30th Canadian Symposium on Theoretical and Computational Chemistry

CSTCC 2024, HALIFAX

Canadian Association of Theoretical Chemists

30th Canadian Symposium on Theoretical and Computational Chemistry

CSTCC 2024, HALIFAX

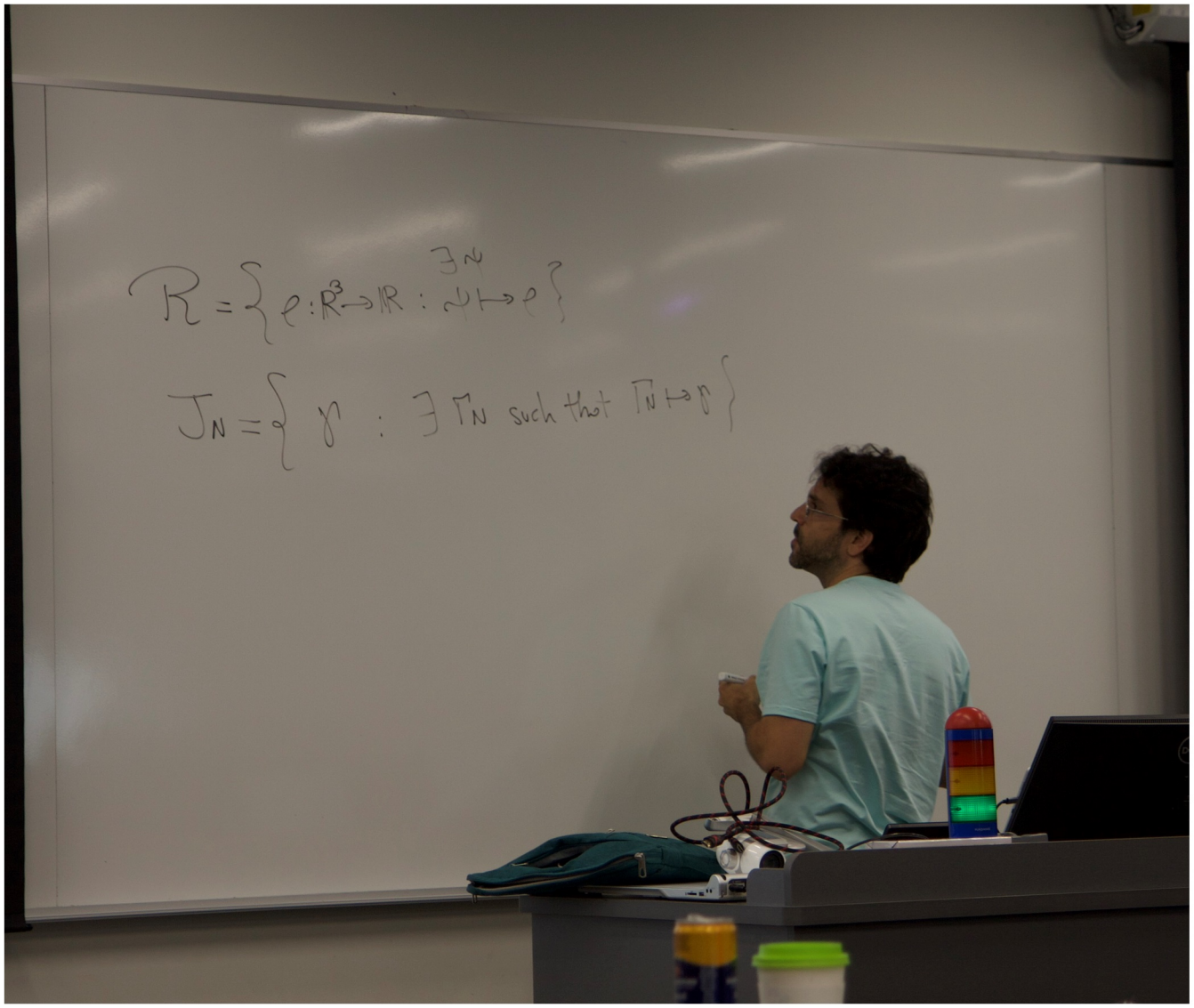
Canadian Association of Theoretical Chemists

ORGANIZERS
Erin Johnson
Ryan MacDonell
Stijn De Baerdemacker

DAY 1

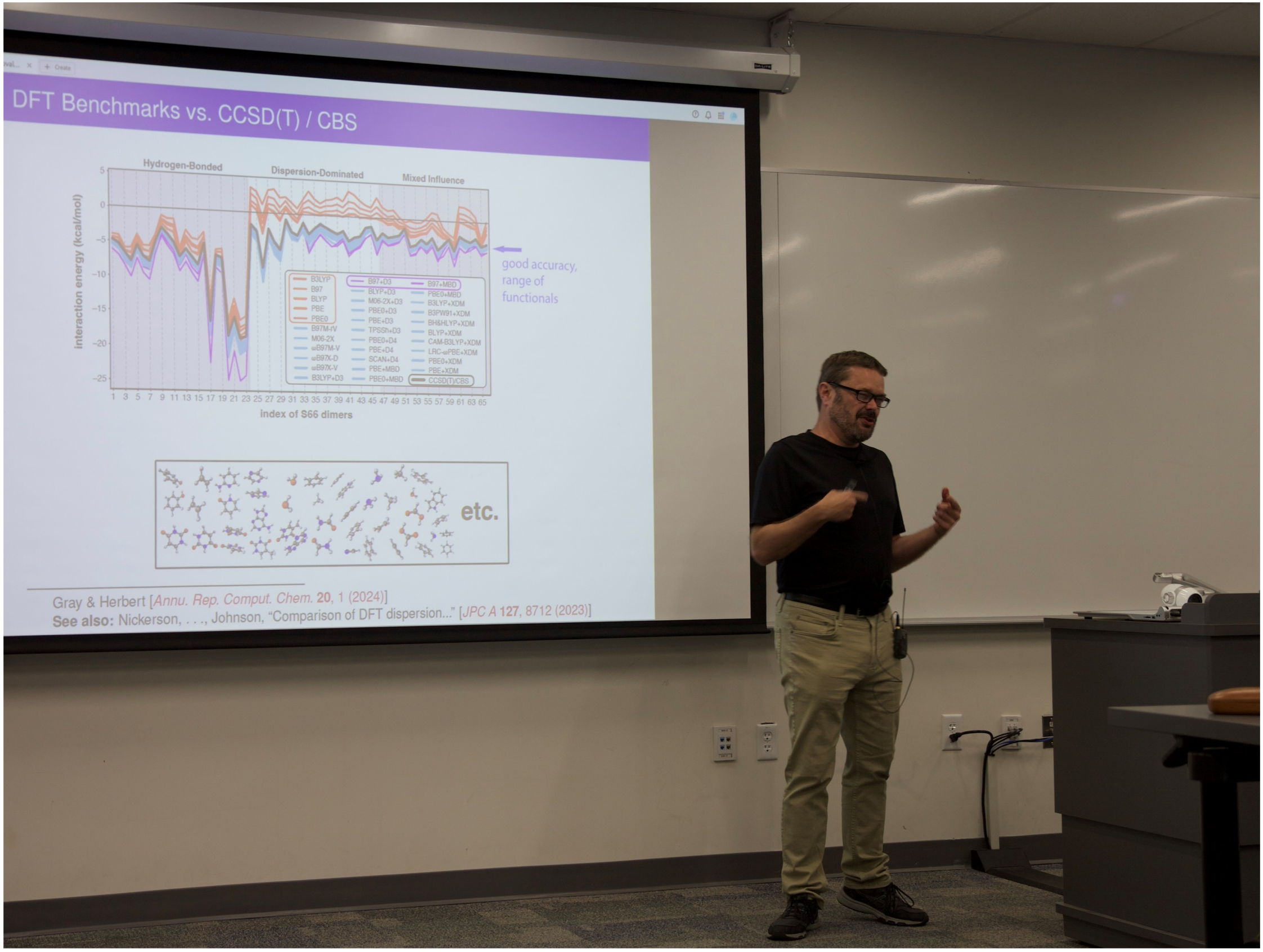
Josh Hollet

Kieron Burke



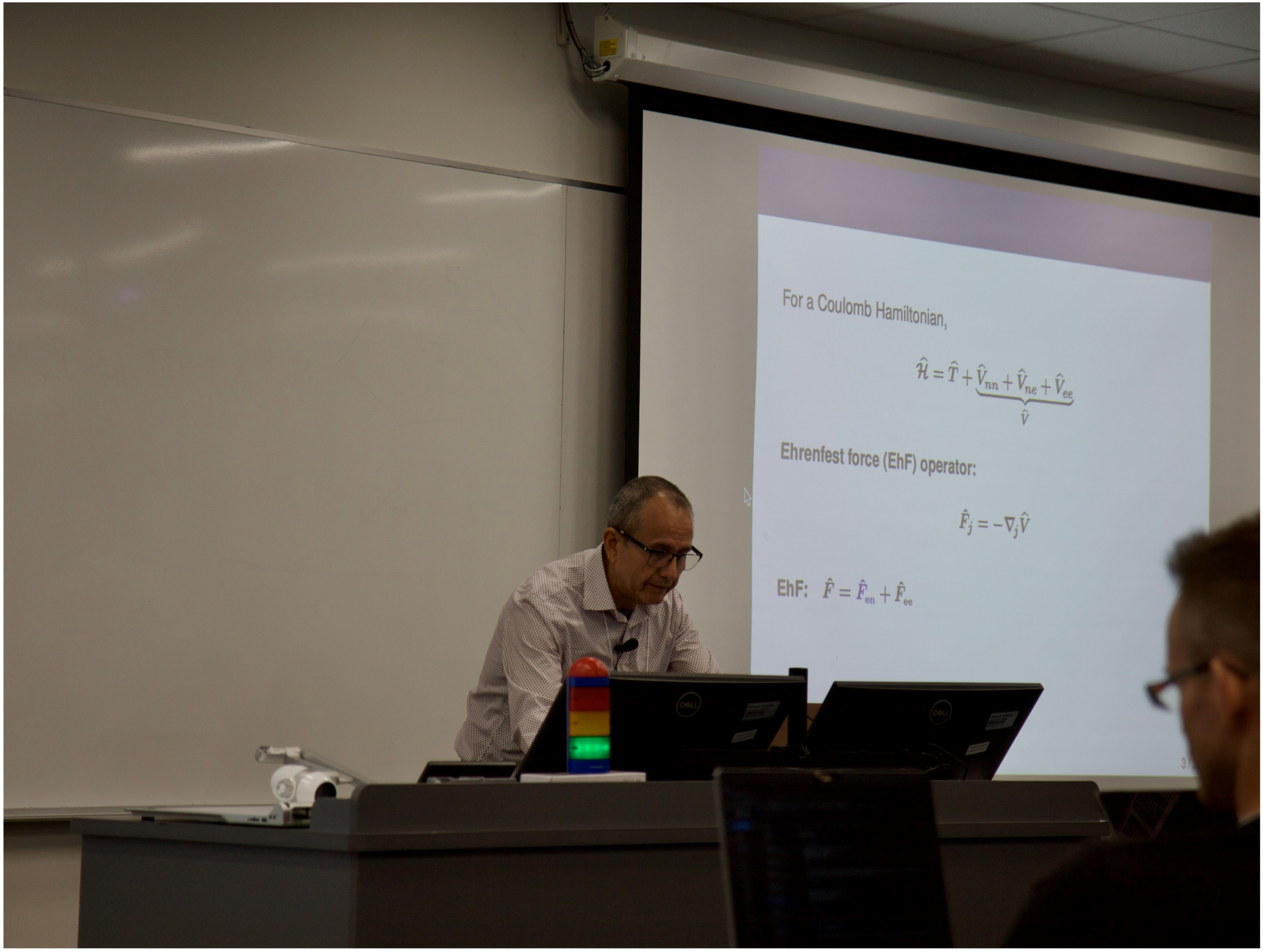
Augusto Gerolin

Gino DiLabio

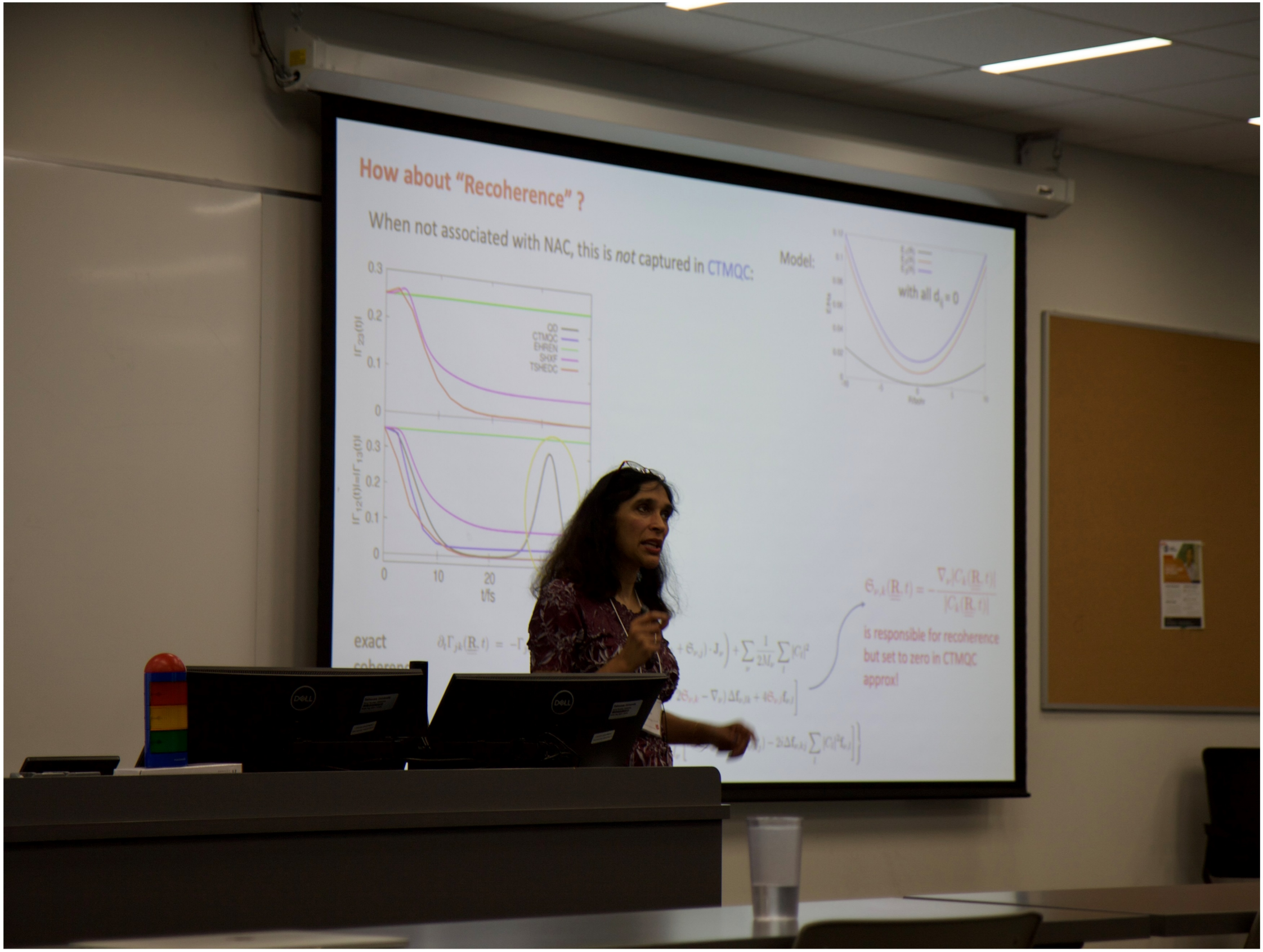


JOHN HERBERT

Stacey Wetmore



Jesús Hernández-Trujillo

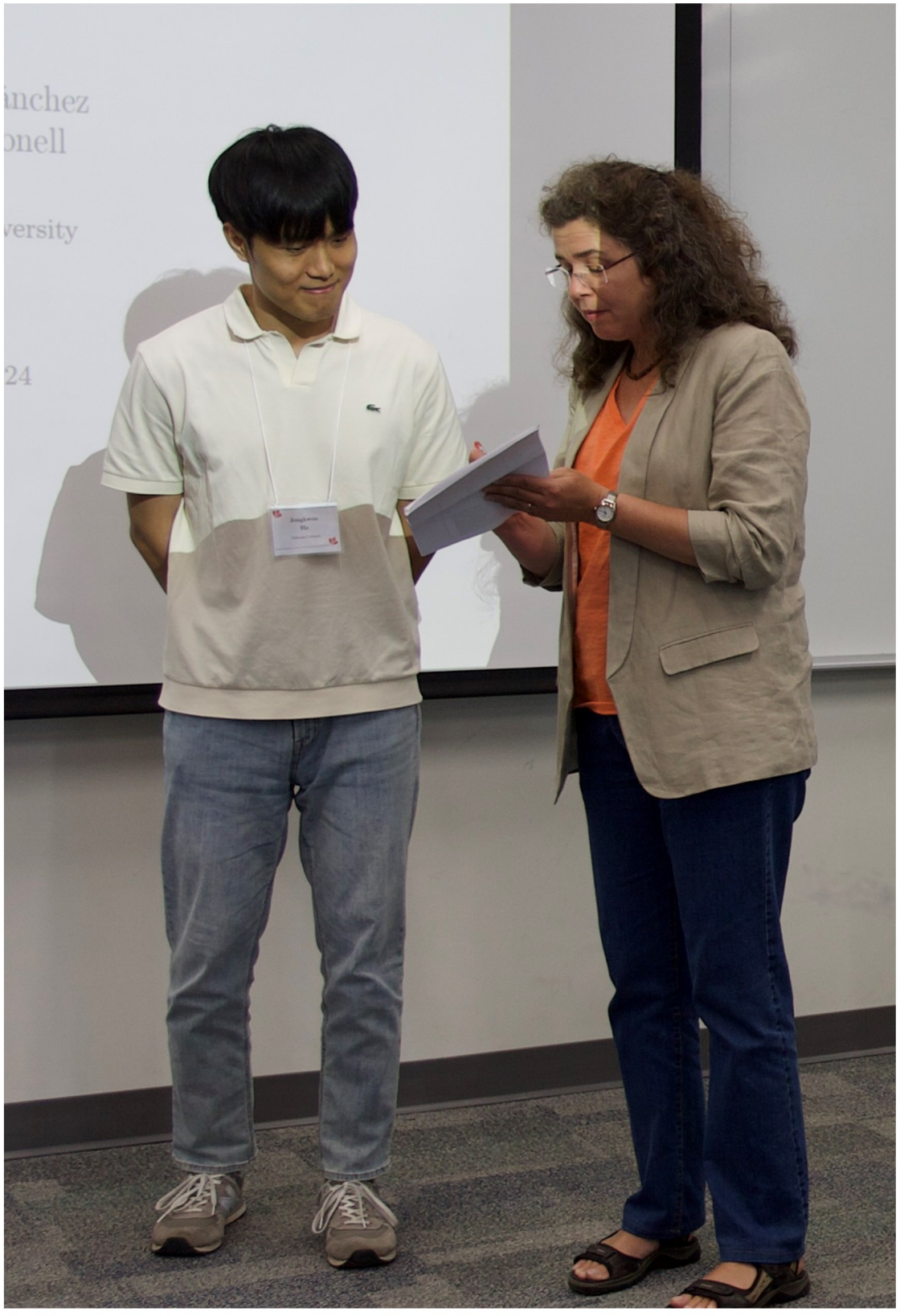


Neepa Maitra

ARTUR IZMAYLOV

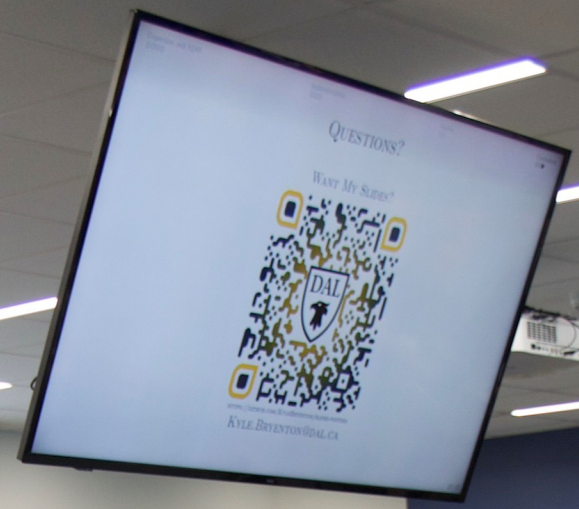
Toby Zeng

Alex Brown

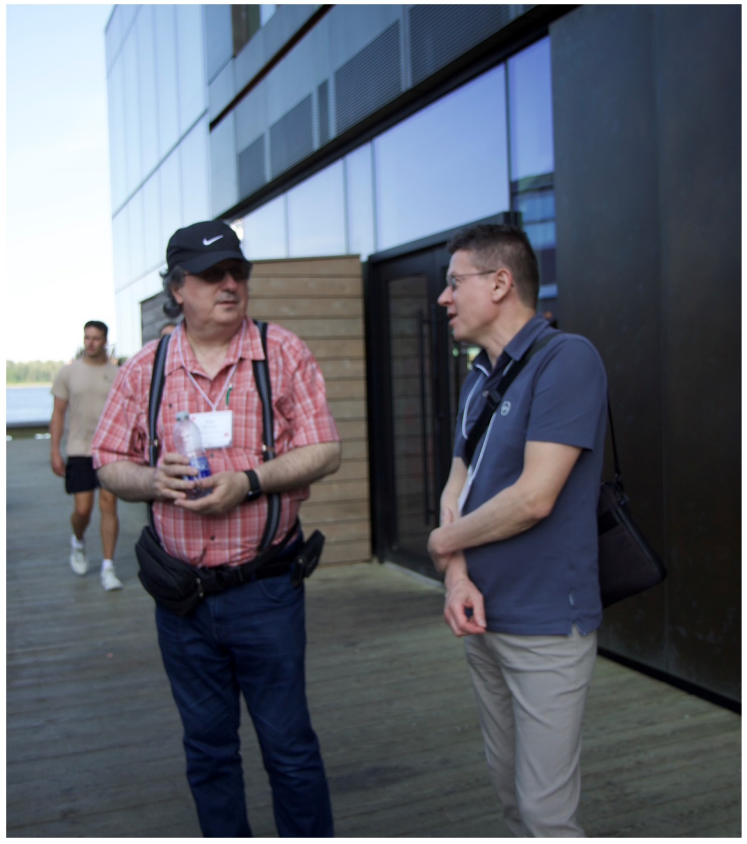


Nelaine Mora-Diez

Clockwise from top left: Edith Leal-Sánchez, Jonkwon Ha, Martha Yaghoubi Jouybari, Amir Ayati, Kyle Bryenton


Questions?
Want My Slides?
DAL
Kyle.Brenton@dal.ca

EXCURSION




CABLE WHARF
KITCHEN MARKET PATIO


ICMU
INTERNATIONAL CENTRE
FOR MATHEMATICS
IN UKRAINE


deuter
RACE


GANT

Russel Boyd and Plenary Lecturer Axel Becke

DAY 2

Viktor Staroverov

Richard Bowles

Josef Zwanziger


Zohreh
Khodadad


efano
Morgan
Acknowledgements
Eva
Ethan
Nisha
Biswas
Xiaoyu
Trevor
Masashi
Francesco
Josiah
Samad
Stefano
Morgan
MAP
CDAC

Eva Zurek


Summary
FHI-aims
ELSI
ELPA
Electronic Structure Library
Efficient, accurate framework for general-purpose electronic structure theory.
Common libraries (ELPA, ELSI & supported libraries, libxc etc.) furnish essential parts of the numerics, bridge to other projects.
Key scalability improvements for exact exchange: Hybrid DFT beyond 10,000 atoms.
Layered perovskites: Atomic structure, electronic & spin properties, electronic doping all within reach of dispersion-corrected, spin-orbit coupled hybrid DFT.
CHOISE
AUTOMATIC CAUTION DOOR

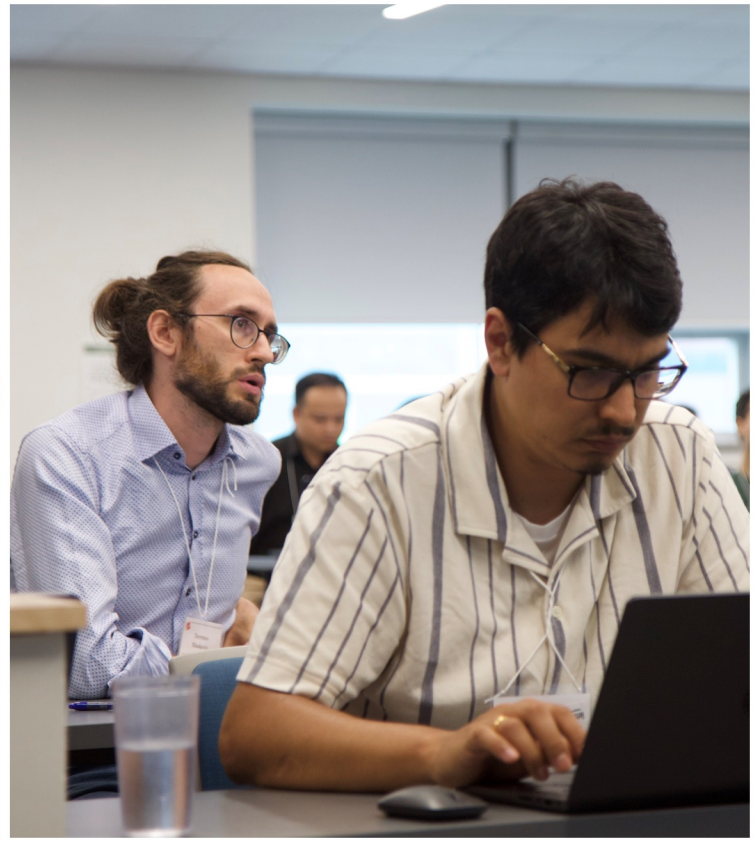
Volker Blum

Oleksandr Voznyy

Jason Pearson

Rodrigo Vargas-Hernández

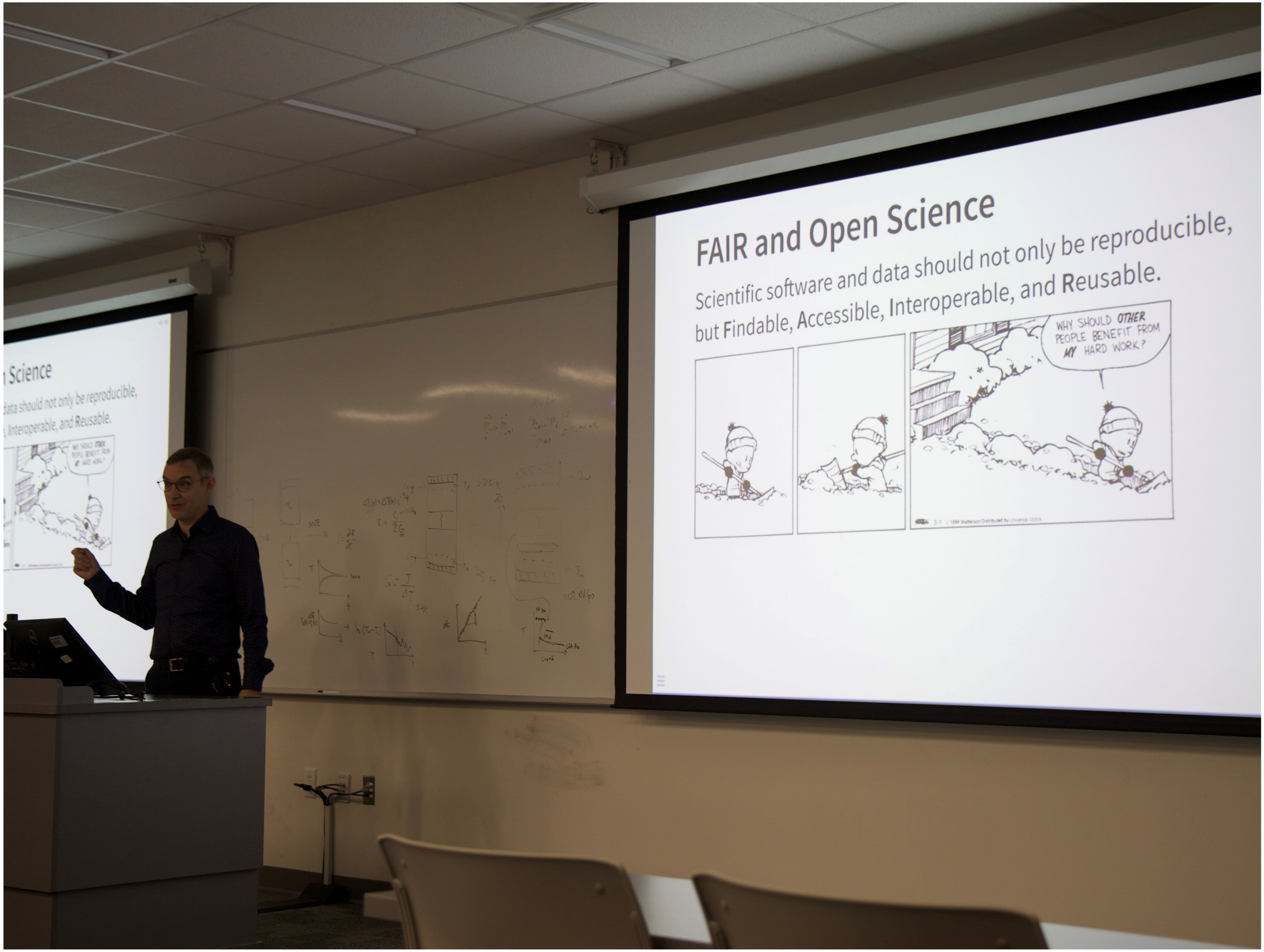
Clockwise from top left: Alastair Price, Gilles Peslherbe, Amer El-Samman



Clockwise from top left: Fanwang Meng, Mostafa Javaheri Moghadam, Mehdi Shamekhi, Jonathan Wang, Ehsan Ghasempouri

BANQUET

DAY 3



CATC Medal Lecturer Paul Ayers

Paul Ayers and Tom Woo

Patrick Bultinck

Farnaz Heidar-Zadeh and Paul Johnson

Piotr Piecuch

Lee Thompson

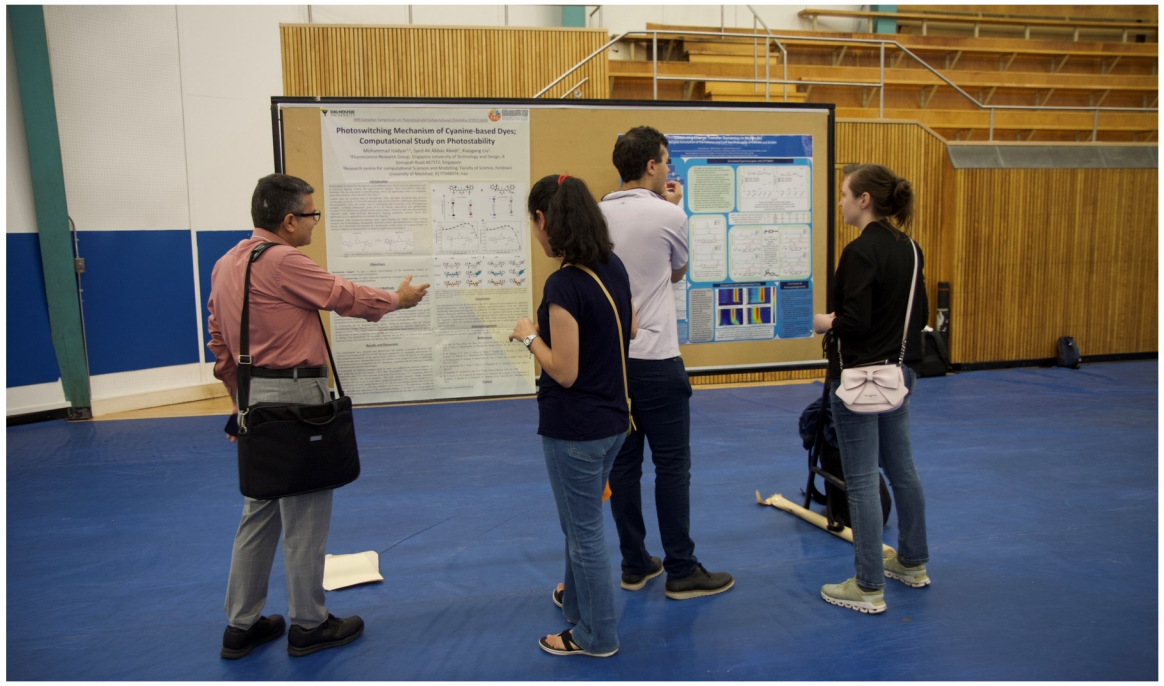
Thomas Baker and Kade Head-Marsden

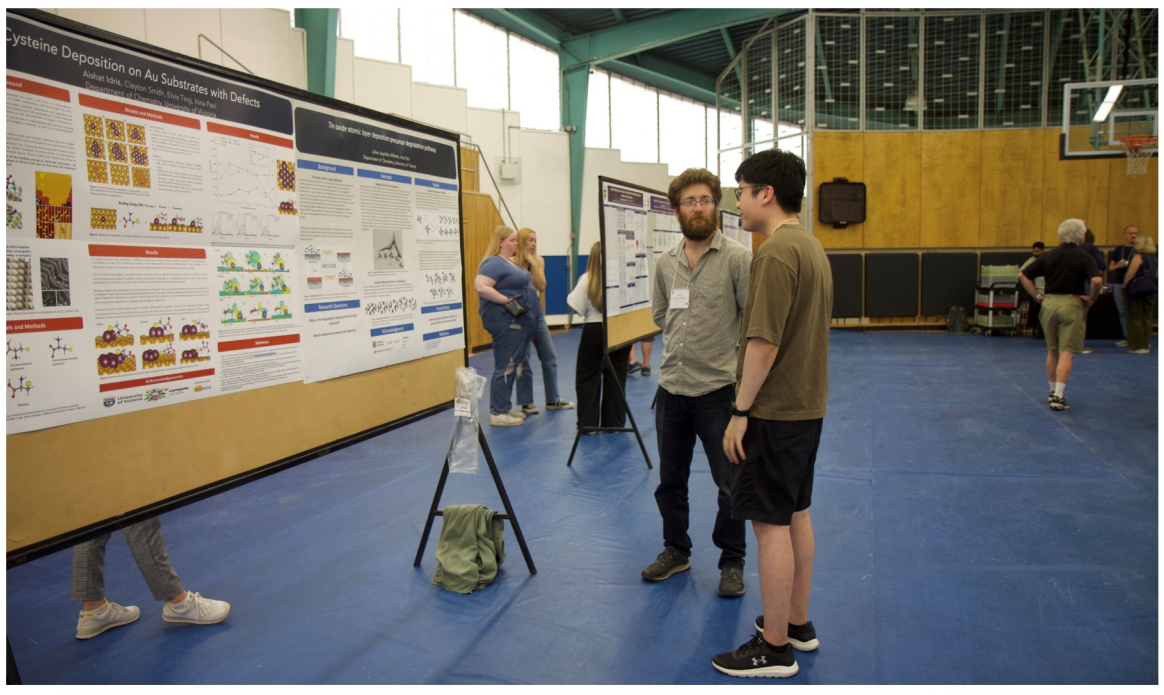
Matthias Degroote

Jakob Kottmann

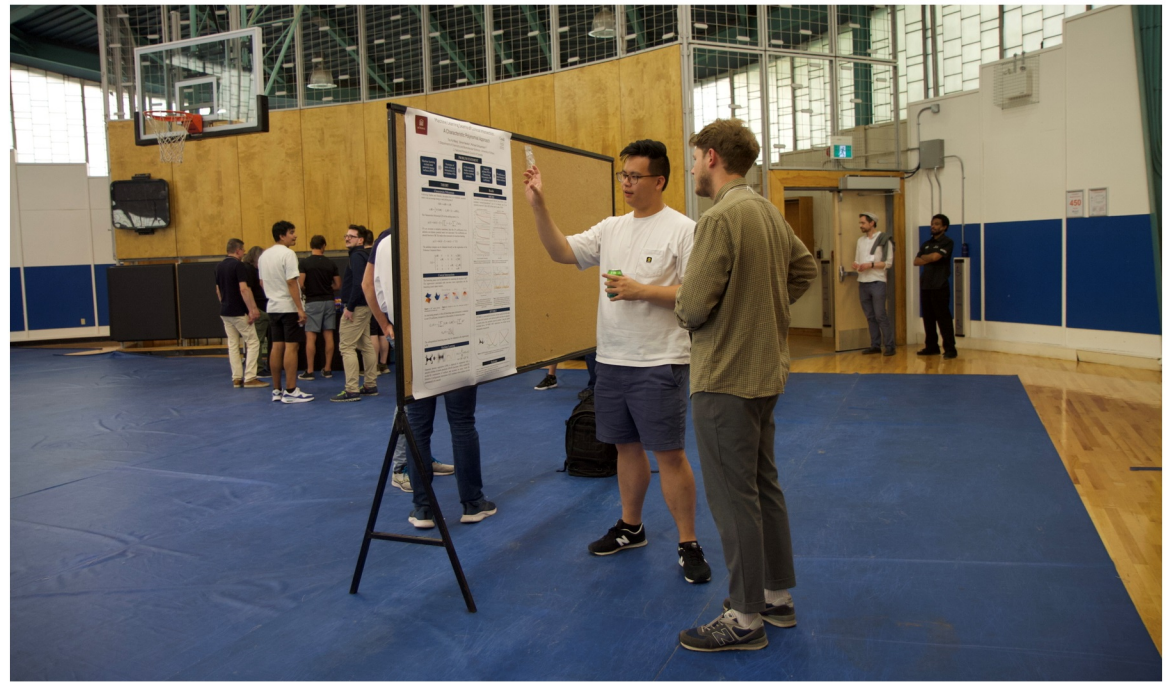

Marriott Hotel

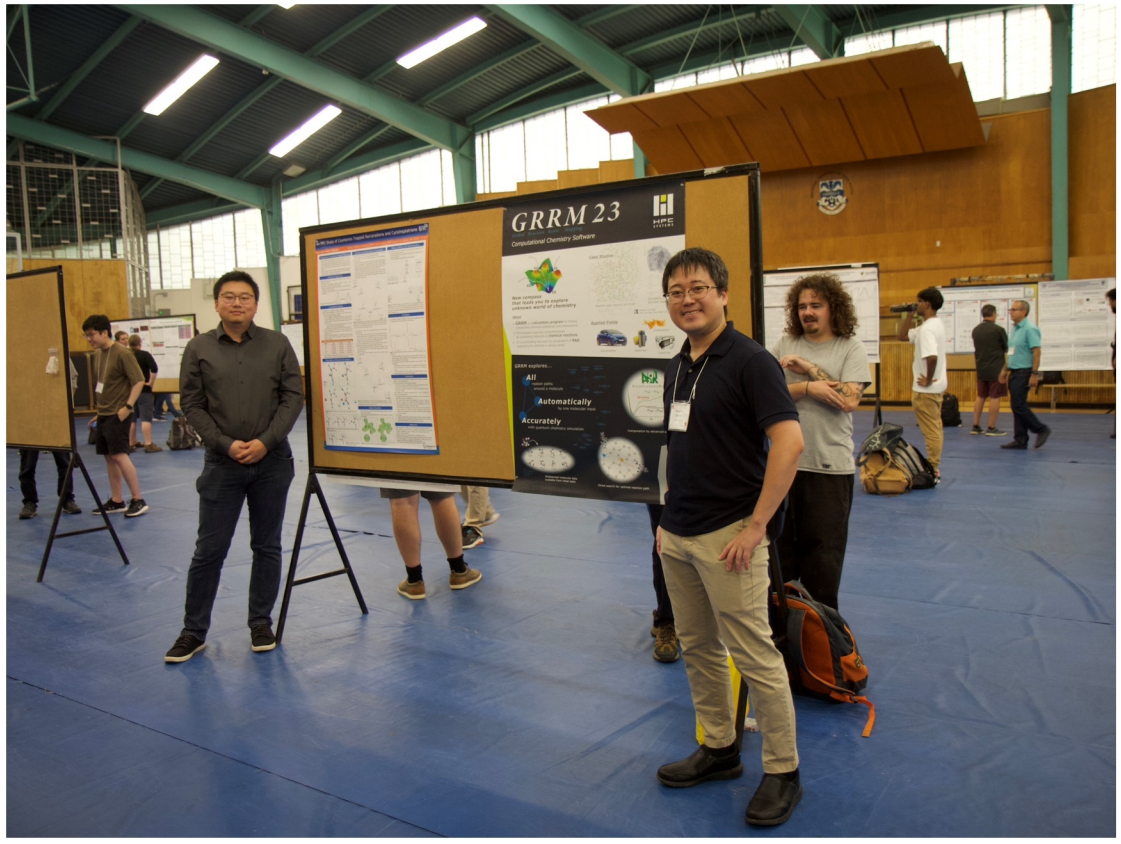
POSTERS

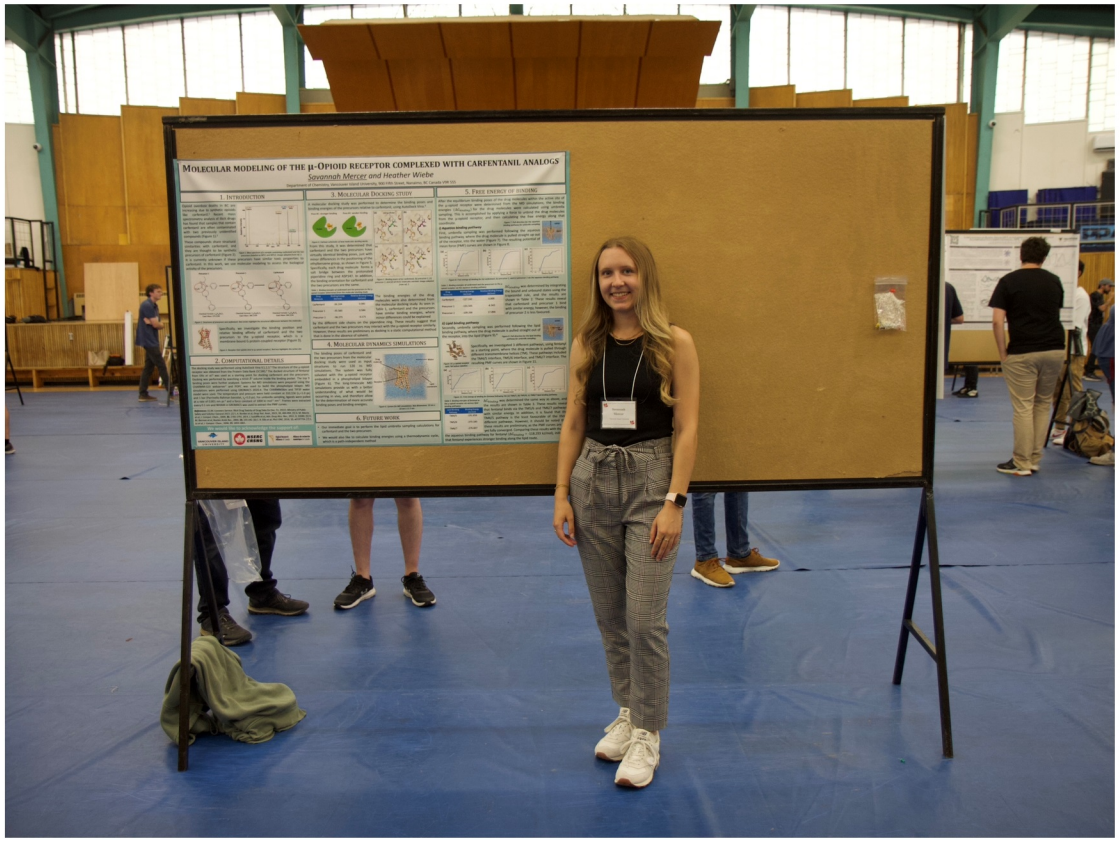

Photoswitching Mechanism of Cyanine-based Dyes; Computational Study on Photostability

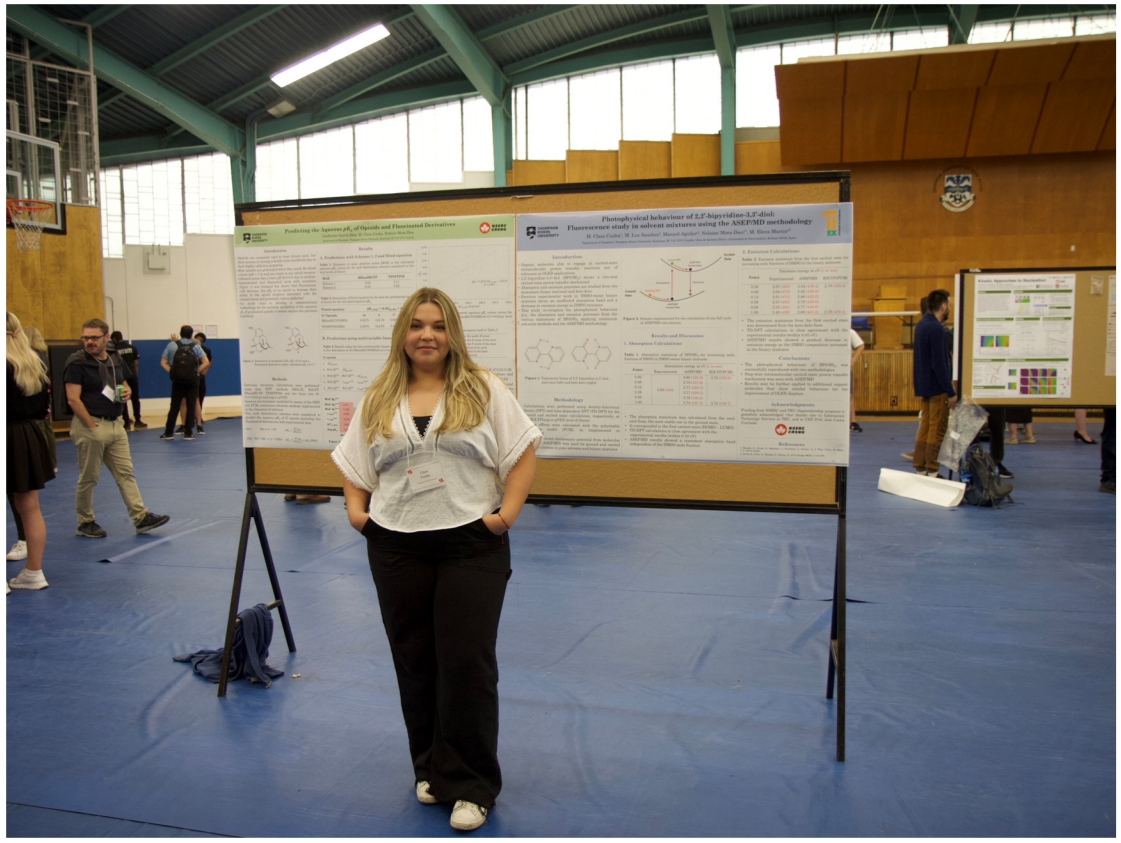

Cysteine Deposition on Au Substrates with Defects
Aishat Idris, Clayton Smith, Elvia Ting, Inna Paci
Department of Chemistry, University of Surrey
Tin oxide atomic layer deposition precursor deposition setting
Background
Results
Research Questions
Conclusions
Acknowledgements

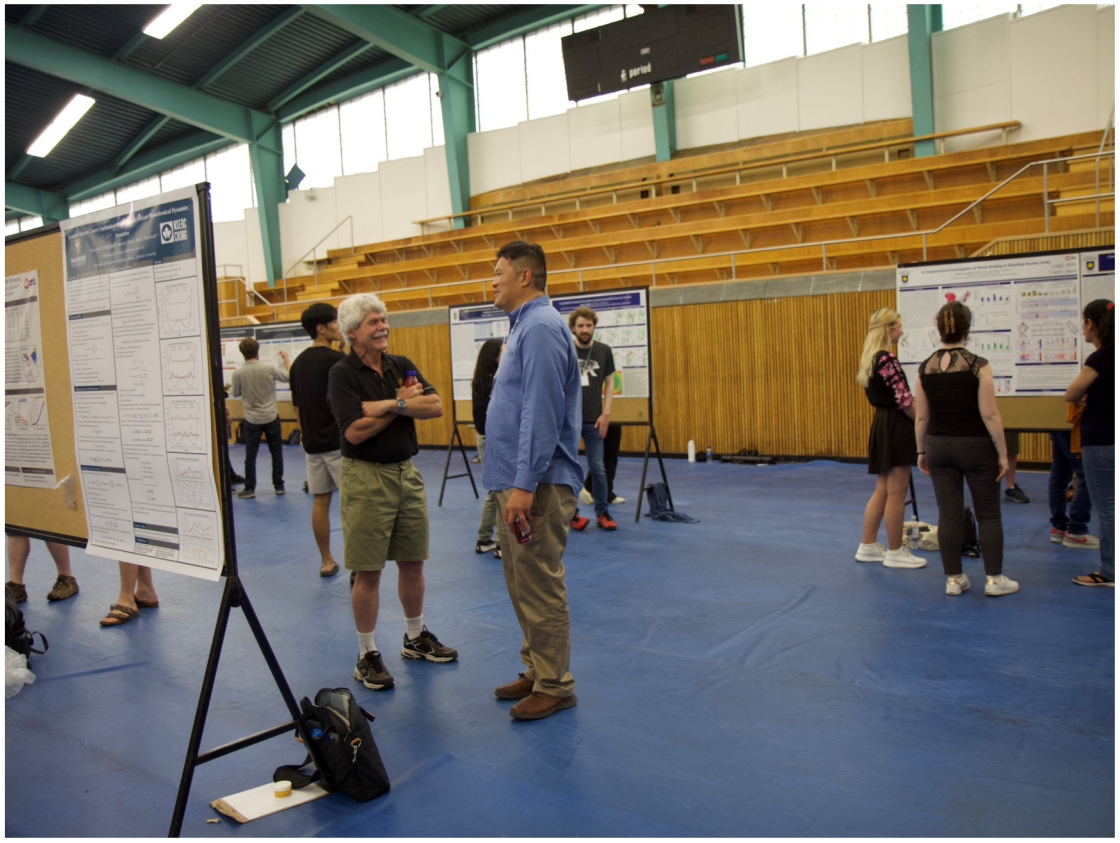

Dynamic Heterogeneities in Confinement
ABSTRACT
DYNAMICS
DYNAMICAL HETEROGENEITIES
MODEL & METHODS
FUTURE WORK
STRUCTURE

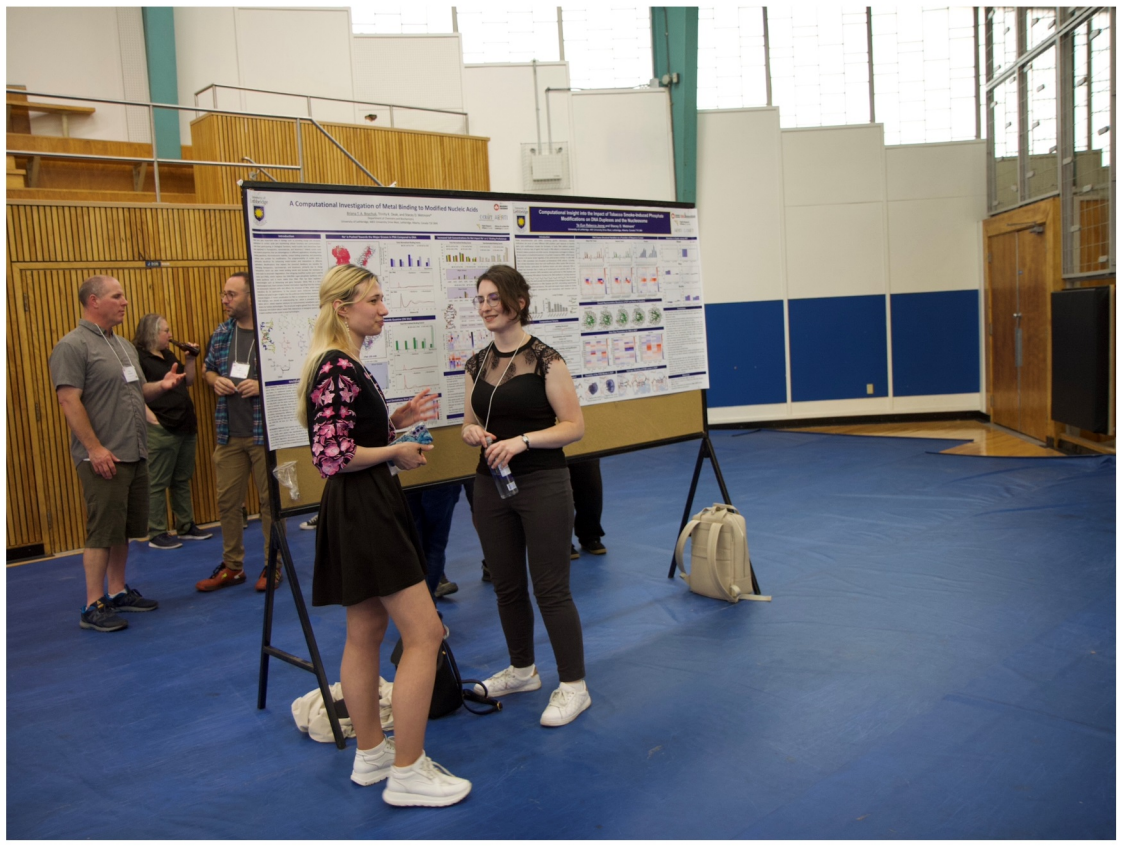


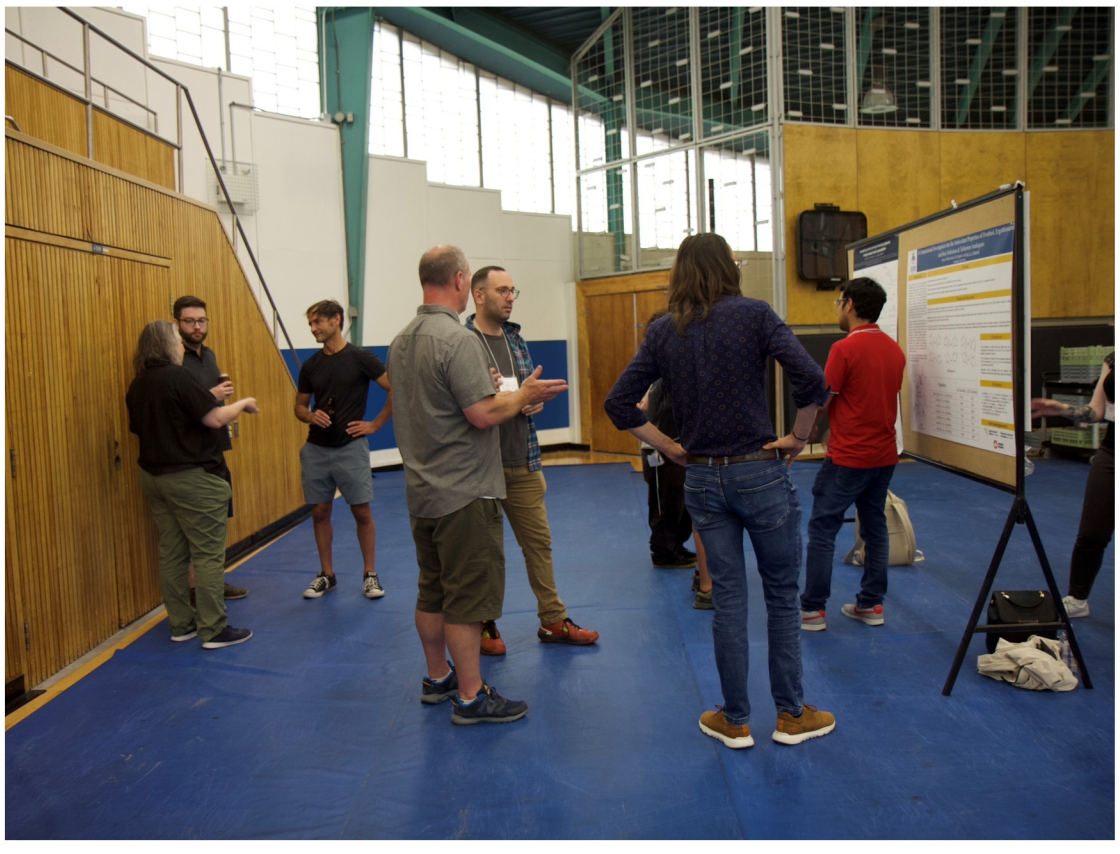

GRRM 23
Computational Chemistry Software
All
Automatically
Accurately

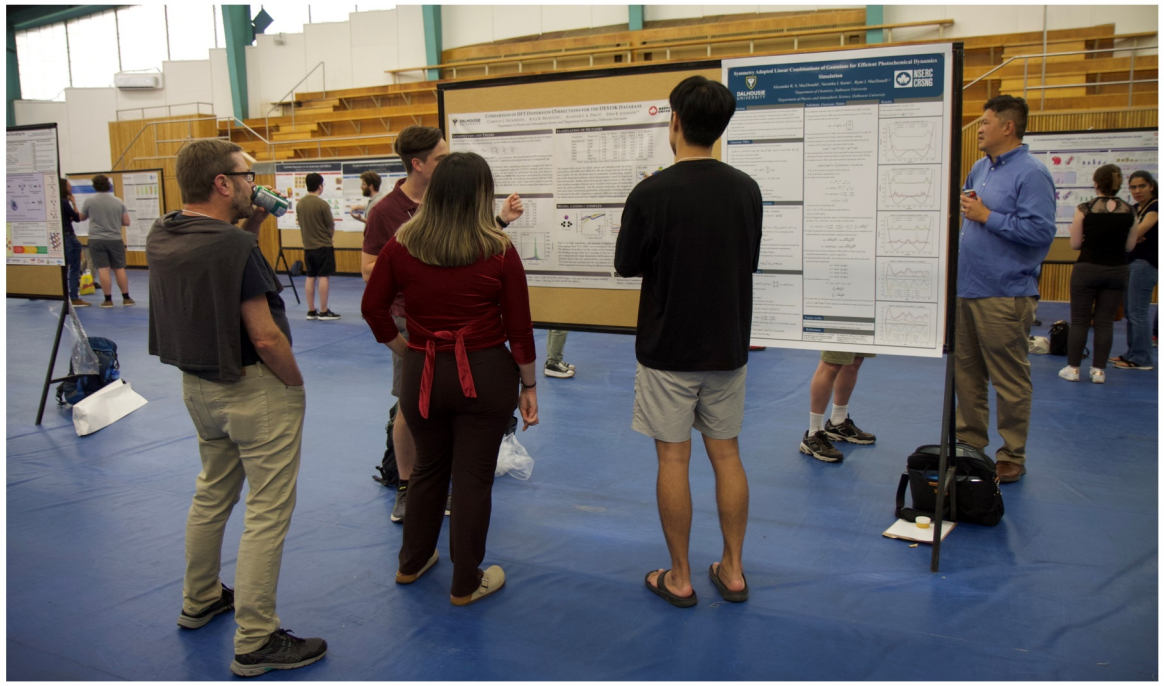

MOLECULAR MODELING OF THE μ-OPIOID RECEPTOR COMPLEXED WITH CARFENTANIL ANALOGS
Savannah Mercer and Heather Wiebe
1. INTRODUCTION
2. COMPUTATIONAL DETAILS
3. MOLECULAR DOCKING STUDY
4. MOLECULAR DYNAMICS SIMULATIONS
5. FREE ENERGY OF BINDING
6. FUTURE WORK

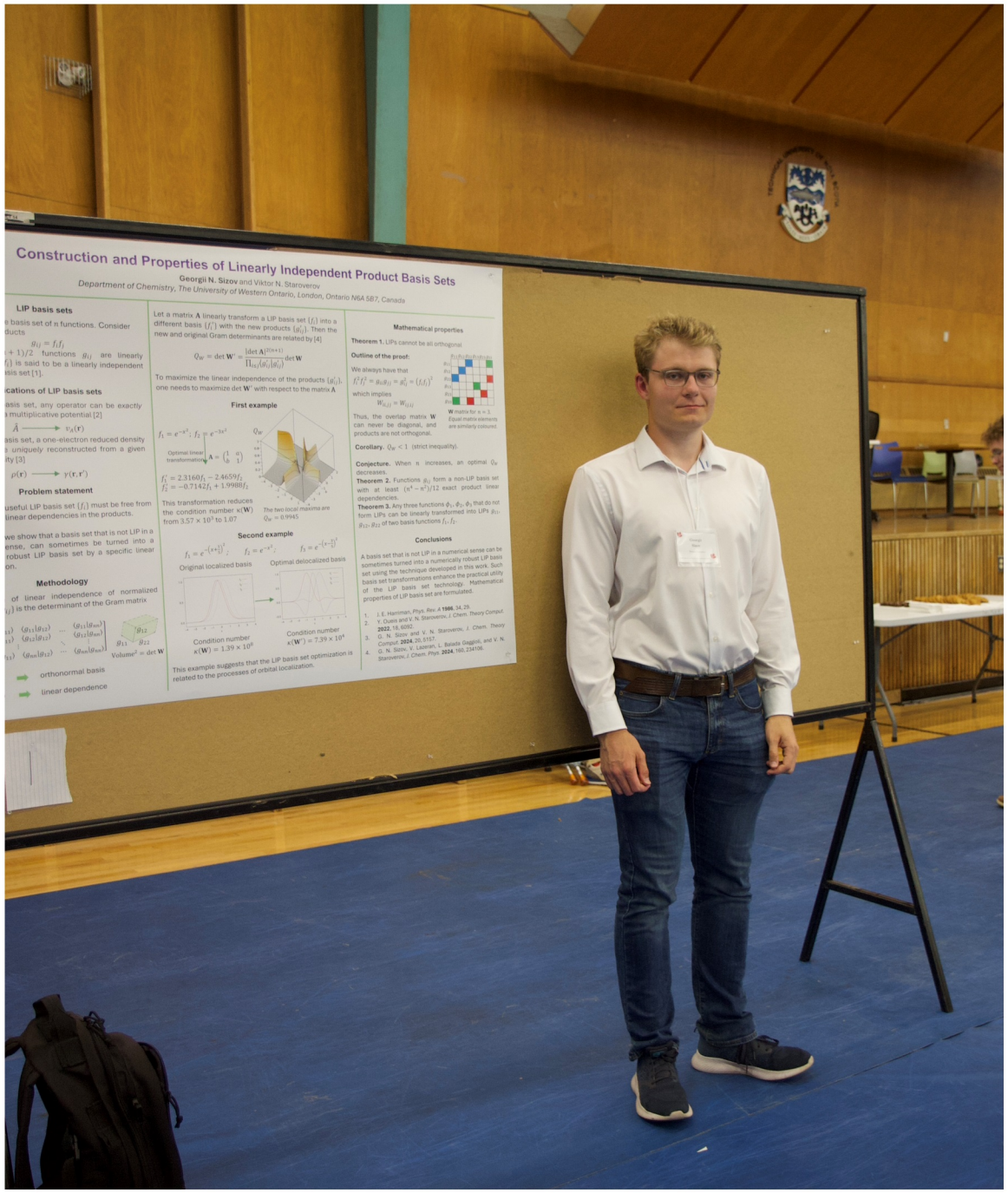

Predicting the Aqueous pK_a of Opioids and Fluorinated Derivatives
Photophysical behaviour of 2,2'-bipyridine-3,3'-diol: Fluorescence study in solvent mixtures using the ASEP/MD methodology

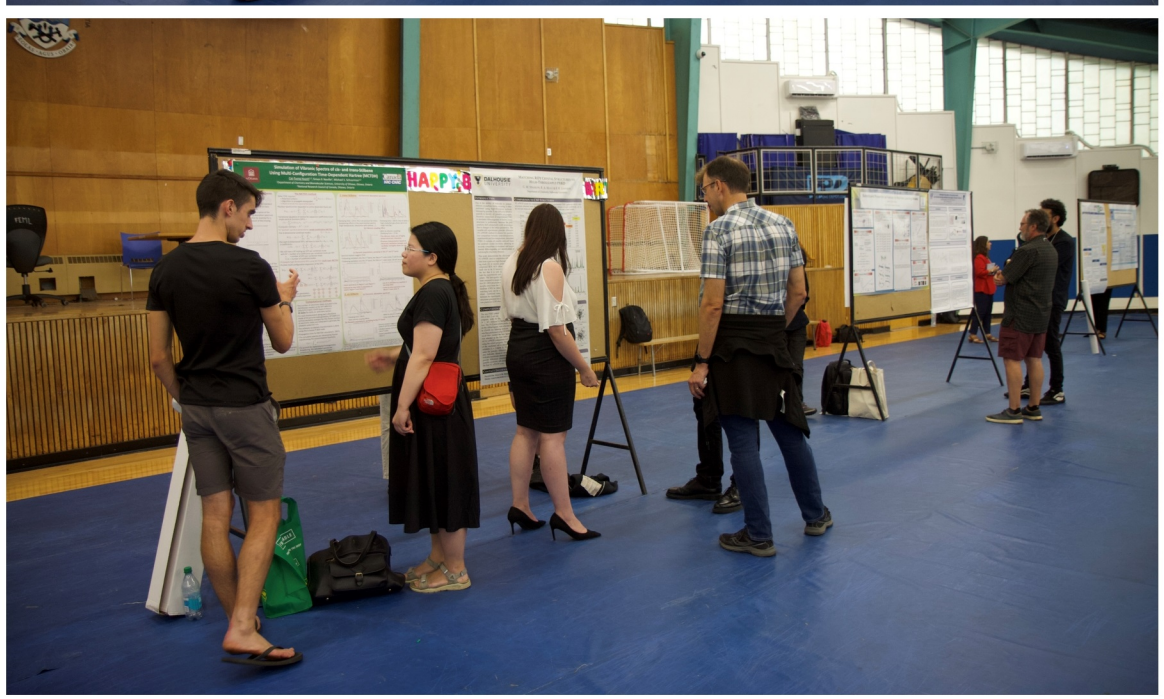



A Computational Investigation of Metal Binding to Modified Nucleic Acids
Computational Insight into the Impact of Tobacco Smoke-Induced Proximity Modifications on DNA Duplexes and the Nucleosome

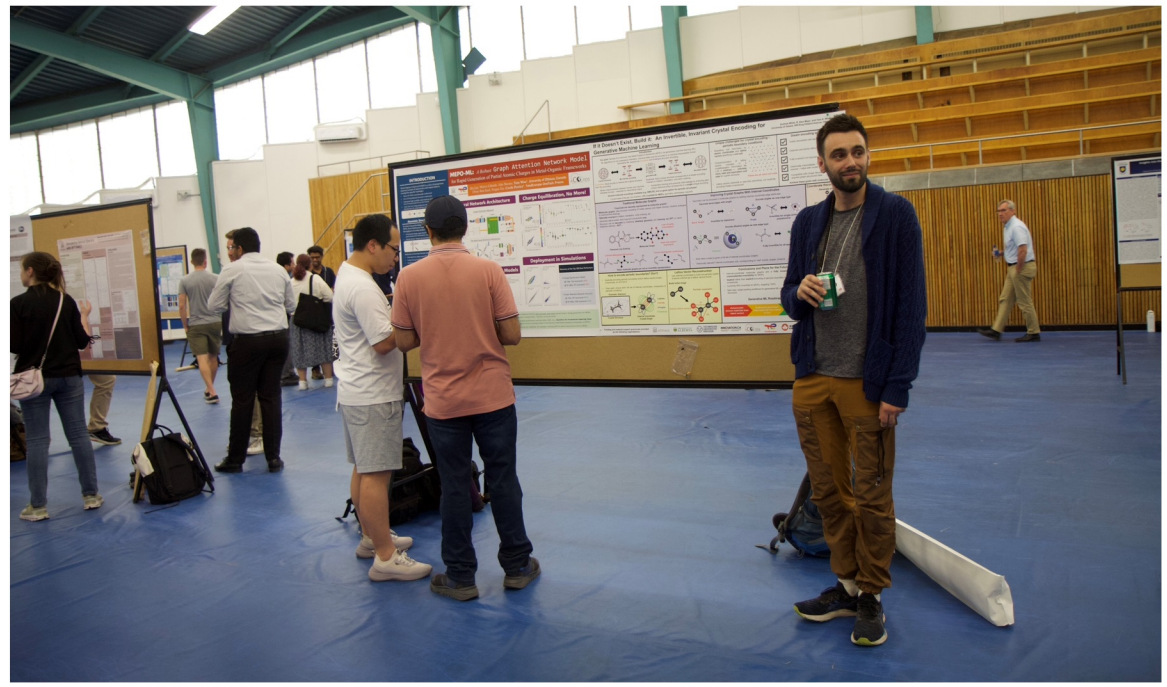




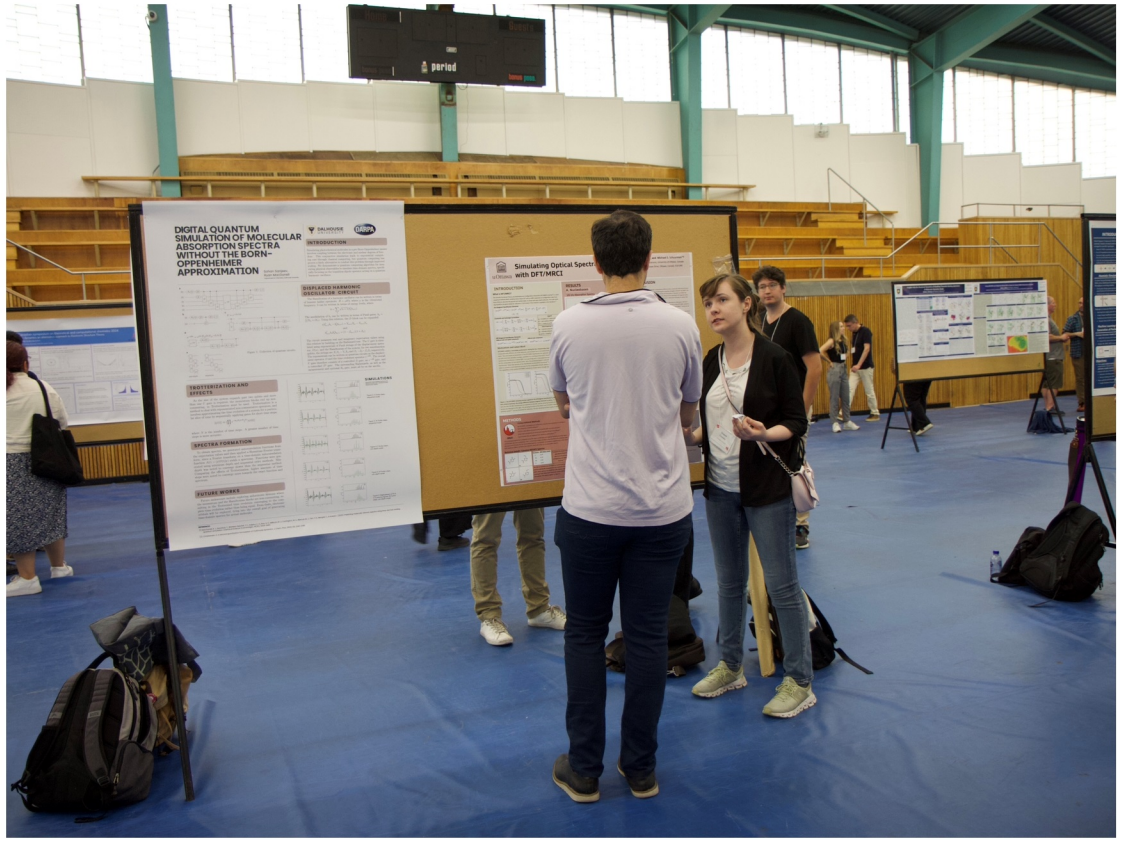

Construction and Properties of Linearly Independent Product Basis Sets
Georgii N. Sizov and Viktor N. Staroverov
Department of Chemistry, The University of Western Ontario, London, Ontario N6A 5B7, Canada
LIP basis sets
Problem statement
Methodology
orthonormal basis
linear dependence
First example
Second example
Original localized basis
Optimal delocalized basis
Mathematical properties
Conclusions

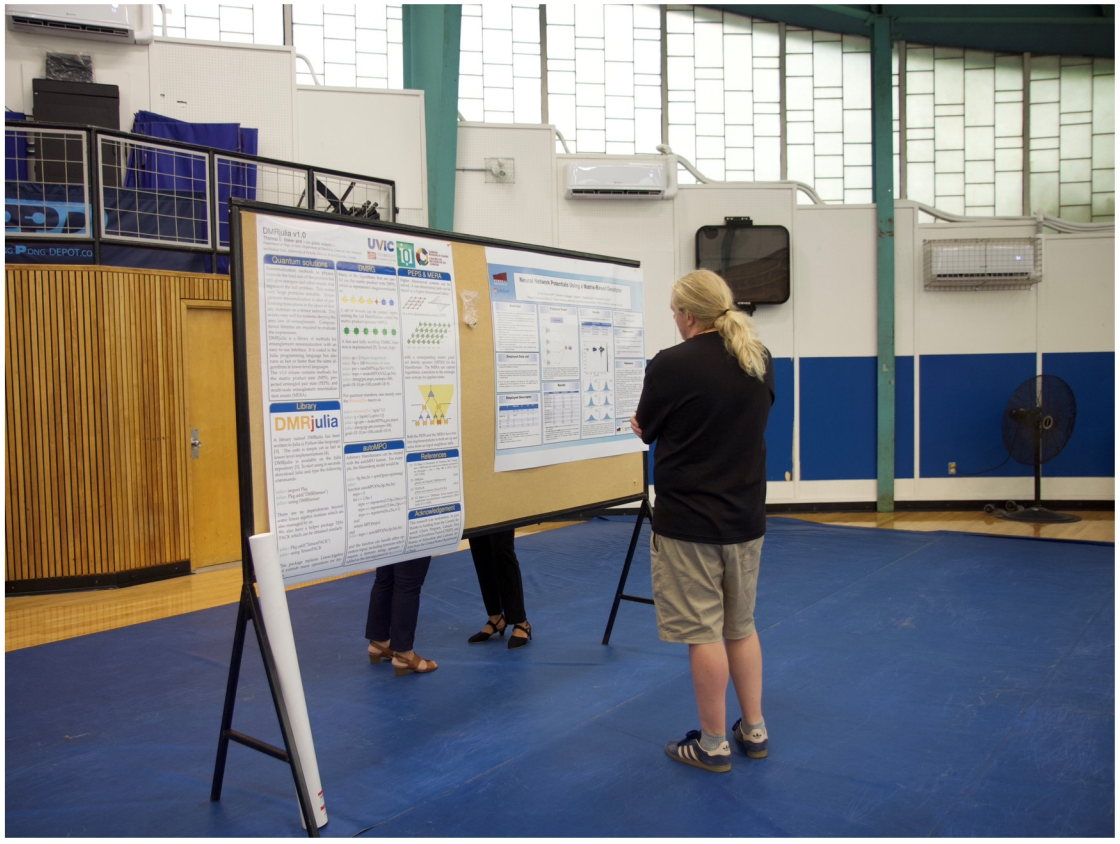

HAPPY

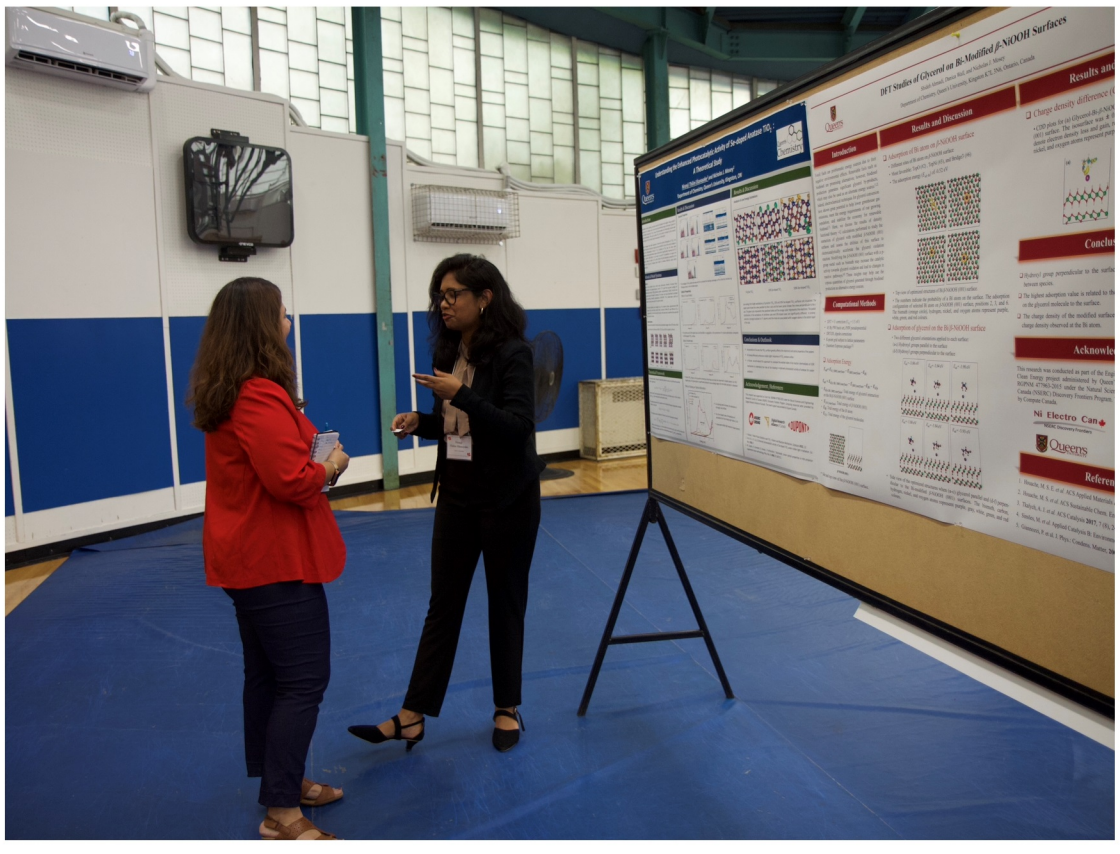

UNIVERSITY OF ALBERTA
Parametrization of a Molecular Excitonic Quantum Battery Model
Abstract
Methodology
Introduction
Dark State
References
ACKNOWLEDGEMENTS

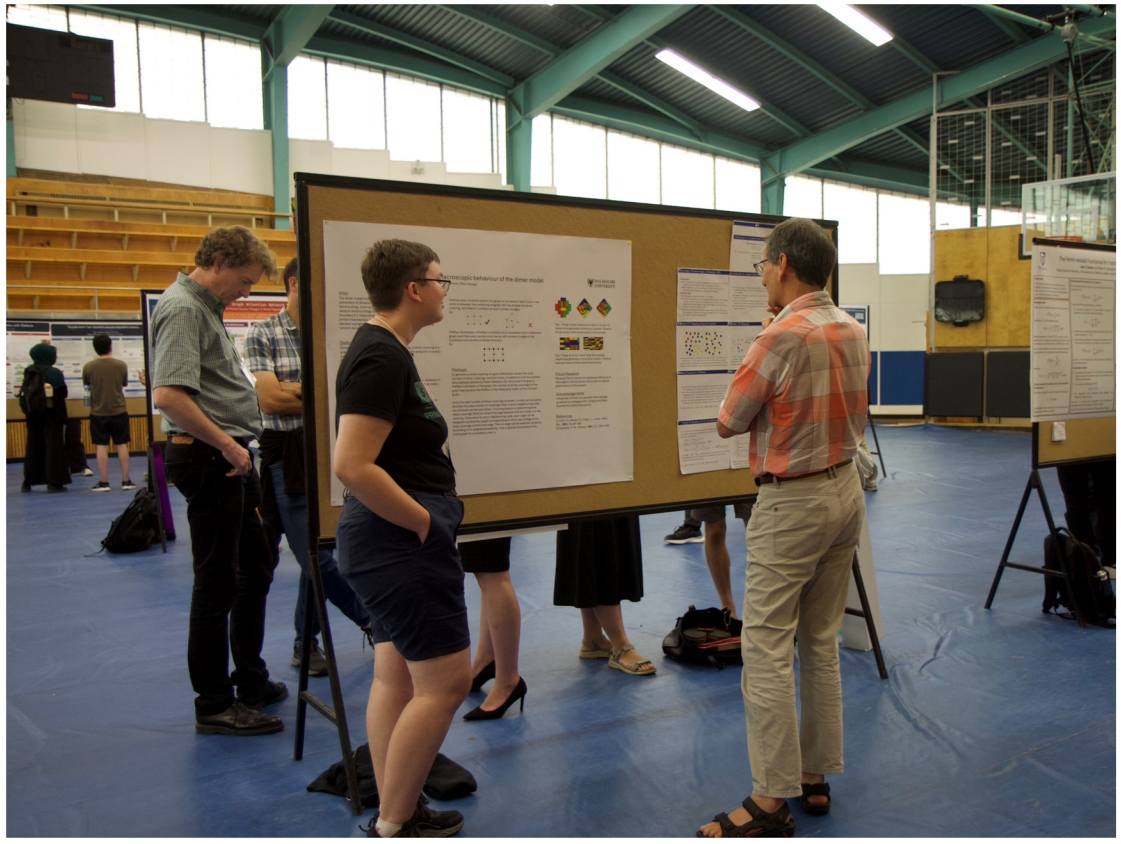

MHPO-MLP: A Robust Graph Attention Network Model
Charge Equilibration, No More!

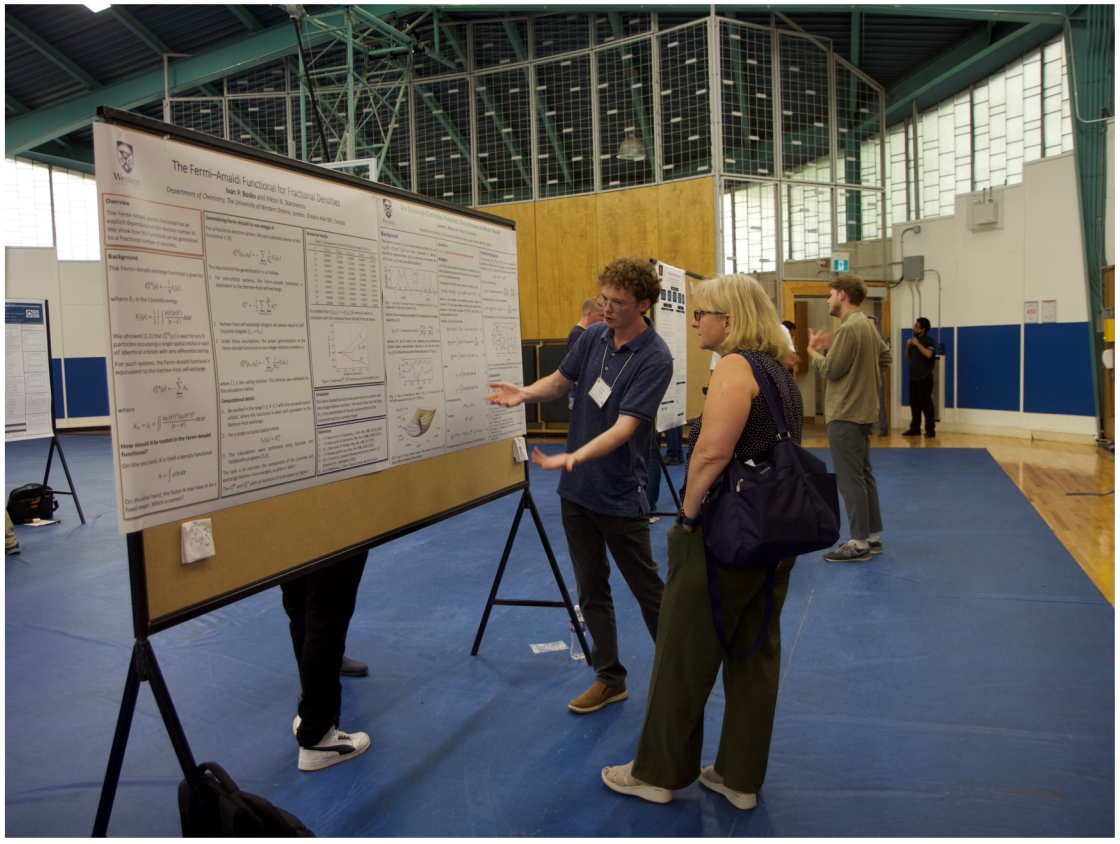

Substituent Properties as Features in Machine Learning Models

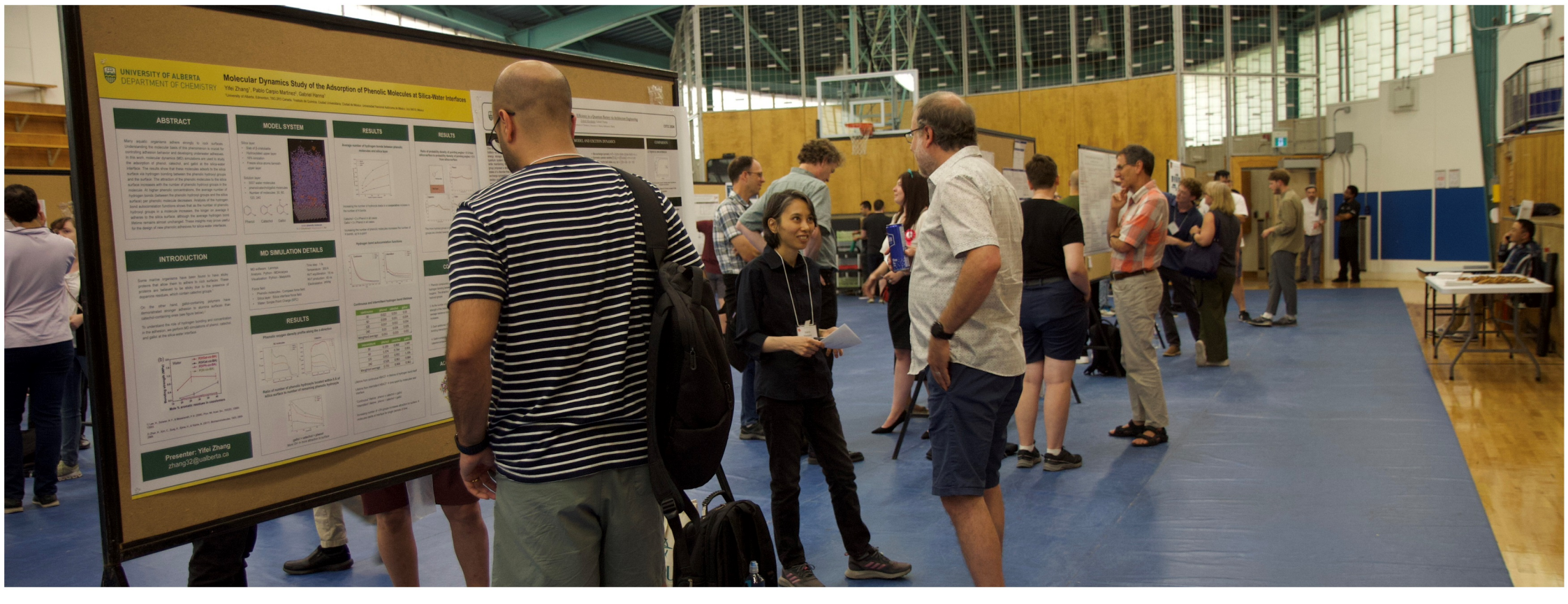

DIGITAL QUANTUM SIMULATION OF MOLECULAR ABSORPTION SPECTRA WITHOUT THE BORN-OPPENHEIMER APPROXIMATION
Simulating Optical Spectra with DFT/MRCI

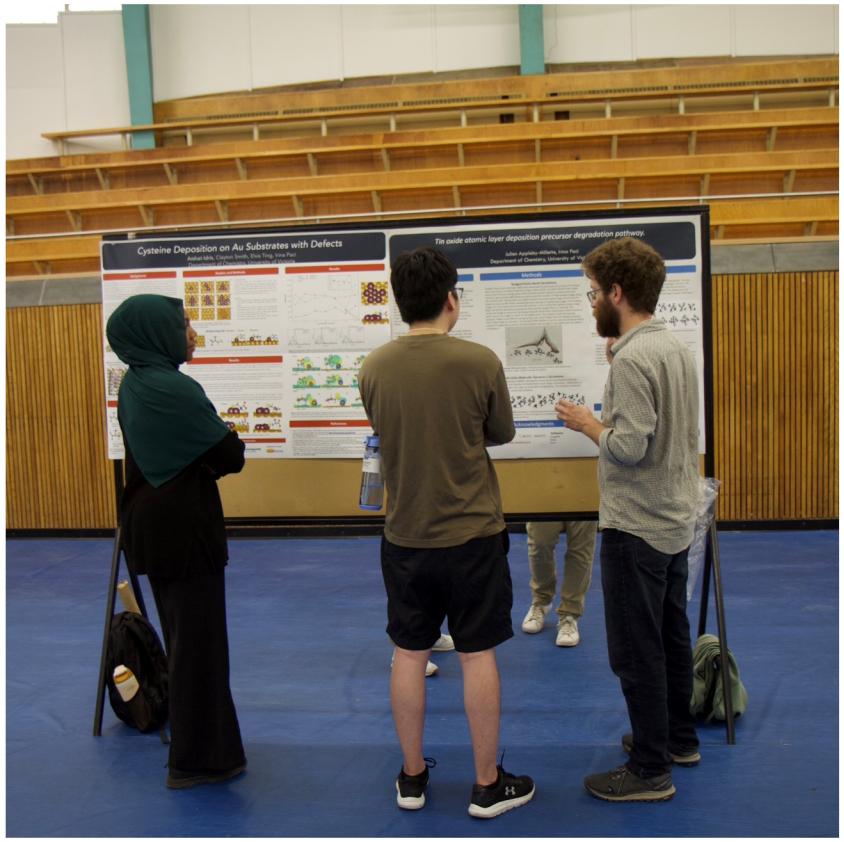

DMRjulia v1.0
DMRjulia

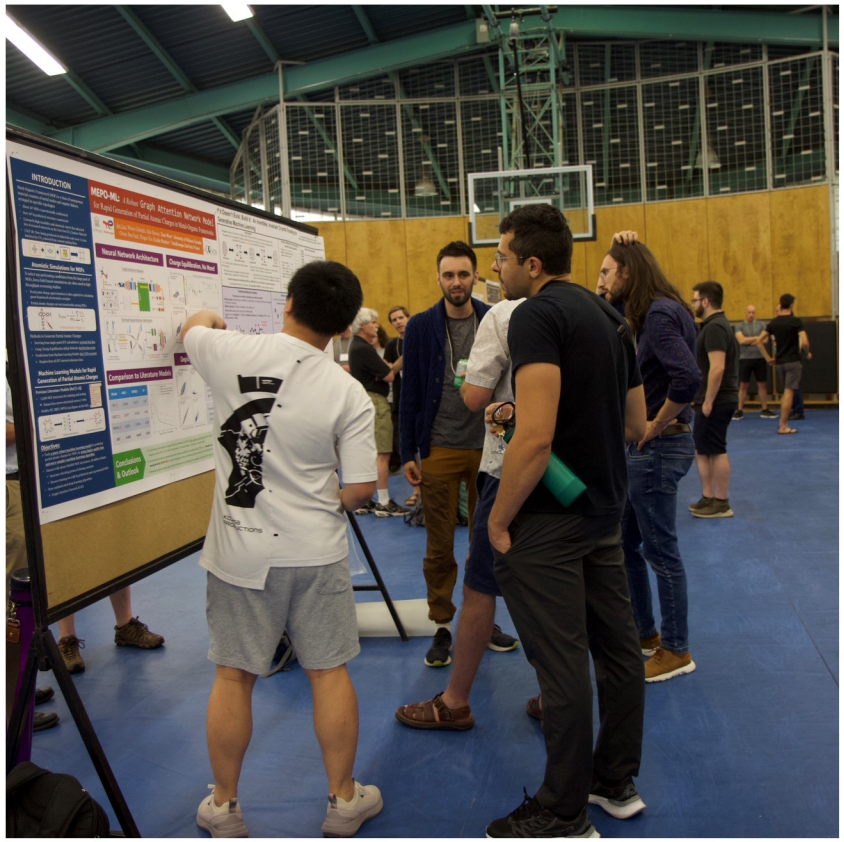

DFT Studies of Glycerol on Bi-Modified β-NiOOH Surfaces
Results and Discussion
Introduction
Computational Methods

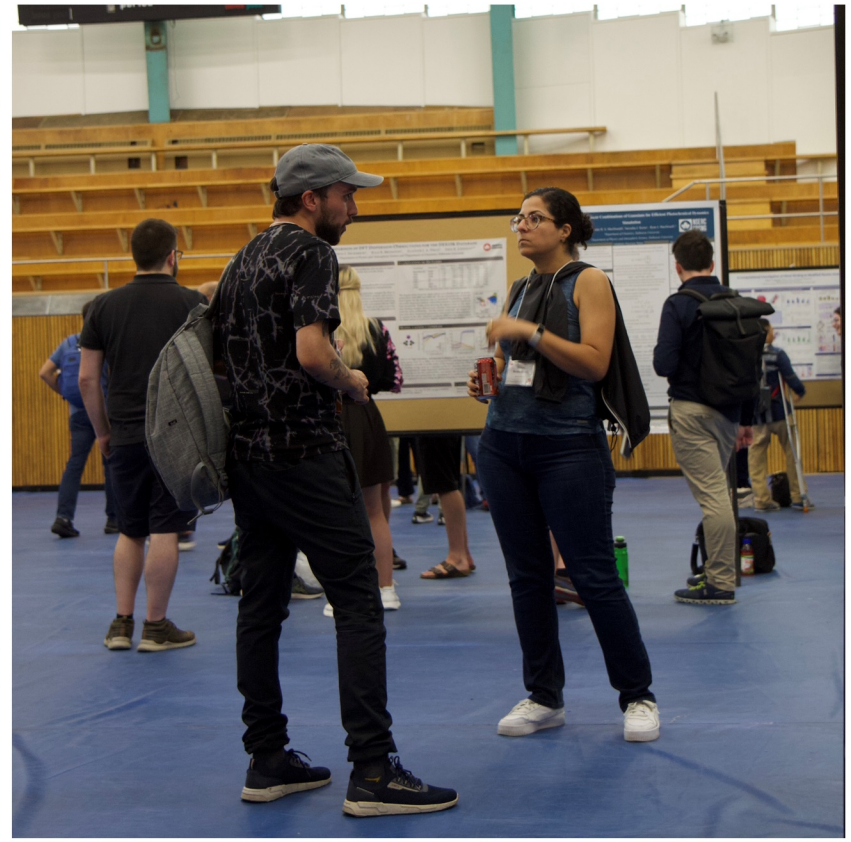

Microscopic behaviour of the dimer model


The Fermi–Amaldi Functional for Fractional Densities
Ivan P. Bosko and Viktor N. Staroverov
Department of Chemistry, The University of Western Ontario, London, Ontario N6A 5B7, Canada
Overview
Background
Generalizing Fermi–Amaldi to non-integer N
Results
Conclusions


UNIVERSITY OF ALBERTA
DEPARTMENT OF CHEMISTRY
Molecular Dynamics Study of the Adsorption of Phenolic Molecules at Silica-Water Interfaces
Yifei Zhang, Pablo Carpio Martinez, Gabriel Hanna
ABSTRACT
MODEL SYSTEM
RESULTS
INTRODUCTION
MD SIMULATION DETAILS
RESULTS
Presenter: Yifei Zhang
zhang32@ualberta.ca


Cysteine Deposition on Au Substrates with Defects
Tin oxide atomic layer deposition precursor degradation pathway.
Methods
Results
Acknowledgments

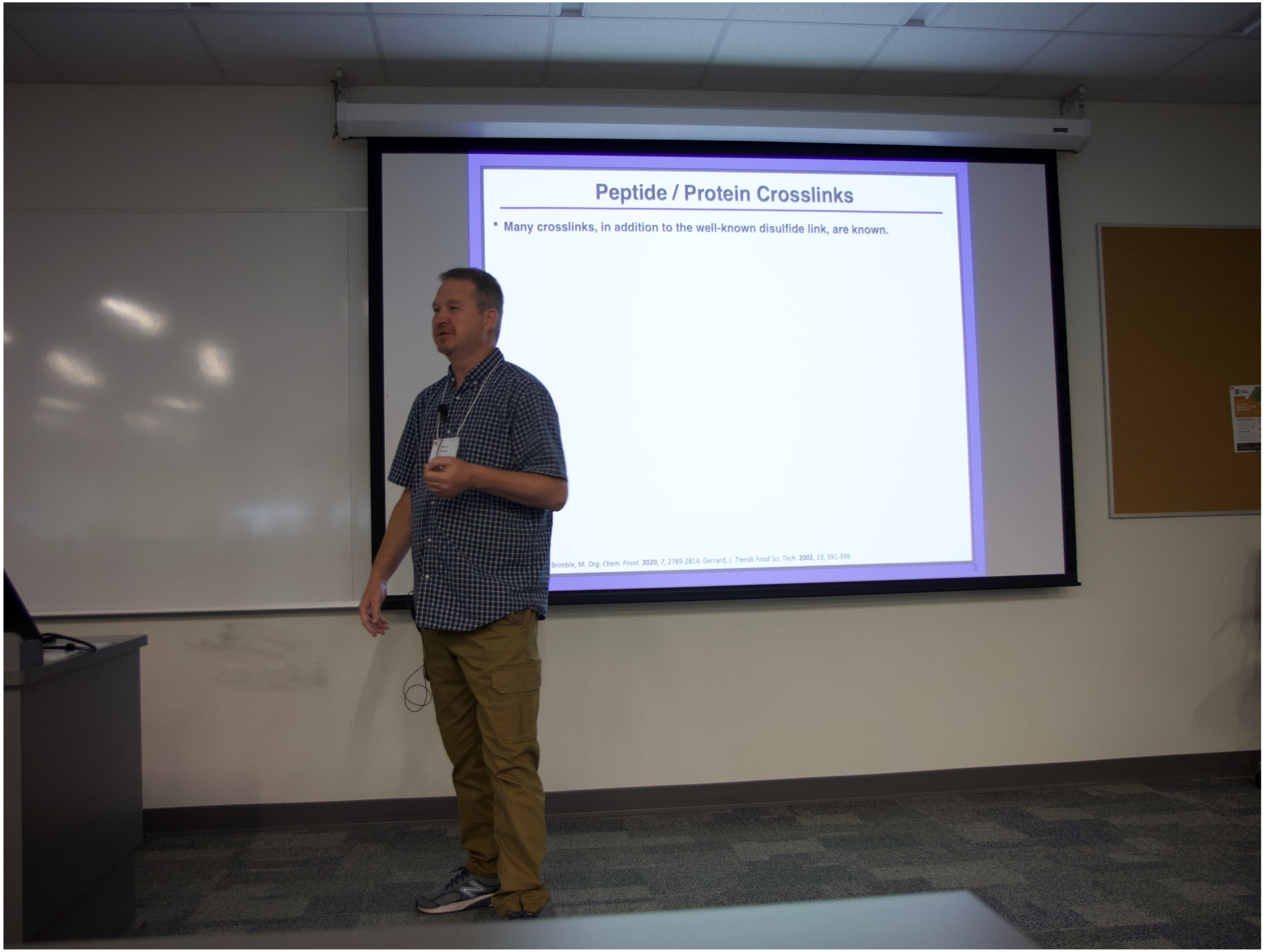

INTRODUCTION
MEPO-ML:
Neural Network Architecture
Charge Equilibration, Re-Norm
Comparison to Literature Models
Conclusions & Outlook
Objectives



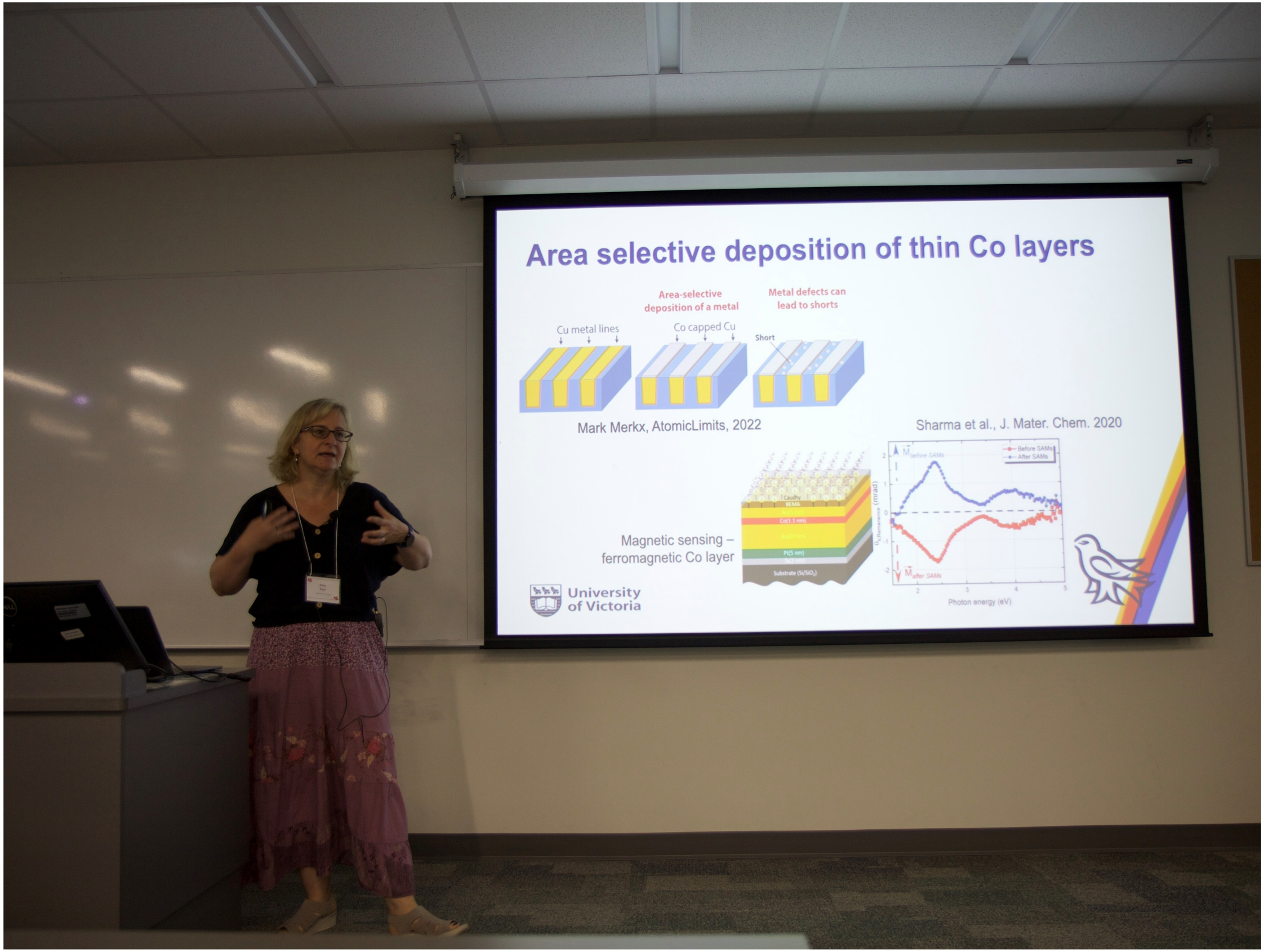
Francesco Gentile

DAY 4

Heather Wiebe


Peptide / Protein Crosslinks
• Many crosslinks, in addition to the well-known disulfide link, are known.
Brimble, M. Org. Chem. Front. 2020, 7, 2789-2814. Gerrard, J. Trends Food Sci. Tech. 2002, 13, 391-399.

James Gauld


Area selective deposition of thin Co layers
Area-selective deposition of a metal
Metal defects can lead to shorts
Cu metal lines
Co capped Cu
Short
Mark Merkx, AtomicLimits, 2022
Sharma et al., J. Mater. Chem. 2020
Magnetic sensing – ferromagnetic Co layer
Caudhy
BEMA
Co(1.1 nm)
Pt(5 nm)
Substrate (Si/SiO2)
Before SAMs
After SAMs
Photon energy (eV)
University of Victoria

Irina Paci

Gregory Beran

Conrard Tetsassi Feugmo

Jochen Autschbach

Michael Schuurman


Farnaz
Heidar-Zadeh

Terry Blaskovits

Simon Neville

Best Poster Award (Runner-Up): David Samuvel Michael

Best Poster Award (Runner-Up): Jun Luo

Best Poster Award: Vivek Das

Best Contributed Talk Award: Kyle Bryenton

Photography
Stijn De Baerdemacker
Leanne D. Chen

Design
Leanne D. Chen