Carlo (QMC) for Planar Rotors
- P11(a) Nan Song, Ondrej Demel and Marcel Nooijen**
(University of Waterloo)
Construction of Orbital Domains in Cluster in Molecule Calculations
- P11(b) Tobias Serwatka, Pierre-Nicholas Roy**
(University of Waterloo)
Quantum Phase Transition In One-Dimensional Water
- P12(a) Robert Wodraszka, Tucker Carrington Jr.**
(Queen's University)
Solving The Schroedinger Equation on a General Potential Energy Surface with The MCTDH Method Using a Rectangular Collocation Approach That Employs a Nondirect Product Basis and Grid
- P12(b) Matthew Schmidt, Pierre-Nicholas Roy**
(University of Waterloo)
A Path Integral Molecular Dynamics Investigation into Hydrogen Clathrates: From Rigid to Flexible Cages
- P13(a) Anirudh Krishnadas, René Fournier**
(York University)
Melting-Like Transitions Modelling in Clusters using Artificial Neural Network
- P13(b) Gilles-Alex Dessap Pefete, Simon Foucault, Nicolas Grenier, Emrik Dauphinais, Frédéric Orban, Josée Maurais and Patrick Ayotte**
(Université de Sherbrooke)
Prevention and Intervention Strategies for The Mitigation of Fugitive Dust Emission from Mining Residues Storage Sites
- P14(a) Amir Hemmati, Xenia Medvedeva, Feng Li, Anna Klinkova**
(University of Waterloo)
Nanoelectrocatalysis in Confined Space: the Matter of Stability and Electrochemical Activity
- P14(b) Sakina Fatima, Melinda Recchia**
(University of Waterloo)
Molecular Interactions Driving RNA Binding to hnRNPA1 Implicated in Neurodegeneration

P15(a) Max Walton-Raaby, Tyler Floen, Guillermo Garcia-Diez, Nelaine Mora-Diez, Subha Kalyaanamoorthy
(University of Waterloo)
Calculating The Aqueous pKa of Phenols: Predictions for Antioxidants and Cannabinoids

P15(b) Christian Ieritano, Alexander Haack, W. Scott Hopkins
(University of Waterloo)
Kinetic vs Thermodynamic Control within Differential Mobility Spectrometry: An Unexpected Observation from Alpha-Acids

P16(a) Tsun Hei Arthur Enoch, Courtney Kates, W. Scott Hopkins, Terry McMahon
(University of Waterloo)
Investigation of Dodecaborate Cages Complexing with Diaminoalkanes

P16(b) Mohamad H. Al-Jabiri¹, Mihael Erakovic², Aran Insausti³, Marko Cvitaš², Wolfgang Jäger¹**
(¹University of Alberta, ²Ruder Boškovic Institute, ³Universidad del País Vasco)
A Rotational Spectroscopic and Theoretical Study of Tunneling in Substituted Benzoic Acid Heterodimers

P17(a) Rodney Smith**
(University of Waterloo)
Distortions and Defects in Electrocatalysts for Oxygen Evolution

P17(b) Toby Zeng**
(York University)
General Spin-Orbit Jahn-Teller Hamiltonian Formalism In One-Electron Representation

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:**

<i>Airways Transit:</i>	519-886-2121	https://secure.airwaystransit.com
<i>Waterloo Taxi:</i>	519-747-7777	https://unitedtaxi.ca/contact-us.html
<i>United Taxi:</i>	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.

IQC Foyer = Second floor QNC. Here we have our 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 \$5 – \$6. Everything is within walking distance.

