OpenMOLCAS 2024, Toronto, Canada

Conference Information
Date: June 22 – 24, 2024
Venue: Rm 428 Lash Miller Building, University of Toronto
ZOOM link for virtual presentations: https://yorku.zoom.us/j/97947179380

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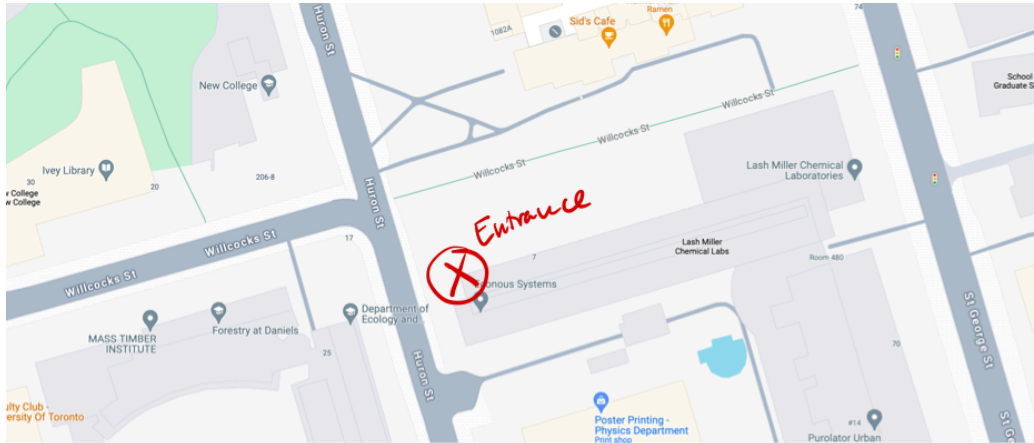
Program (v for virtual presentation)		
22 June (Saturday)		
9:00 am - 9:30 am	**Nike Dattani**	Set-up, and opening remarks
9:30 am - 10:15 am	**Meng Wang**	Accelerating Molcas Executions Through Intelligent Caching Mechanisms
10:15 am - 11:15 pm	**Ed Valeev**	Massively Parallel Quantum Chemistry: research platform for the post-Moore world
11:15 pm - 1:15pm		Lunch
1:15 pm - 2:00 pm	**Emil Zak (v)**	Simulation of quantum chemistry Hamiltonians with relativistic effects on fault-tolerant quantum computers
2:00 pm - 3:00 pm	**Bert de Jong (v)**	NWChemEx, moving computational chemistry to the exascale
3:00 pm - 3:15 pm		Break
3:15 pm - 4:00 pm	**Arta Safari**	Recent Progress in Stochastic Complete Active Space Second-Order Perturbation Theory
4:00 pm - 4:45 pm	**David Poole**	A modular, composite framework for the utilization of reduced-scaling Coulomb and Exchange construction algorithms
4:45 pm - 5:00 pm		Closing remarks
5:00 pm - 10:00 pm		Dinner at Center Island ($9 ferry ticket + dinner). 9:05pm return ferry is best for seeing the 9:07pm sunset over the Toronto skyline.
23 June (Sunday)		
10:00 am - 11:00 am	**Geoff Hutchison (v)**	Computational Chemistry and Open Source: Babel, Avogadro and the Wider Ecosystem
11:00 am - 12:00 pm	**David Sherrill**	The Psi4 Software Ecosystem
12:00 pm - 2:00 pm		Lunch
2:00 pm - 3:00 pm	**Martin Head-Gordon (v)**	MP2 made better and faster: New developments in regularization and local correlation
3:00 pm - 3:45 pm	**Alexander Davis**	Electronegativity differences as voltages that equalize charge
3:45 pm - 4:00 pm		Break
4:00 pm - 5:00 pm	**Devin Matthews**	Recent Developments in CFOUR
5:00 pm - 5:15 pm		Closing remarks
24 June (Monday)		

9:15 am - 10:00 am	**Shahidul Islam**	A decoy ACE2 shows significant efficacy against SARS-CoV-2 Omicron variants and related viruses: A computational-experimental approach
10:00 am - 10:45 am	**Irene Conti (v)**	Computational Tool as a Multifunctional Time-Resolved Spectrometer: The Thiobases Test Case
10:45 am - 11:00 am	**Tuhin Samanta (v)**	An intermediate phase between jammed and unjammed amorphous solids
2:00 pm - 11:00 pm	Day trip to Niagara Falls and back	

A note from the organizing team

Dear Attendees,

Welcome to Toronto! We thank you for attending the 12th annual OpenMolcas meeting! The conference will be held at Room 428 Lash Miller Building, University of Toronto, St. George Campus, Downtown Toronto. Step by step instructions are given below to guide you to the building and the room:

1) Please use the entrance at the **Huron - Willcocks corner**

2) Proceed to the 4th floor up the stairs:

3) Through this door on the 4th floor

4) Straight and then to the right in this corridor:

5) Straight and to the left in this corridor:

6) Final destination, Chemical Physics Theory Group lounge:

Yours truly,

The Organizing Committee