

The 39th Annual
Symposium on
Chemical Physics
at the
University of Waterloo

November 7-9, 2025

Acknowledgements

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

Faculty of Science, University of Waterloo
Department of Chemistry, University of Waterloo
Waterloo Institute for Nanotechnology

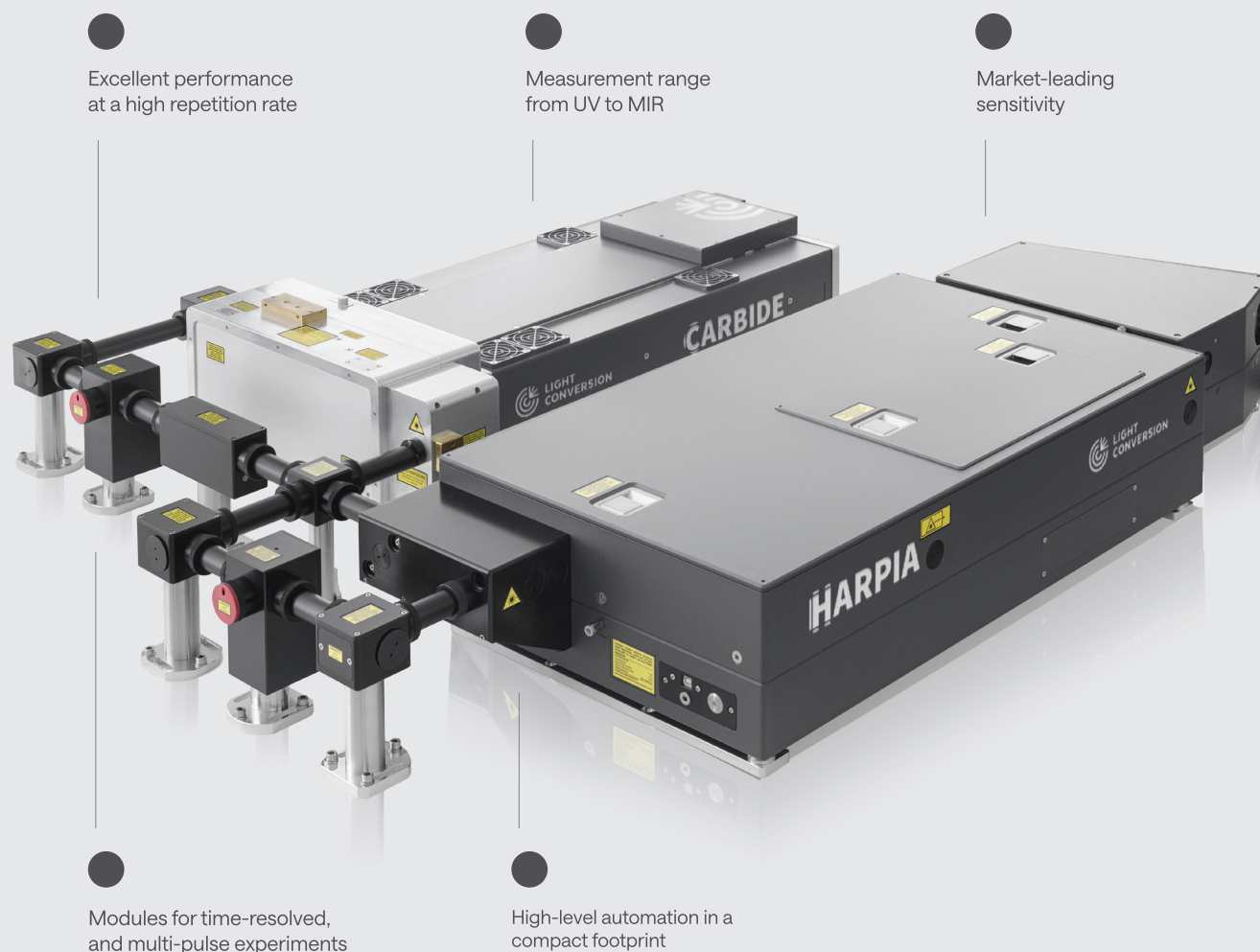
Canadian Journal of Chemistry (<https://cdnsiencepub.com/journal/cjc/>)

Industry sponsors:

Light Conversion USA (<https://LightCon.com/>) – Platinum

Intlvac (<https://www.intlvac.com/en-us/>) – Platinum

Ultrafast Spectroscopy System



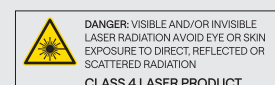
Specifications

Configuration	UV-VIS	UV-VIS-NIR	MIR
Probe spectral range	350 – 1100 nm ¹⁾	350 – 1600 nm ¹⁾	2000 – 13 000 nm ²⁾
Pump range	240 – 2200 nm ²⁾		450 – 2200 nm ³⁾
Delay range (resolution)	8 ns (8.3 fs)		4 ns (4.2 fs)
Temporal resolution	≤ laser pulse duration or better		
Laser repetition rate	1 – 100 kHz		
Maximum data acquisition rate	3850 Hz		100 kHz
Modes	Reflection and transmission		

¹⁾ Pump-probe measurements using Yb-based laser systems may exhibit blind spots at 515 nm and 1030 nm, corresponding to the second harmonic and fundamental wavelength of the laser, where strong pump scattering can interfere with accurate detection.

²⁾ The range is determined by the OPA's output spectrum.

³⁾ The wavelength range is configurable to 240 – 700 nm. Contact sales@lightcon.com for more details.



Tabletop Transient Absorption Spectroscopy System



Specifications

Modes	Transmission and reflection
Probe spectral range	460 – 910 nm
Probe polarization control	Linear (0 – 180°)
Pump wavelengths	515 nm, 343 nm
Delay range (resolution)	7.5 ns (10 fs)
Temporal resolution	≤ 290 fs
Laser repetition rate	60 kHz, any fundamental repetition rate division
Maximum data acquisition rate	3850 Hz
Dimensions	870.5 × 388 × 346 mm

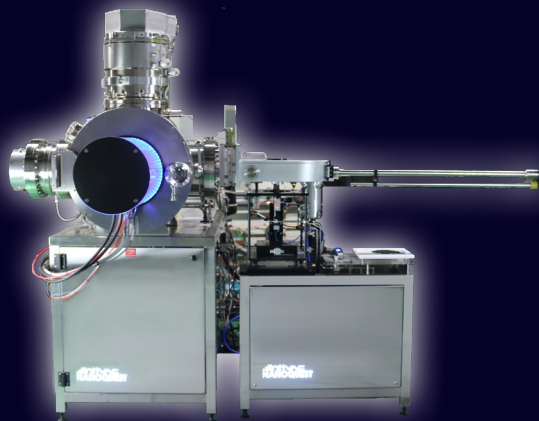
CLASS 1
LASER PRODUCT

INTLVAC'S LITHIUM NIOBATE FOUNDRY



AEGIS DLC

Advanced Etch Masking



NANOQUEST II

High-Aspect-Ratio Nanostructuring



NANOCHROME IV

Durable Pattern Transfer

FABRICATING THE FUTURE OF PHOTONICS

Intlvac's Lithium Niobate Foundry is a dedicated suite of advanced vacuum process tools engineered to unlock the full potential of LiNbO_3 for photonic, quantum, and microelectronic applications. From precision etch masking to high-aspect-ratio nanostructuring and durable pattern transfer, our platform enables accurate, scalable, and repeatable fabrication workflows.

Available as a fully integrated cluster tool, as individual modules, or an on-demand service. The foundry also supports other waveguide materials such as Ta_2O_5 and Al_2O_3 .



Intlvac
THIN FILM
intlvac.com



Leybold's Solutions for Every Lab Need

Every great discovery starts with the right tools. Whether you're exploring the frontiers of physics, engineering, or chemistry, Leybold is here to fuel your breakthroughs with precision and reliability.



leyboldcanada.com

IntIVAC
Providing Technology Solutions
Exclusive Canadian Distributor

WATERLOO INSTITUTE FOR NANOTECHNOLOGY

Quantum Nano Centre

\$160-million highly-advanced community laboratory
for nano-metrology and nano-fabrication



UNIVERSITY OF
WATERLOO



WATERLOO INSTITUTE FOR
nanotechnology

A GLOBAL CENTRE OF EXCELLENCE FOR NANOTECHNOLOGY AND ITS APPLICATIONS



120 WIN FACULTY MEMBERS

14 DEPARTMENTS

17 RESEARCH CHAIRS

43 PARTNERS IN 16 REGIONS

258,762

TOTAL CITATIONS*

10,975

PAPERS PUBLISHED

*2008 - 2025



Smart & Functional Materials

nanomaterials | nanoparticles | quantum dots |
carbon nanotubes | biomaterials | nanocellulose

Therapeutics & Theranostics

tissue engineering | minimally invasive treatment |
immunotherapy | medical imaging | drug delivery

Connected Devices

IOT sensors | flexible electronics | photonic-devices |
nano-systems | human-interface machines | wearables

Next Generations Energy Systems

energy devices | batteries | fuel cells | catalysis |
low-carbon technologies | artificial photosynthesis

Discover your research potential with a **\$10,000** Nanofellowship
from the Waterloo Institute for Nanotechnology

NANOFELLOWSHIP COMPETITION

Application Deadline:
February 1st

Open to new and current **MSc** and **PhD** students pursuing nanotechnology research at the University of Waterloo in one (or more) of WIN's four focus areas.

- **\$10,000** in additional funding to supplement research support provided by the supervising faculty member.
- Open to **domestic** and **international** applicants.

Nanotechnology Focus Areas

- Smart and Functional Materials
- Connected Devices
- Next Generation Energy Systems
- Theranostics and Therapeutics



Scan for more info



UNIVERSITY OF
WATERLOO



WATERLOO INSTITUTE FOR

nanotechnology

nano.uwaterloo.ca/nanofellowships

Symposium on Chemical Physics

at the University of Waterloo

November 7-9, 2025

IMPORTANT NOTE FOR SCP 2025 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.

The Lecture in **Memory of Giacinto Scoles** is 60 min, including 15 min for discussion and introduction.

Invited talks are 45 min, including 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 7, 2025 – P.M.

EIT-1015

Chair: **Scott Hopkins**

7:30 – 7:45 **Christian Ieritano**

(University of Waterloo)

1 Compound, 4 Peaks: The Curious Case of How Protonation Can Induce Chirality within Achiral Molecules

7:45 – 8:00 **(T1) Ivan Bosko, V. N. Staroverov**

(University of Western Ontario)

Density Functionals with Explicit Dependence on Electron Number

8:00 – 8:15 **(T2) Matthew Schmidt**, M. Lecours, C. Boone, J. Steffen, N. Raymond, P. Bernath

(University of Waterloo)

Atmospheric Chemistry Experiment: 20⁺ Years of Spectroscopy Opening Atmospheres

8:15 – 8:30 **(T3) Praveen Jayakumar**¹, T. Zeng², A. Izmaylov¹

(¹University of Toronto, ²York University)

How to Unitarily Transform Electronic Hamiltonians?

8:30 – 8:45 **(T4) Christian Viernes**, Germán Sciaini

(University of Waterloo)

Tracking Electronic and Nuclear Orders in a Strongly Coupled Charge Density Wave

8:45 – 9:00 **(T5) Samihat Rahman**, Mark Wilson

(University of Toronto)

Exploring Carrier-Based PbS Quantum Dot Films to Improve Solid-State Photon Upconversion

9:00 – 11:30 WELCOME RECEPTION – Federal Hall (FED 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 – FED) and another drink ticket is for the Refreshments & Poster Session (Saturday evening – EIT Upstairs Foyer).

Chair: **W. Scott Hopkins (and Dino Deligiannis)**

9:00 – 10:00 The Plenary Roger E. Miller Lecturer: Takamasa Momose

(University of British Columbia)

*Exploring Molecular Clusters with Helium Droplet Spectroscopy: From
Molecular Superfluidity to Biomolecular Interactions*

10:00 – 10:15 (T7) Justin Laroche¹, T. Putaud¹, F. Gatti¹, P-N. Roy², P. Ayotte¹

(¹Université de Sherbrooke, ²University of Waterloo)

*Effects of Confinement on Highly Forbidden Ortho-H₂O to Para-H₂O
Isomerization*

10:15 – 10:45 COFFEE BREAK

Chair: **Pierre-Nicholas Roy**

10:45 – 11:45 The Robert J. Le Roy Plenary: Françoise Remacle

(Université Liège)

Tuning Electron-Nuclei Entanglement with Attopulses for Controlling Molecular Dynamics

11:45 – 12:00 J. Sylvester, C. D. Alcorn[†], S. Sasidharanpillai, **Peter R. Tremaine**

(University of Guelph, [†]Present: University of New Brunswick)

Uranyl Chloride Complexation under Hydrothermal Conditions by Raman Spectroscopy

12:00 – 12:15 **(T6) You Li**, T. Carrington Jr.

(Queen's University)

A Numerical Method for Computing Vibrational Spectra that Obviates Integrals by Using the Weighted and Chopped Rectangular Collocation Method with Contracted Basis Functions

12:15 – 1:30 **LUNCH** – EIT Foyer

Chairs: **Marcel Nooijen**

1:30 – 2:30 In Memory of Giacinto Scoles: Kevin Lehmann

(University of Virginia)

Giacinto and Me: Four Decades of Collaboration and Friendship

2:30 – 2:45 Myongin Oh

(Memorial University of Newfoundland)

*Covalent: A Machine-Learning-Driven Protocol for Collective Variable
Discovery in Biomolecular Simulations*

2:45 – 3:00 (T7) Simon Godin, Ke Zou

(University of British Columbia)

*Novel Nickel-Nitrogen-Nickel (Ni-N-Ni) Magnetic Defect Centers in Nickel Oxide
(NiO)*

3:00 – 3:15 J. Shi, H. Nguyen, M. Voronich, Stella Consta

(Western University)

Electrostatic Properties and Reaction Acceleration in Droplets

3:15 – 3:30 (T8) Thomas Putaud, J. Laroche, P-N. Roy, X. Michaut, P. Ayotte

(Université de Sherbrooke)

Nuclear spin conversion of water isotopologs in confined environments

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 8, 2025, from 3:30 P.M. EIT Upstairs Foyer

POSTER SESSION

Chair: **Marcel Nooijen**

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)***

Chair: **W. Scott Hopkins**

9:15 – 10:00 Michael Van Stipdonk

(Duquesne University)

Going where few dare to: Combining Ion Trapping Mass Spectrometry and Computational Chemistry to Investigate the Intrinsic Chemistry and Structure of Uranium Species

10:00 – 10:15 (T9) Leon Daniel¹, R. Zheng², D. Sutarma¹, C. Viernes², Y. Ding³, T. Fabunmi¹, G. Bacher¹, M. Heuken⁴, H. Kalish⁴, A. Vescan³, P. Kratzer¹, M. Schleberger¹, G. Sciaini²

(Universität Duisburg-Essen¹, University of Waterloo², ³RWTH Aachen University, ⁴AIXTRON SE)

Defect-Engineered Competition Between Exciton Annihilation and Trapping in MOCVD WS₂

10:15 – 10:30 (T10) Miguel Albaladejo, S. Ambrico, V. Xia, M. Imran, M. Wilson

(University of Toronto)

Template-Mediated synthesis of AgBiS₂ Nanocrystals for Solar Cells via Cation Exchange Reactions

10:30 – 11:00 COFFEE BREAK

Chair: **Pierre-Nicholas Roy**

11:00 – 11:45 Ryan MacDonell

(Dalhousie University)

Ab Initio or Ab Initiation't? Unraveling Approximations in Excited-State Chemistry and Nonadiabatic Dynamics

11:45 – 12:00 (T11) Ruofei Zheng¹, A. A. Petruk¹, J. Tordiff², P. Price², P. Concepcion², D. Homeniuk², K. Pichugin¹, M. Salomons², G. Sciaini¹

(¹University of Waterloo, ²National Research Council)

Cathodoluminescence-SEM: A Window into Nanoscale Light Emission

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

POSTER SESSION:

Saturday, November 8, 2025 – 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) Jikai Zhu, T. Carrington Jr

(Queen's University)

VSCF with Collocation and Pruned Grids

P1(b) Luca Corneo, T. Carrington Jr

(Queen's University)

Collocation Methods to Calculate Vibrational Spectra with Complicated Kinetic Energy

P2(a) Jacob Chausse, P-N Roy

(University of Waterloo)

Quantifying Nuclear Quantum Effects in Water-filled Carbon Nanotube and its Quasiphase Transition

P2(b) Jingwen Zhou, L. D. Chen

(University of Guelph)

Ammonia and Urea Electrooxidation: Mechanisms and Catalyst Design

P3(a) Julia Coveny, B. J. R. Laframboise, J. Zhou, and L. D. Chen

(University of Guelph)

DFT Investigation of Pt-M Alloys for the Electrocatalytic Oxidation of Ammonia

P3(b) Conrad Moore, V. N. Staroverov

(University of Western Ontario)

Shapes of Electron-Nucleus Cusps in Approximate Wavefunctions

P4(a) Smik Patel, P. Jayakumar¹, T. Zeng², R. Huang¹, A. F. Izmaylov¹

(University of Toronto¹, York University²)

Quantum Seniority-Based Subspace Expansion: A Near-Term Quantum Algorithm for Electronic Structure

P4(b) Henry Lim, B. Paget, L. D. Chen

(University of Guelph)

DFT Investigation of Ammonia Oxidation Reaction on CeO₂ (111), (110), (100) Facets

P5(a) Illia Voropai, M. Nooijen

(University of Waterloo)

Configurational Coupled Cluster

P5(b) Farjad Raza, P-N Roy

(University of Waterloo)

Quantum Interactions between Vibrational Rotors

P6(a) Muna Abdulaziz¹, K. Pichugin², T. Whistle¹, T. George¹, G. Sciaini², and L. Trevani¹

(Ontario Tech University¹, University of Waterloo²)

Exploring Ti and Ta as Adhesion Layers for Pt Thin Film Electrodes for Hydrothermal Applications

P6(b) Tuhin Ghosh, J. Gao

(Brock University)

Hot Carrier Harvesting Enables Open-Circuit Voltages (V_{oc}) Beyond the Band Gap (E_g)

P7(a) Harmanjot Singh Grewal, R.J. Dwayne Miller

(University of Toronto)

Ultrafast Studies on a Cyanobacterial Chloride pump and its proton pumping mutant

P7(b) Nithin Aaron, P-N Roy

(University of Waterloo)

Simulating Flexible Water Clusters using Path Integral Monte Carlo with Normal-Mode Sampling

P8(a) George McBane, S. Schaertel

(Grand Valley State University)

Pressure Broadening Studies of the 3-0 Overtone Band of CO Perturbed by Neon and Nitrogen

P8(b) Estêvão Vilas Boas de Oliveira, P-N Roy

(University of Waterloo)

Path Integral Monte Carlo for Planar Rotor Lattices

P9(a) Georgii Sizov, V. N. Staroverov

(University of Western Ontario)

Limitation-Free Method for Recovering Potentials from Their Matrix Representations

P9(b) Jiayang Jiang, S. Keramati, Z. Huang, W. Song

(University of Toronto)

Ultrafast electron Diffraction with Phase Change Materials: Sb_2Te_3

P10(a) Tyler Lott, J. Andrianasolo, K. Froese, A. Arjuna, S. Benourджа, T. Maksyuta, K. Pichugin, and G. Sciaini

(University of Waterloo)

Advanced Methods in Electron Microscopy

P10(b) Linjun Wang, J. Lin, and A. F. Izmaylov

(University of Toronto)

Predicting Accuracy of Electronic Structure Methods Based on Violation of Exact Conditions

P11(a) Marko Voronych, S. Constat

(University of Western Ontario)

Taylor Cone Formation in Molecular Clusters: A Simulation-Based Assessment of Electrostatic Theory

P11(b) Patrick Ayotte, J. Maurais, C. Wespiser, R. Robidas

(Université de Sherbrooke)

Trapping Intermediates of the NO₂ Hydrolysis Reaction on Ice

P12(a) Toby McConville, C. T. Feugmo

(University of Waterloo)

Physics-Informed Neural Networks for EIS Analysis

P12(b) Jim Martin¹, D. Meng¹, D. Z. Chan²

(University of Waterloo¹, University of Oxford²)

Humpty-Dumpty is Three-Dimensional: The Role of Transverse Fields in Stern-Gerlach Interferometry

P13(a) Zach Hoang, K. Mitchell-Koch

(University of Manitoba)

Exploring the Effect of Internal Protein Dynamics on Allosteric Regulation in CsrA

P13(b) Julian Carl Puentespina, K. Mitchell-Koch

(University of Manitoba)

Hydration Layer Dynamics of MHC-I

P14(a) Christine Duong¹, L. Markmann¹, H. Zhao², G. A. Baker³, K. R. Mitchell-Koch¹

(University of Manitoba¹, University of Minnesota², University of Missouri³)

Development of CHARMM Forcefield Compatible Parameters for Synthesized Ionic Liquids to Investigate the Biosurfactant Activity of Candida Antarctica Lipase B (CALB)

P14(b) Dawson McLachlan, S. Hopkins

(University of Waterloo)

Investigating Discrepancies of Collision Cross Section Calculations of Per- and Polyfluoroalkyl Substances

P15(a) Rashne Vakharia, W. S. Hopkins.

(University of Waterloo)

MS-Based Separation of O-Desmethylenlafaxine and Tramadol for Environmental Monitoring

P15(b) Alma Bravo Rivero, K. Mitchell-Koch

(University of Manitoba)

Enzyme And Solvent Shell Dynamics of Subtilisin Carlsberg in Organic solvents

P16(a) Duong (Lily) Phan, Jace Trosky, K. Mitchell-Koch

(University of Manitoba)

Developing computational methods to identify mosquito olfactory genes targeted by model insect repellants

P16(b) Leo Markmann, I. Asakereh, H. Rezasoltani, N. Duong, M. Khajehpour, K. Mitchell-Koch

(University of Manitoba)

Mechanistic Insights into Protein Helix Stabilization by TFE and Other Short-Chain Alcohols: A Computational and Spectroscopic Study

P17(a) Amirhossein Rashidi, H. Gao, M. Vashishta, P. Djuricanin, T. Momose

(University of British Columbia)

Trapping Ammonia Molecules in a Fabry-Perot Microwave Cavity

P17(b) Rees Hughes, M. Hasham, M. W.B. Wilson

(University of Toronto)

Dynamic Trap Emission from Individual CdSe/ZnS Quantum Dots

P18(a) Xinran Liu, R. Smith

(University of Waterloo)

Unraveling and Controlling Metal-Support Interactions in Oxide-Supported Platinum Catalysts

P18(b) Jixi Zhang, R. Smith

(University of Waterloo)

Thermal Decay Kinetics of Monolayer MoS₂ in Controlled Environments

P19(a) Megan Dawson, P-N Roy

(University of Waterloo)

Simulating Furanoside Conformations with Path Integral Molecular Dynamics

P19(b) Azharuddin Mohammed, M. Nooijen

(University of Waterloo)

Property Extraction in Time Dependent Coupled Cluster Theory

P20(a) Christopher Ryan, W. S. Hopkins

(University of Waterloo)

CO₂ as a Protective Gas in LC×DMS Separation of Fragile PFAS Compounds

P20(b) Spencer Spiegelman¹, A. Zarrine-Afsar^{2,3}, D. Vlaminc^{2,3}, F. Talbot^{2,3}, W. S. Hopkins¹

(¹University of Waterloo, ²University of Toronto, ³University Health Network)

Predictive Modeling of Spectral Fingerprints for Mouse Organ PIRL-MS Data

P21(a) Sahar Moghadamy, J. Gao

(Brock University)

Chiral Organic Semiconductor Photodetector Development

P21(b) Areeba Iqbal, J. Gao

(Brock University)

Exciton Dynamics in Two-Dimensional Chiral Perovskite Nanostructures

P22(a) Griffin Loeb sack¹, N. J. A. Coughlan¹, Y. Li¹, N. Mashmoushi¹, Y. Xiao¹, M. Guna², B. B. Schneider², J. C. Yves Le Blanc², W. S. Hopkins¹

(¹University of Waterloo, ²SCIEX)

The Product of NH₃ Loss from Gas Phase Protonated Tyrosine

P22(b) Isabella Sciorilli, N. King, R. Smith

(University of Waterloo)

Surface Characterization of Novel Quadruple Perovskite CaCu₃Fe₄O₁₂

P23(a) Yiming Xiao, J. Featherstone

(University of Waterloo)

Mass Spectrometry Capability at UWMSF

P23(b) Wenxue Zhang, P-N. Roy

(University of Waterloo)

Path Integral Sampling of Discrete Molecular Rotations: Application to Quantum Rotor Assemblies in Beryl

+++++ 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:**

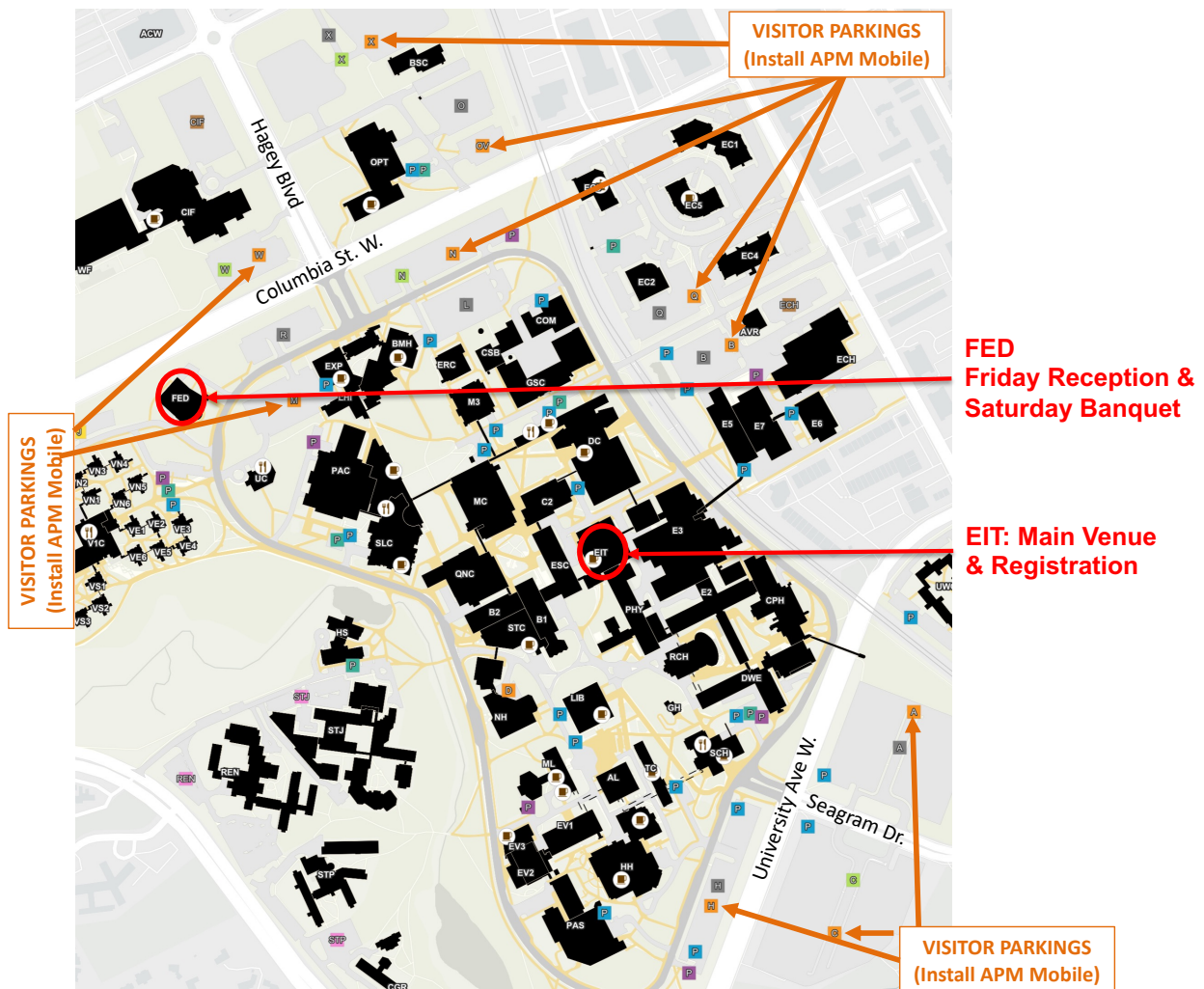
- **Waterloo Taxi: 519-747-7777 | <https://waterlootaxi.ca/>**
- **United Taxi: 519-888-9999 | <https://unitedtaxi.ca/contact-us.html>**

Please note that Waterloo Taxi and United Taxi offer flat rates to and from airport locations, which are usually the most convenient option! Reserve 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 Reception on Friday starting at 9 pm and our banquet dinner on Saturday starting at 6:30 pm.



VISITOR PARKING INFORMATION

Visitor parking lots are highlighted on the map. The University now uses the AMP Mobile Pay system for parking payments. You will need to install the AMP app to pay for parking.

Instructions for setup can be found here:

<https://uwaterloo.ca/sustainable-transportation/visitors/amp-mobile-pay>

Daily parking rates range from **\$7.25 to \$8.30**, depending on the lot. The most convenient and closest lot to EIT is Lot N, though all lots are within walking distance.