

29th Canadian Symposium on Theoretical and Computational Chemistry



CSTCC 2022

Canadian Association of Theoretical Chemists



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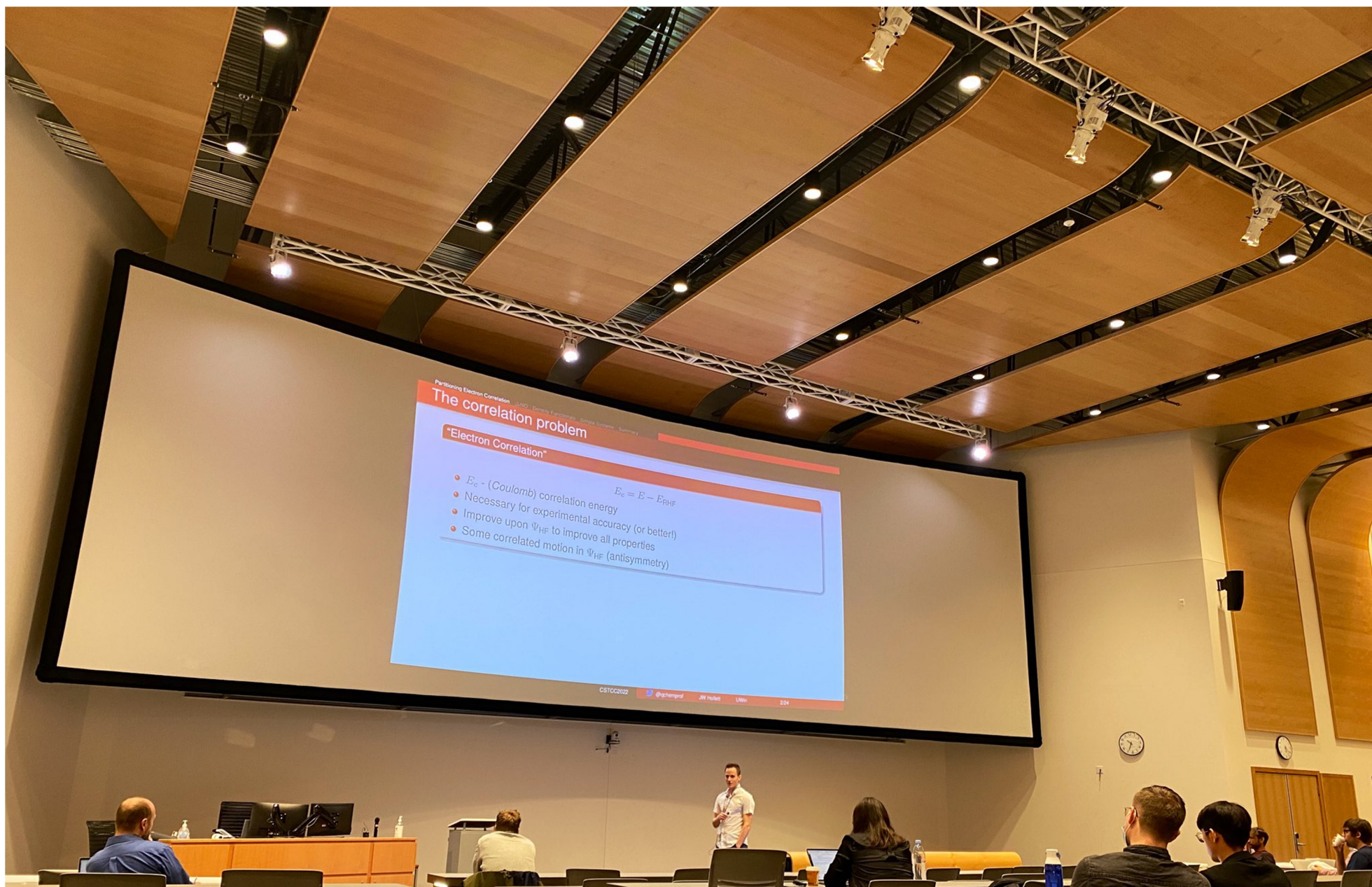
Canadian Association of Theoretical Chemists



Llewellyn Thomas- 1927
Enrico Fermi- 1927

$$T = C_F \int \rho(\mathbf{r})^{5/3} d\mathbf{r}$$

Dennis Salahub



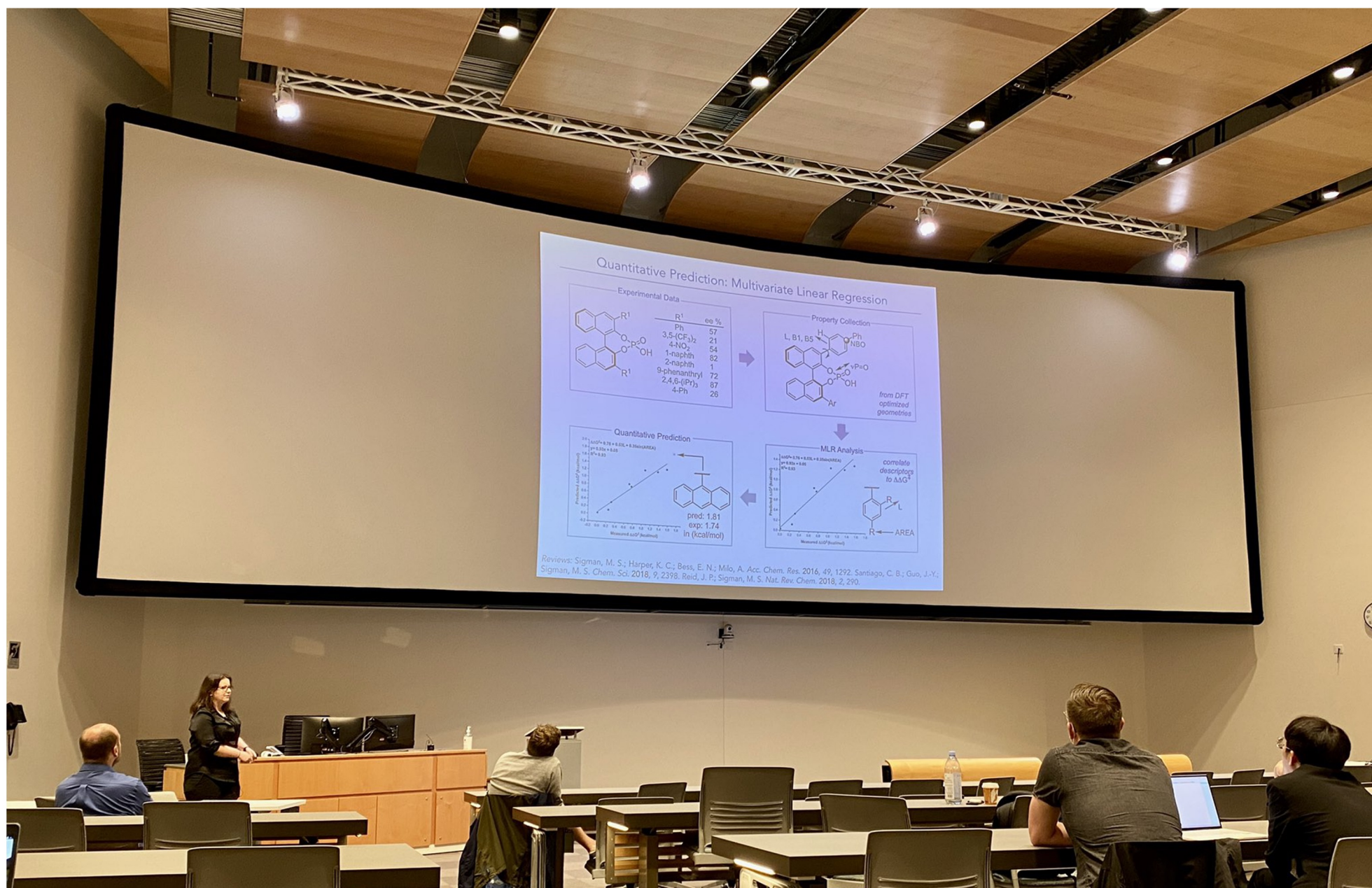
Partitioning Electron Correlation
The correlation problem

"Electron Correlation"

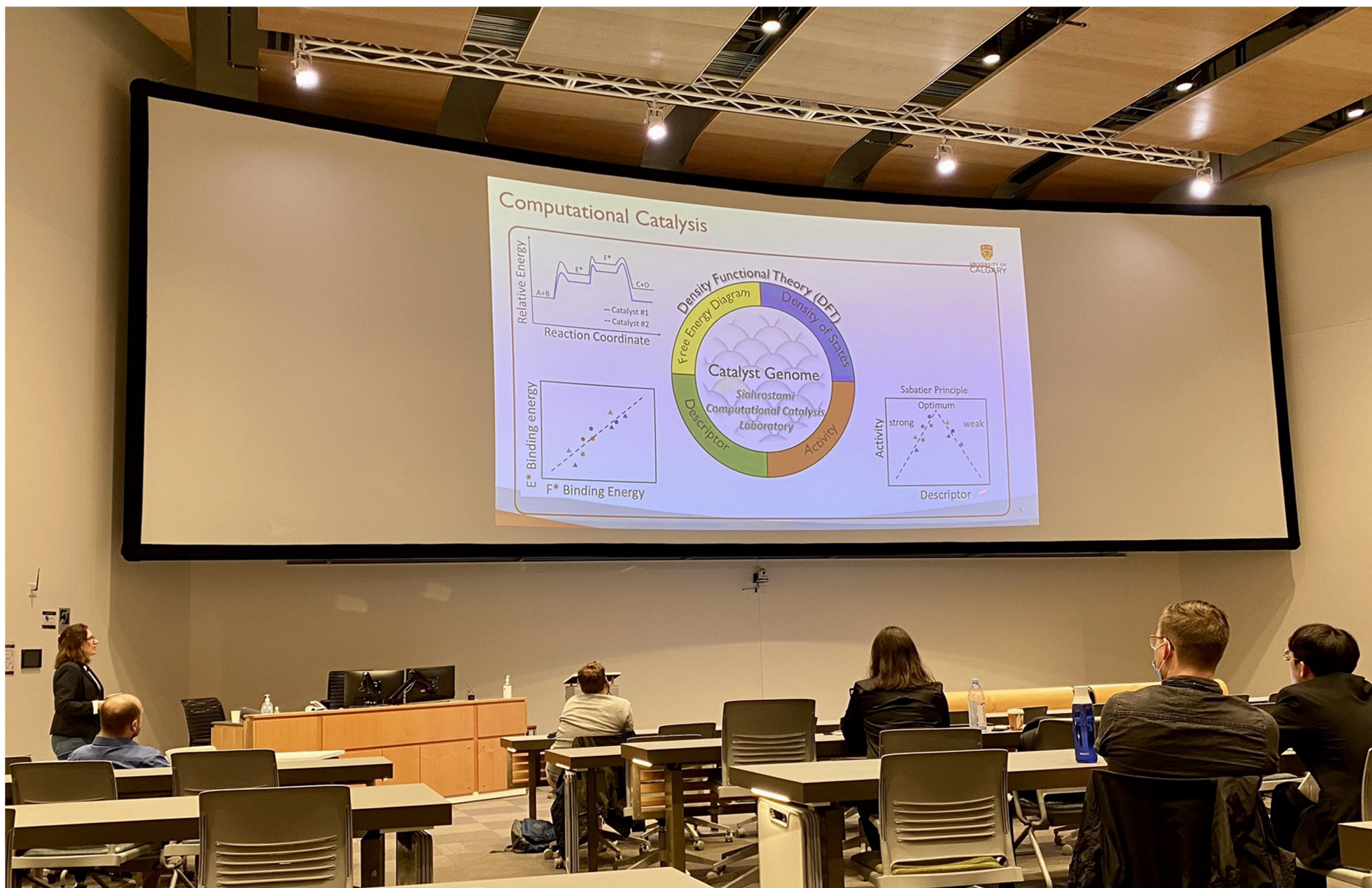
- E_c - (Coulomb) correlation energy
- Necessary for experimental accuracy (or better!)
- Improve upon Ψ_{HF} to improve all properties
- Some correlated motion in Ψ_{HF} (antisymmetry)

$$E_c = E - E_{RHF}$$

Joshua Hollett



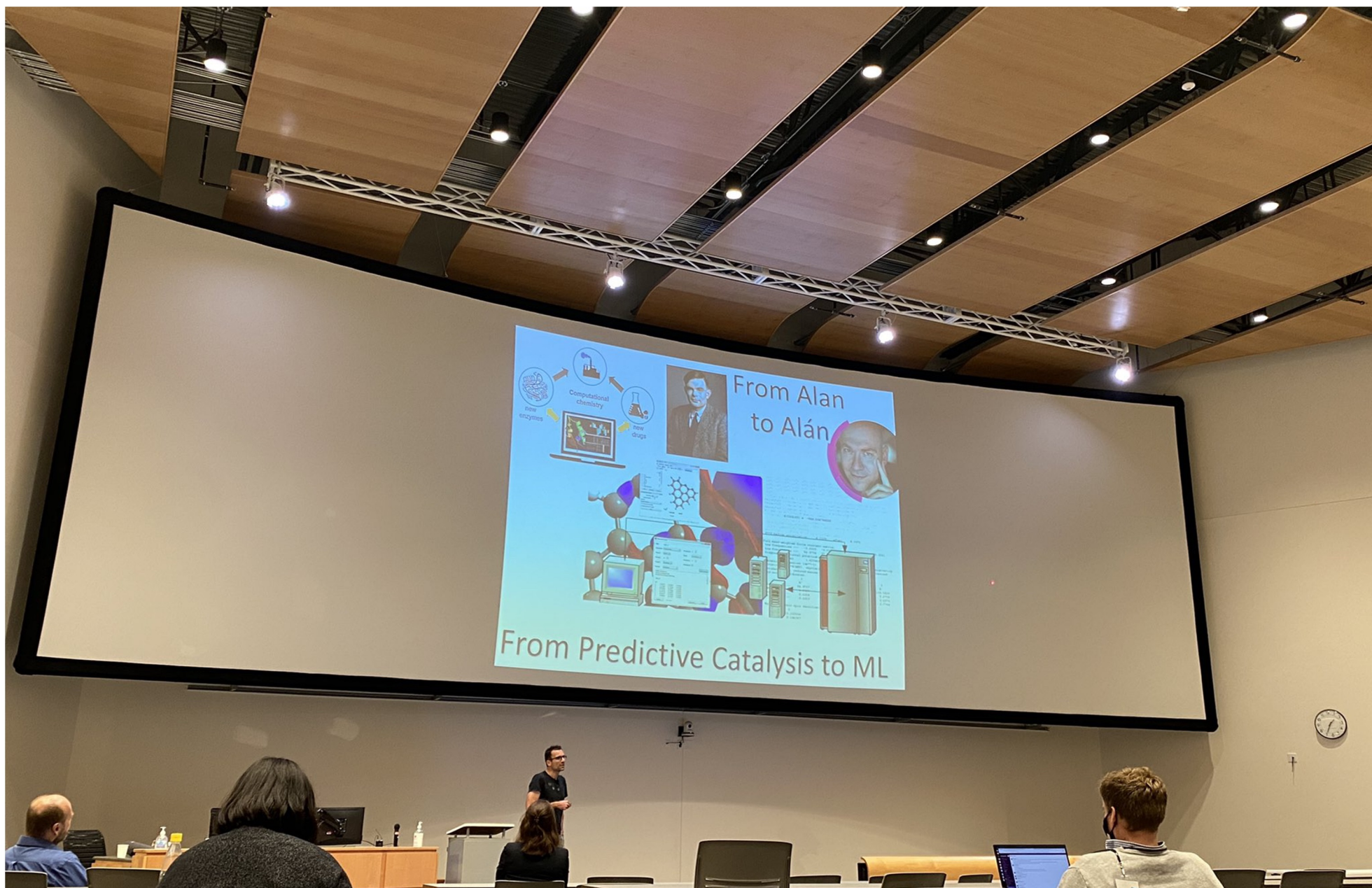
Jolene Reid



Samira Siahrostami



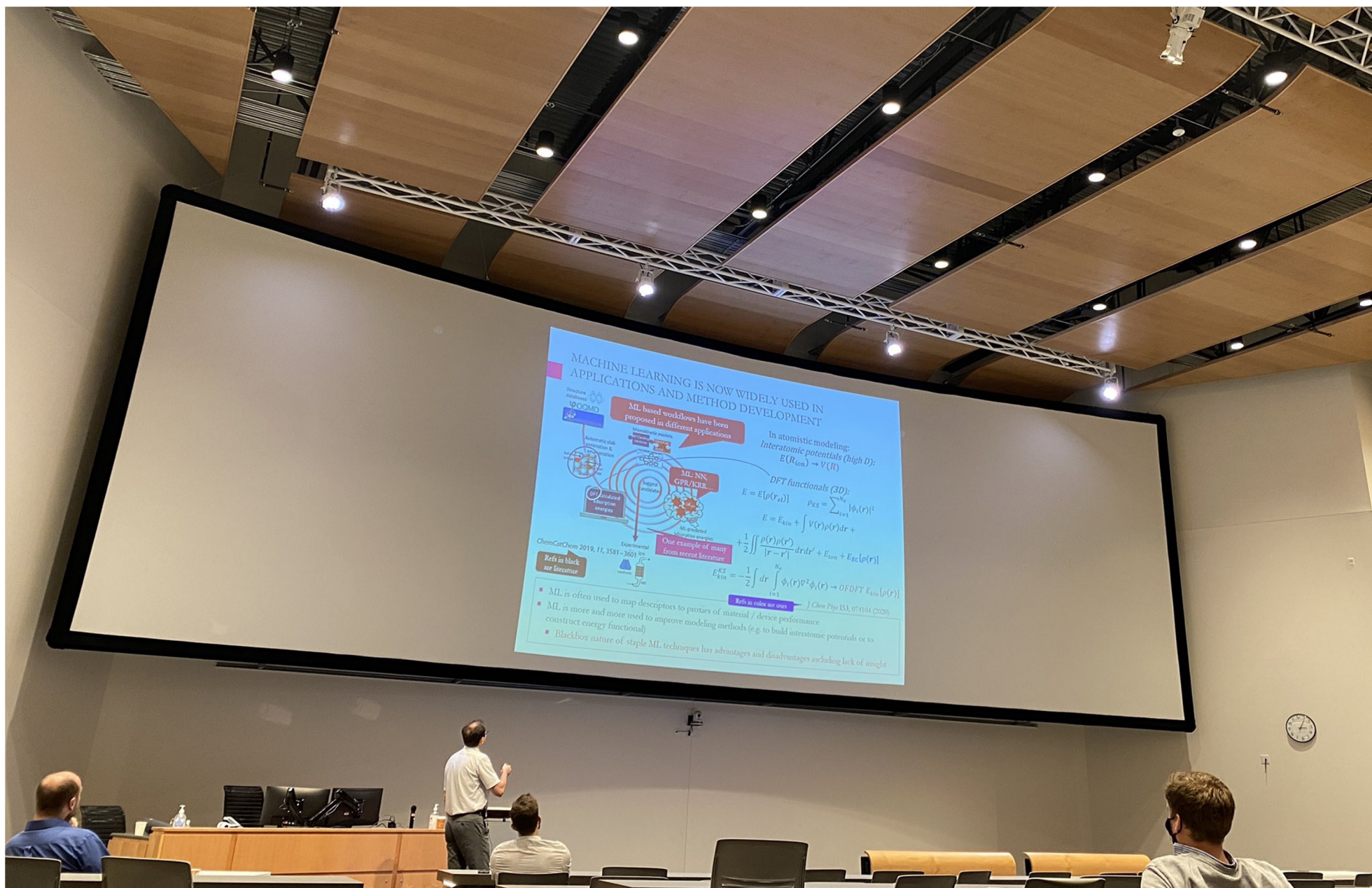
Leanne Chen



Albert Poater



Rachel Otero Crespo



MACHINE LEARNING IS NOW WIDELY USED IN APPLICATIONS AND METHOD DEVELOPMENT

ML based workflows have been proposed in different applications

In atomistic modeling:
 Interatomic potentials (high D):
 $E(R_{ion}) \rightarrow V(R)$

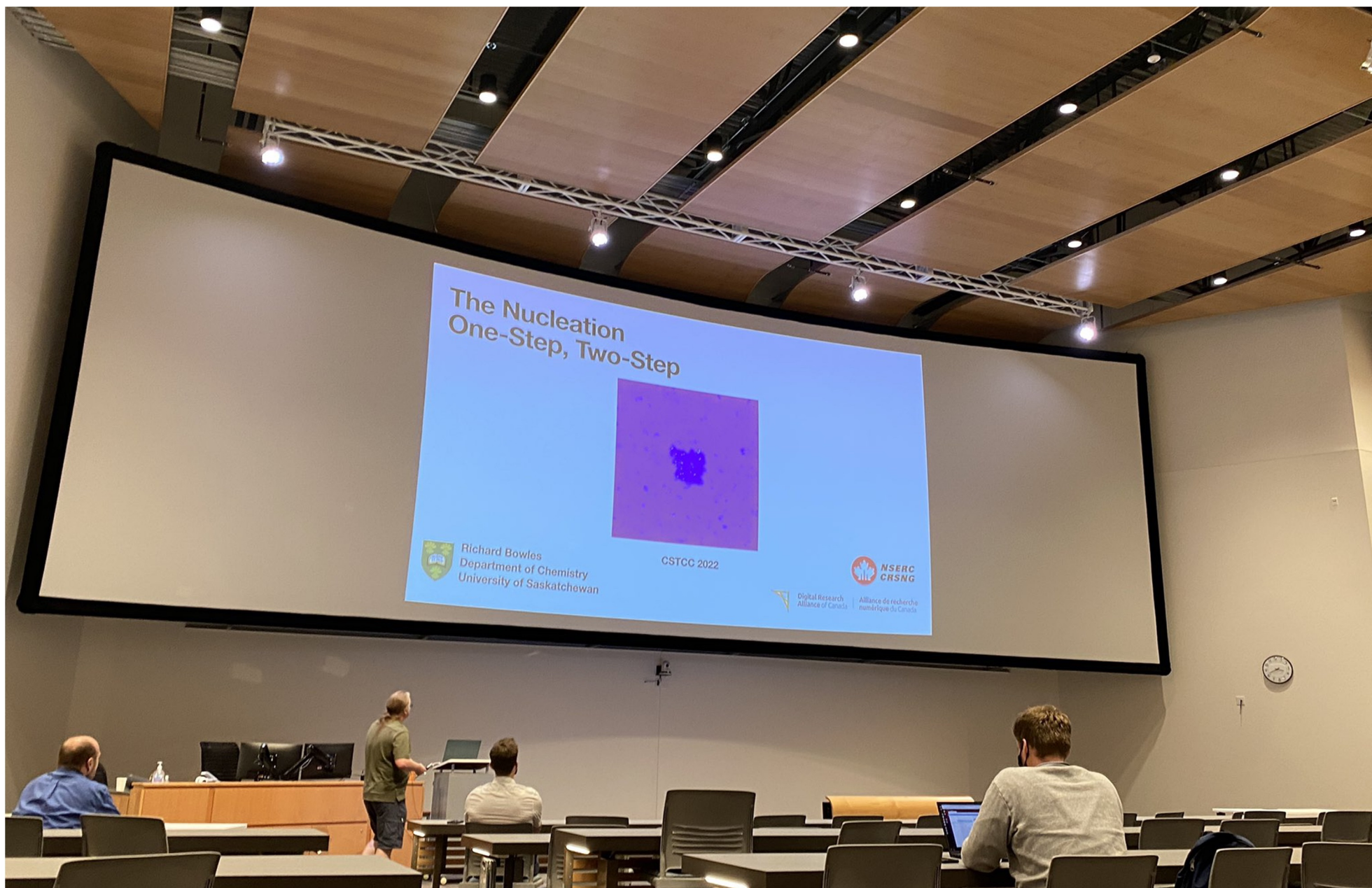
DFT functionals (3D):
 $E = E[\rho(r_{el})]$ $\rho_{el} = \sum_{i=1}^N |\psi_i(r)|^2$
 $E = E_{kin} + \int V(r)\rho(r)dr + \dots$

One example of many from recent literature:
 $E_{kin}^{KS} = -\frac{1}{2} \int dr \int_{i=1}^N \psi_i(r) \nabla^2 \psi_i(r) \rightarrow \text{OFDFT } E_{kin}[\rho(r)]$

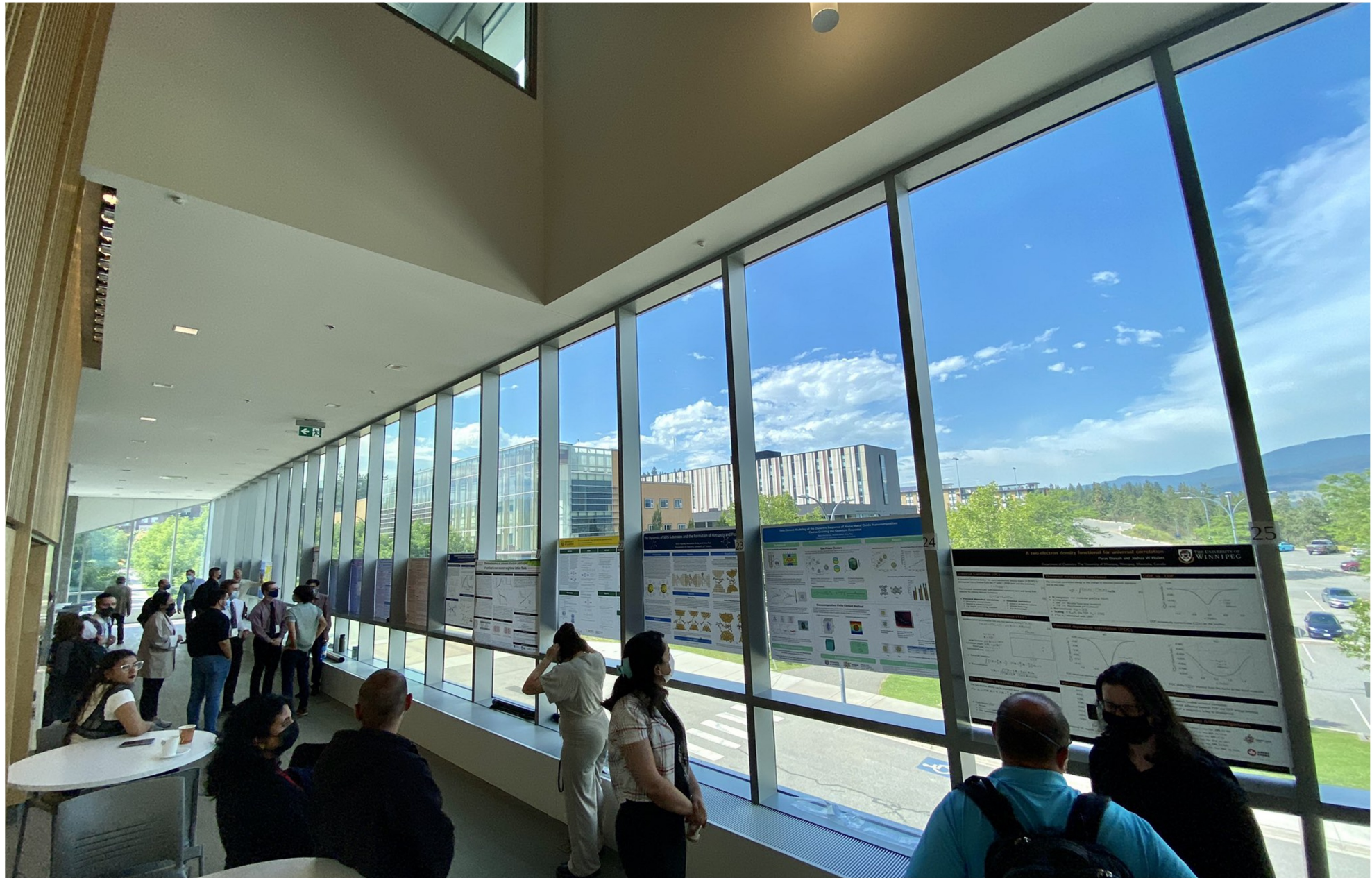
Refs in color are ours: *J Chem Phys* 153, 074104 (2020)

- ML is often used to map descriptors to proxies of material / device performance
- ML is more and more used to improve modeling methods (e.g. to build interatomic potentials or to construct energy functional)
- Blackbox nature of staple ML techniques has advantages and disadvantages including lack of insight

Sergei Manzhos




Richard Bowles



Poster Session


39



UNIVERSITY OF TORONTO

Graph Convolutional Neural Network for Projected Density of States predictions

Ihor Neporozhnyi¹, Zhibo Wang¹, Rochan Bajpai², Oleksandr Voznyy¹
¹University of Toronto, ²Indian Institute of Technology Roorkee



CSTCC 2022

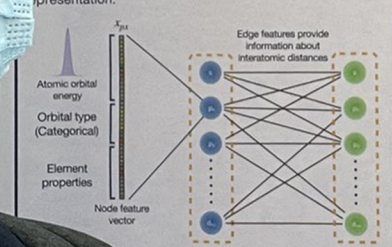
Introduction

It is to discover safe, inexpensive, and defect-tolerant electronic materials. Projected Density of States (PDOS) provide us information about bandgap and shallow states to guide us towards perspective candidates high-throughput exploration of material space.

In this work we present a method that allows us to predict DOS in less than a second for the majority of materials.

Methods

Materials Project database contains 124,000 materials and provides access to orbital projected Density of States data for 88,000 compounds. The incorporation of orbital PDOS data can significantly increase number of training examples for some materials by a factor of 100). To train our model on orbital density data we developed orbital graph material representation.



Results

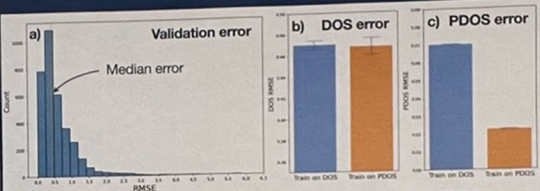
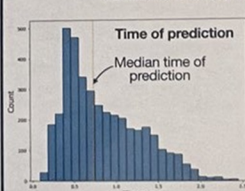


Figure 3 shows the validation error distribution (a), Total DOS validation error (b) and PDOS validation error (c)

Time of prediction




Our model is trained on dataset of 20,000 materials with following selection criteria:

- Non-polarized DOS calculations
- Element range: H — Bi (1 — 83)
- Maximum number of atoms in unit cell: 15

The median validation error of total DOS is 0.47 states/eV. The median time of PDOS prediction for single material is 0.7 seconds which is about **10,000 faster** than using density functional theory (DFT) calculations.

Figure 4. Prediction time distribution


Application



ProDOSMate
 Projected Density of States Material Explorer
<https://prodosmate.herokuapp.com/>

To demonstrate capabilities of our model and provide access to the results of this study, we developed a web application that allows users to predict Projected Density of States from a cif file on the fly in a matter of seconds.

Try it yourself



Predict PDOS in seconds (even on your smartphone)

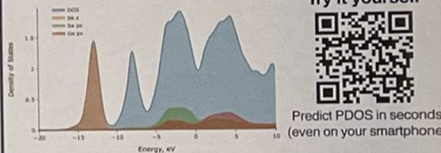


Figure 7 illustrates GeSe PDOS including single orbital electronic density predicted using ProDOSMate application.

References

1. Xie, T. and Grossman, J. C., "Crystal Graph Convolutional Neural Networks for an Accurate and Interpretable Prediction of Material Properties", Physical Review Letters, vol. 120, no. 14, 2018. doi:10.1103/PhysRevLett.120.145301.
2. Jain, A.; Ong, S. P.; Hautier, G.; Chen, W.; Richards, W. D.; Dacek, S.; Cholia, S.; Gunter, D.; Skinner, D.; Ceder, G.; Persson, K. A., "The Materials Project: A Materials Genome Approach to Accelerating Materials Innovation", APL Mater. 2013, 1, No. 011002

Output

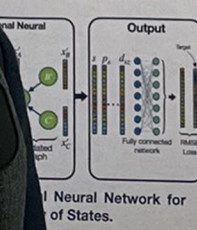


Figure 5. Representative total Density of States validation predictions.

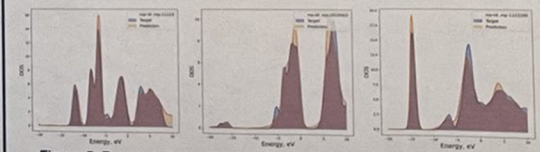
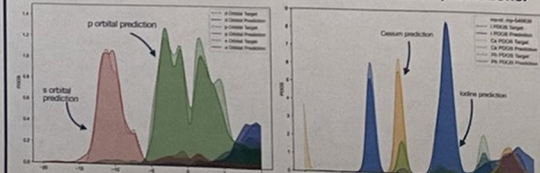



Figure 6. Projected Density of States validation Predictions




References

1. Xie, T. and Grossman, J. C., "Crystal Graph Convolutional Neural Networks for an Accurate and Interpretable Prediction of Material Properties", Physical Review Letters, vol. 120, no. 14, 2018. doi:10.1103/PhysRevLett.120.145301.
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Ihor Neporozhnyi
 Ph.D. Student at UoTf
 Research Assistant at **Clean Energy Lab**
 Neporozhnyi, et. al. "Graph Convolutional Neural Network for Projected Density of States predictions" — In preparation

For future updates connect with me on LinkedIn and Twitter (@ineporozhnyi)



Ihor Neporozhnyi

DFT study of the N₂O functionalization for the preparation of triazolopyridine scaffolds

Roger Monreal-Corona, Emili Besalú, Anna Pla-Quintana* and Albert Poater*

Institut de Química Computacional i Catàlisi and Departament de Química, Universitat de Girona, Catalonia, Spain

rogermonrea198@gmail.com

Introduction

... (text) ...

Objectives

... (text) ...

Computational Details

... (text) ...

Conclusions

... (text) ...

References

... (text) ...

Reaction Mechanism

Reaction Scope

N-Containing Scaffolds

Theoretical Study of the Iron Complexes with Lipoic and Dihydropolipoic Acids

Roger Monreal-Corona, Jesse Biddlecombe, Angela Ippolito, Nelaine Mora-Diez*

Thompson Rivers University, Department of Chemistry, Kamloops, B.C., Canada

Introduction

... (text) ...

Thermodynamic results

Complex	ΔG° (kJ/mol)	logK
[Fe ^{II} (L) ₂] ²⁺	88.3	15.57
[Fe ^{II} (DLA) ₂] ²⁺	11.1	2.04
[Fe ^{II} (DLA)(DLA-2S)] ²⁺	38.4	6.68
[Fe ^{II} (DLA) ₂] ²⁺	28.1	4.94
[Fe ^{II} (DLA)(DLA-2S)] ²⁺	27.2	4.86
[Fe ^{II} (DLA) ₂] ²⁺	21.1	3.79

Kinetic results

Complex	k ₁ (s ⁻¹)	k ₋₁ (s ⁻¹)	k ₂ (s ⁻¹)	k ₋₂ (s ⁻¹)
[Fe ^{II} (L) ₂] ²⁺	1.1 × 10 ⁻¹⁰	1.1 × 10 ⁻¹⁰	1.1 × 10 ⁻¹⁰	1.1 × 10 ⁻¹⁰
[Fe ^{II} (DLA) ₂] ²⁺	1.1 × 10 ⁻¹⁰	1.1 × 10 ⁻¹⁰	1.1 × 10 ⁻¹⁰	1.1 × 10 ⁻¹⁰
[Fe ^{II} (DLA)(DLA-2S)] ²⁺	1.1 × 10 ⁻¹⁰	1.1 × 10 ⁻¹⁰	1.1 × 10 ⁻¹⁰	1.1 × 10 ⁻¹⁰

Conclusions

... (text) ...

References

... (text) ...

Introduction

... (text) ...

Thermodynamic results

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Conclusions

... (text) ...

References

... (text) ...

Roger Monreal-Corona with dual posters





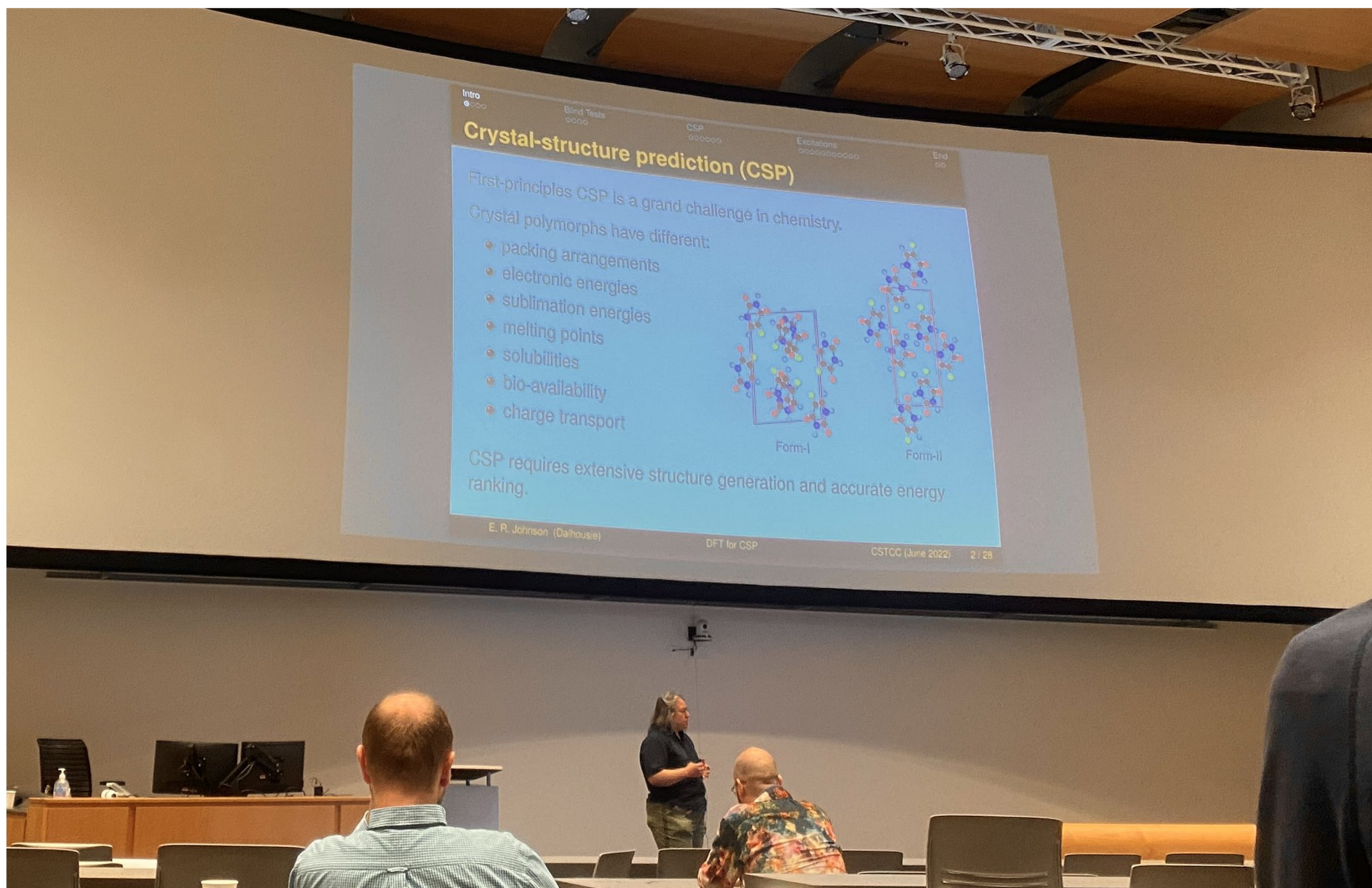
GENERATIVE MODELS FOR DRUG DISCOVERY

Experimental demonstration of AI for drug discovery

MIT Technology Review
10 Breakthrough Technologies 2020
AI-designed molecules



Zhavoronkov, et al, *Nature Biotechnology*, 37, 1038-1040 (2019); see also work by Barzilay lab, Stokes et al, *Cell*, 180, 688 (2020)



Intro
Blind Tests
CSP
Evolution
End

Crystal-structure prediction (CSP)

First-principles CSP is a grand challenge in chemistry.

Crystal polymorphs have different:

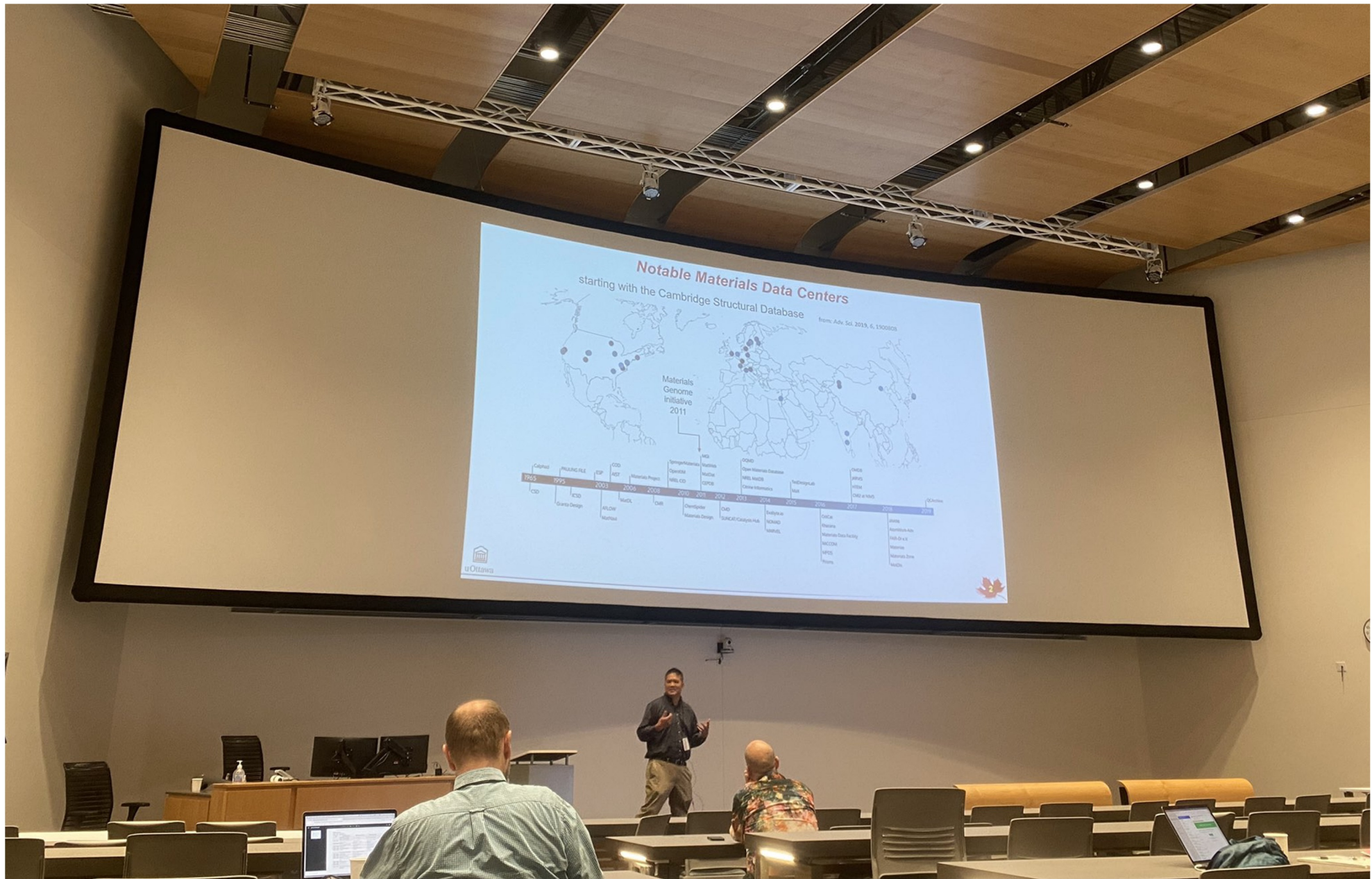
- packing arrangements
- electronic energies
- sublimation energies
- melting points
- solubilities
- bio-availability
- charge transport

Form-I Form-II

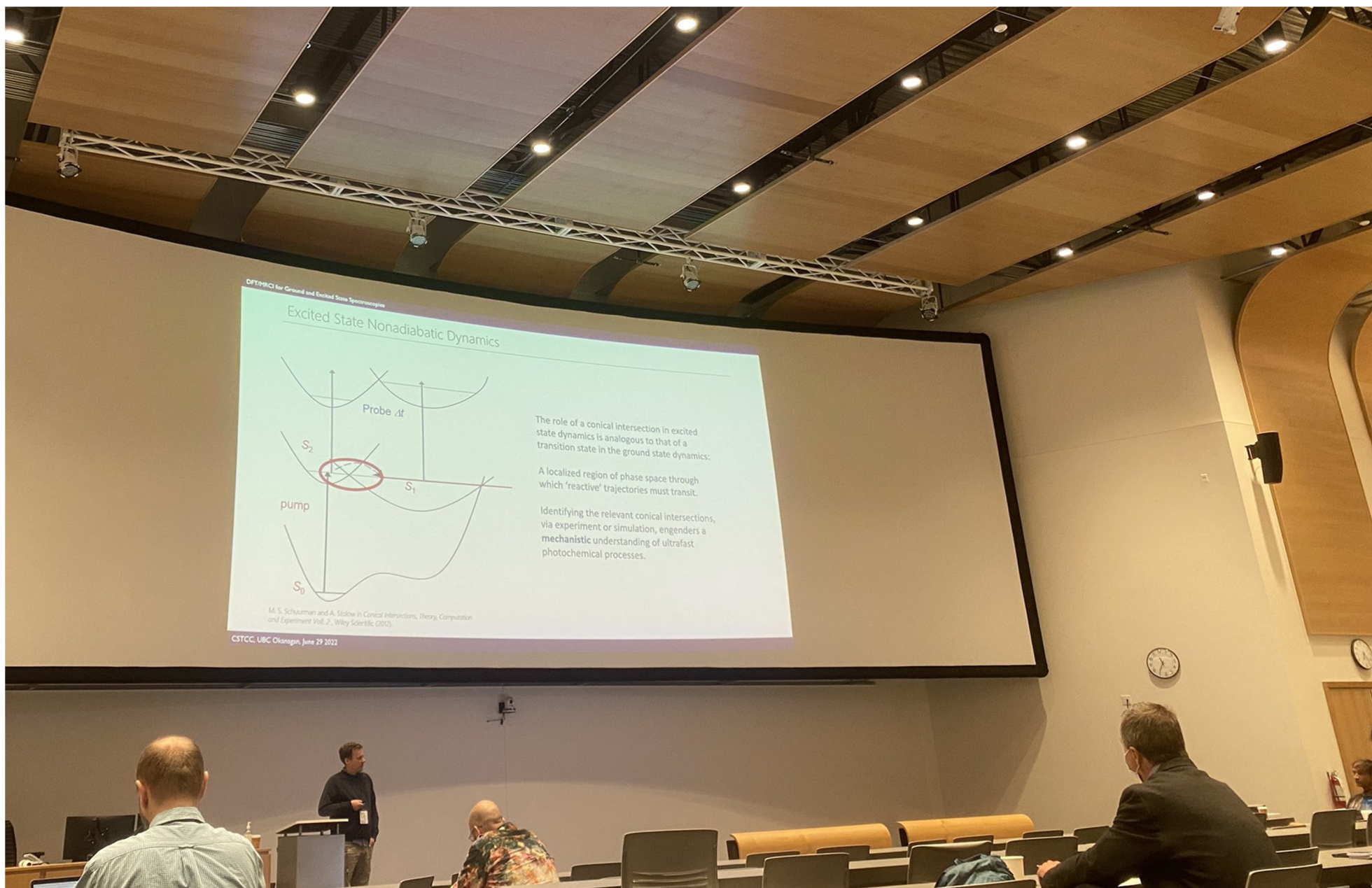
CSP requires extensive structure generation and accurate energy ranking.

E. R. Johnson (Dartmouth) DFT for CSP CSTCC (June 2022) 2 / 28

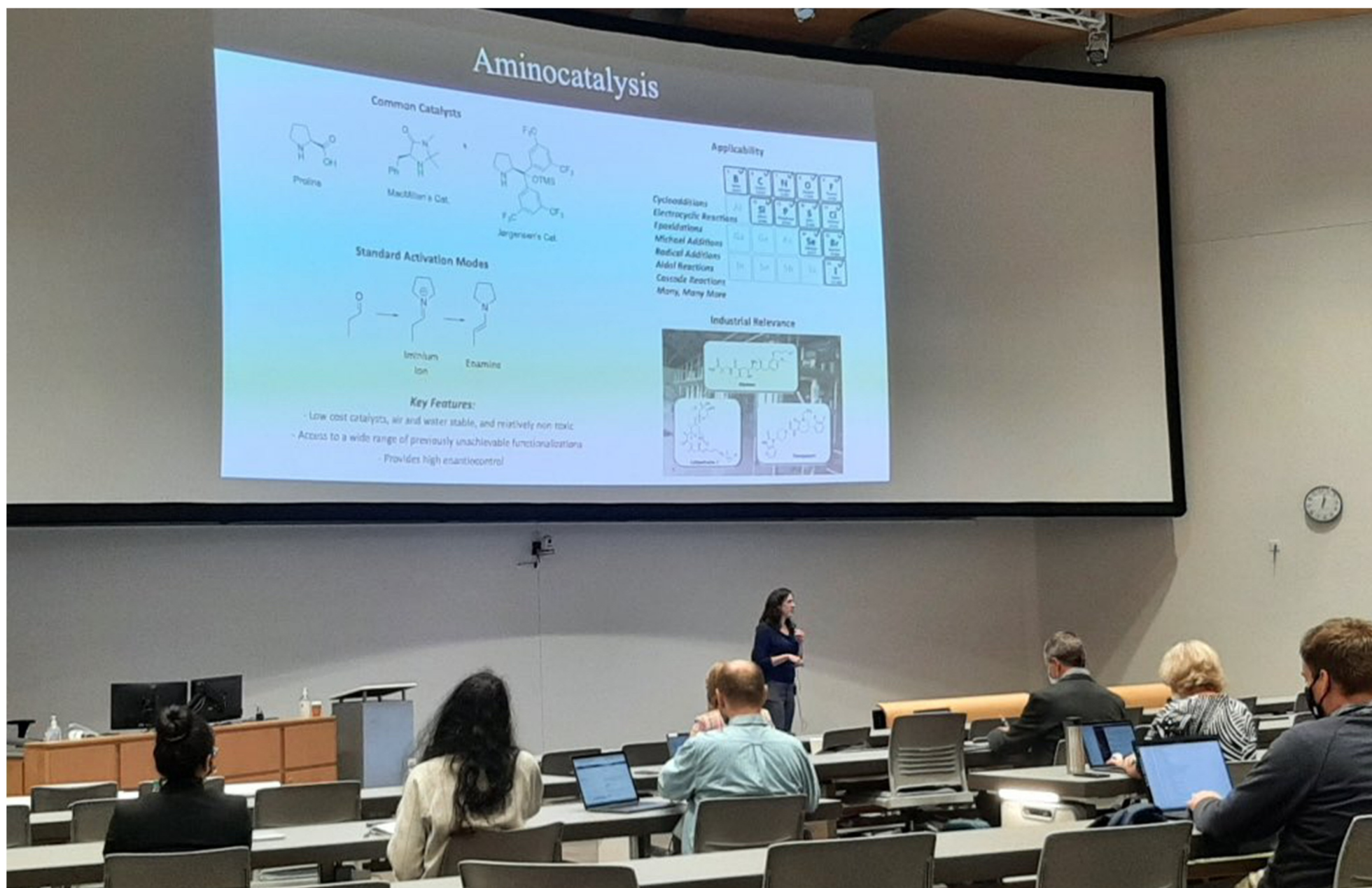
Erin Johnson



Tom Woo

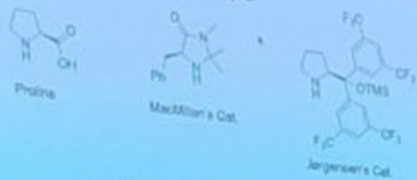


Michael Schuurman

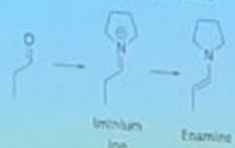


Aminocatalysis

Common Catalysts



Standard Activation Modes



Key Features:

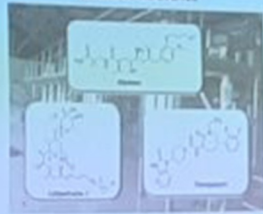
- Low cost catalysts, air and water stable, and relatively non-toxic
- Access to a wide range of previously unachievable functionalizations
- Provides high enantiocontrol

Applicability

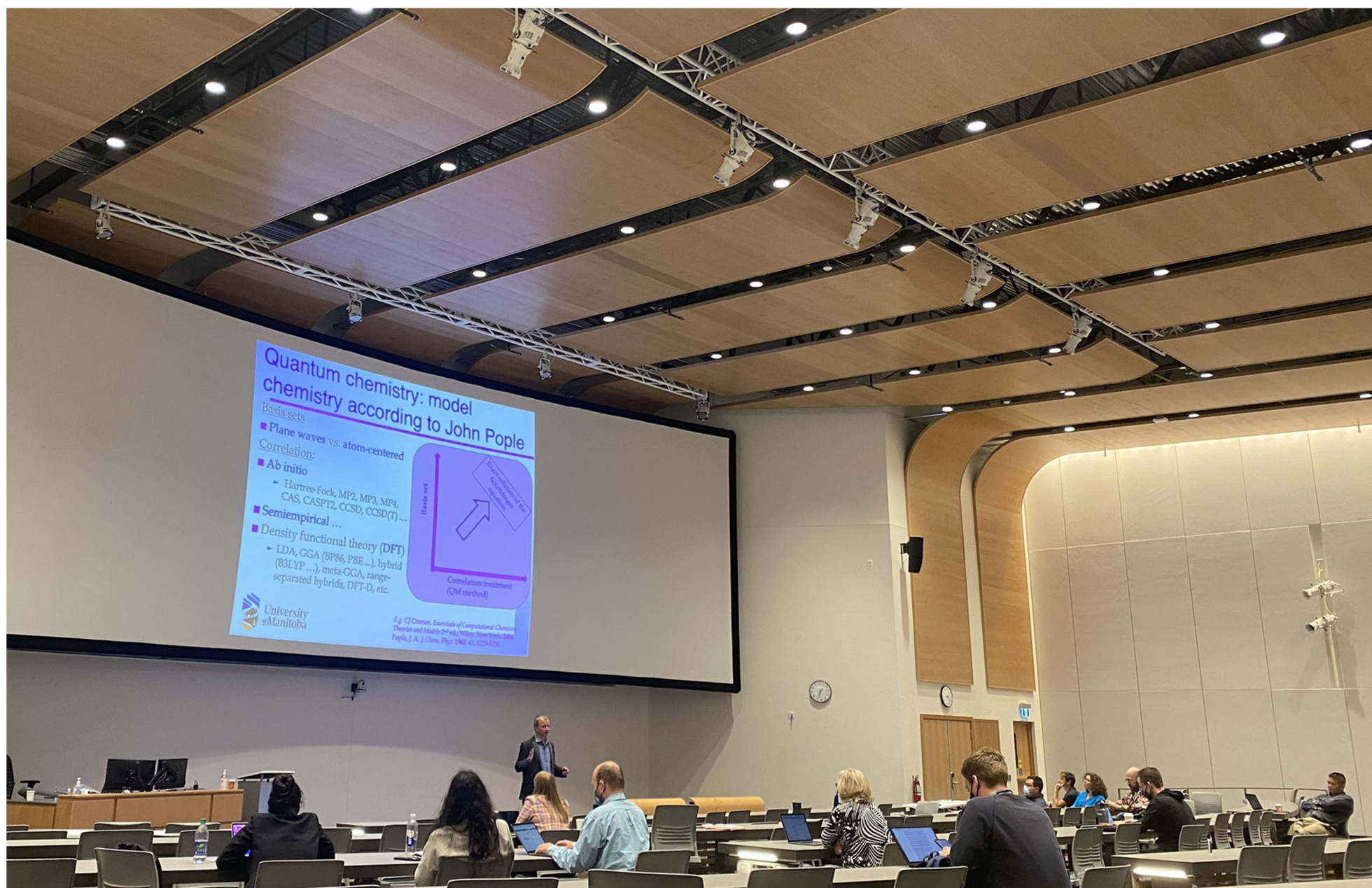
- Cycloadditions
Electrocyclic Reactions
Epoxidations
Michael Additions
Radical Additions
Aldol Reactions
Cascade Reactions
Many, Many More

B	C	H	O	F
N	S	P	A	Cl
Ca	Ga	Al	Se	Br
Fe	Sr	Nb	Sn	I

Industrial Relevance



Rebecca Davis



Quantum chemistry: model chemistry according to John Pople

Basis sets

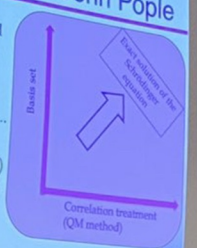
- Plane waves vs. atom-centered

Correlation:

- Ab initio
 - Hartree-Fock, MP2, MP3, MP4, CAS, CASPT2, CCSD, CCSD(T) ...
- Semiempirical ...
- Density functional theory (DFT)
 - LDA, GGA (BP86, PBE ...), hybrid (B3LYP ...), meta-GGA, range-separated hybrids, DFT-D, etc.

University of Manitoba

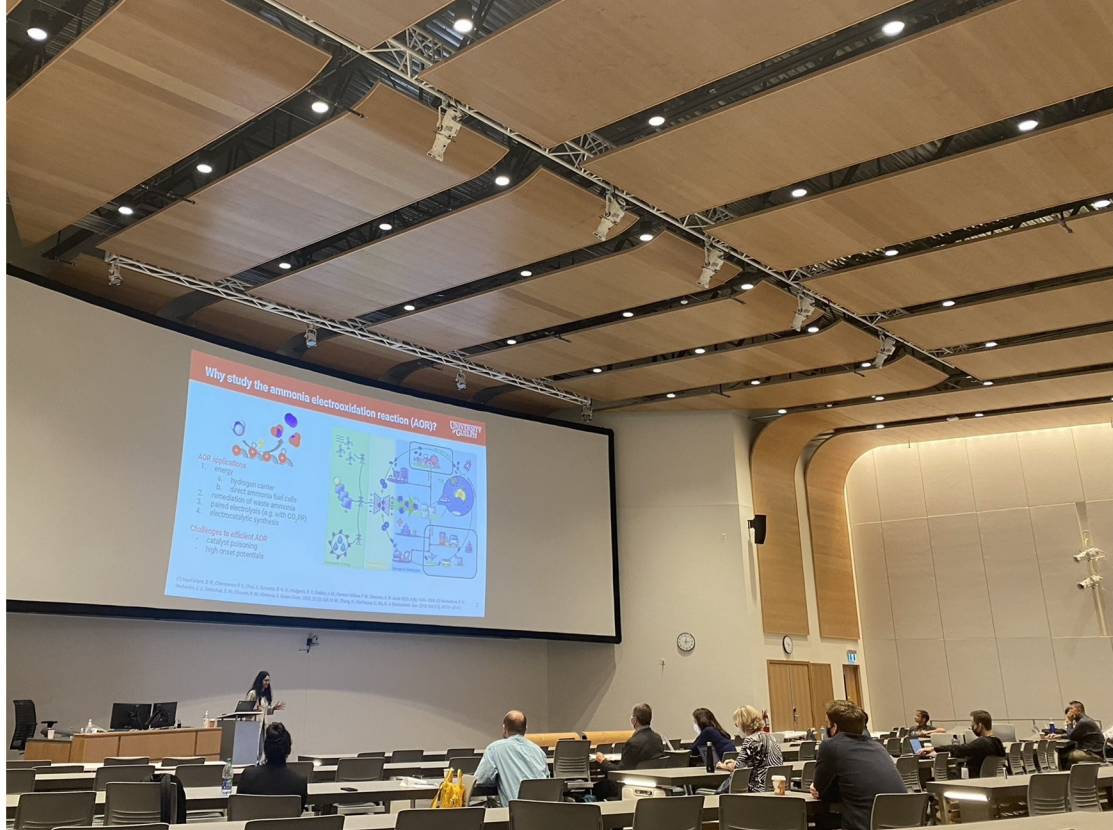
E.g. CJ Cramer, *Essentials of Computational Chemistry: Theories and Models* 2nd ed., Wiley: New York, 2004
Pople, J. A. J. Chem. Phys. 1965, 41, 5205-5232



Georg Schreckenbach



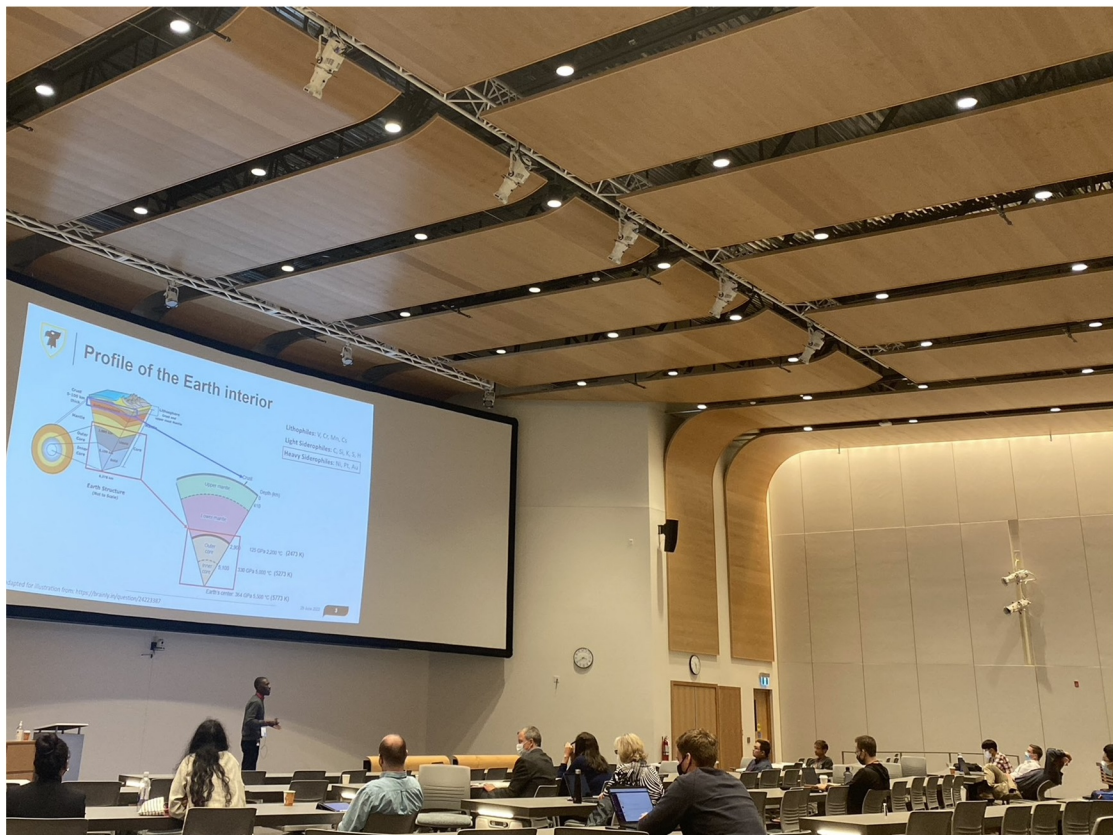
Heather Wiebe



Rachelle Choueiri



Lizandra Barrios Herrera



Adebayo Adeleke



Eduardo Romero-Montalvo











Alex Brown and Gino DiLabio in conversation



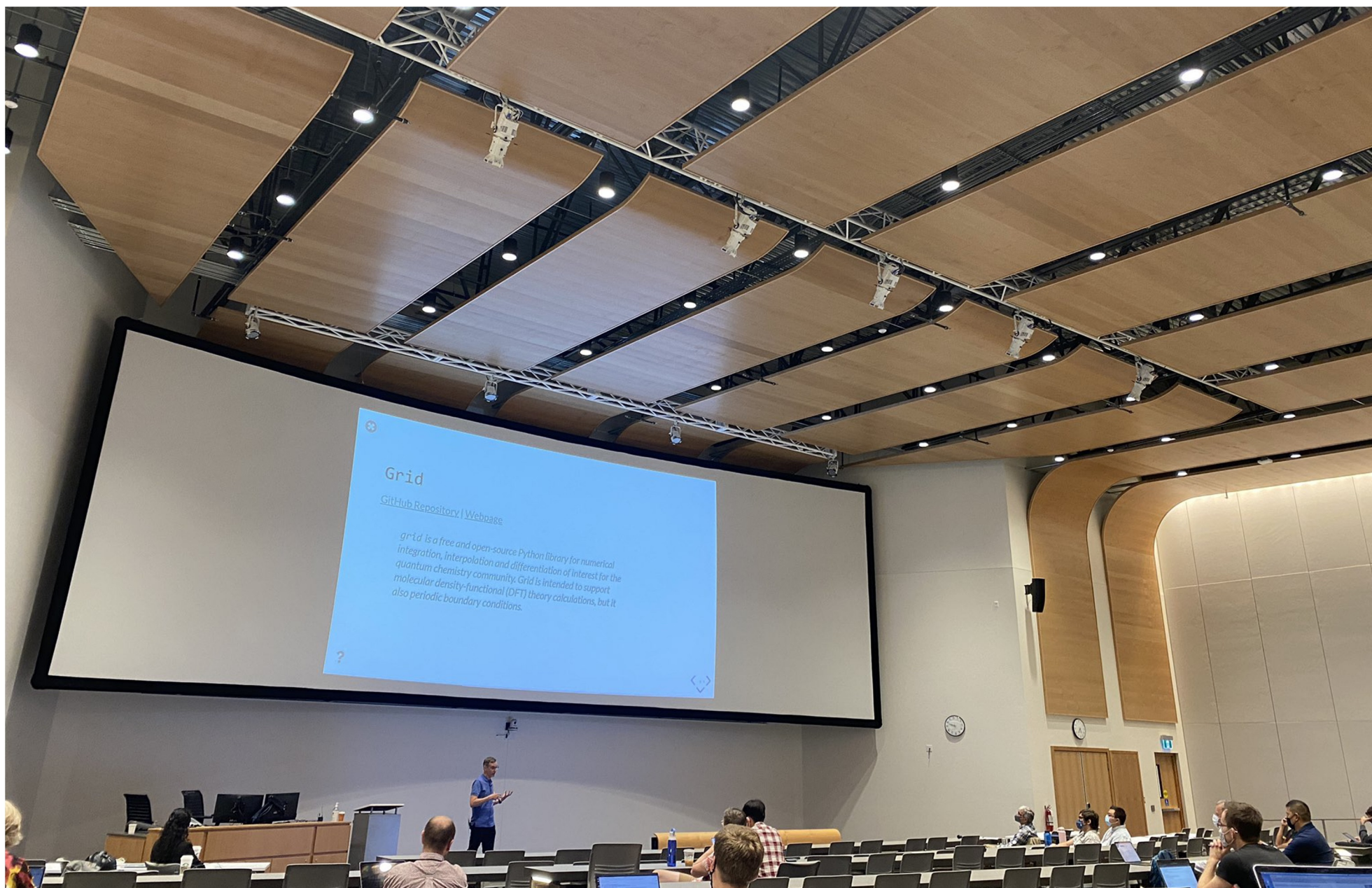
Stacey Wetmore and Alex Brown with Poster Awardees Savannah Mercer and Alastair Price







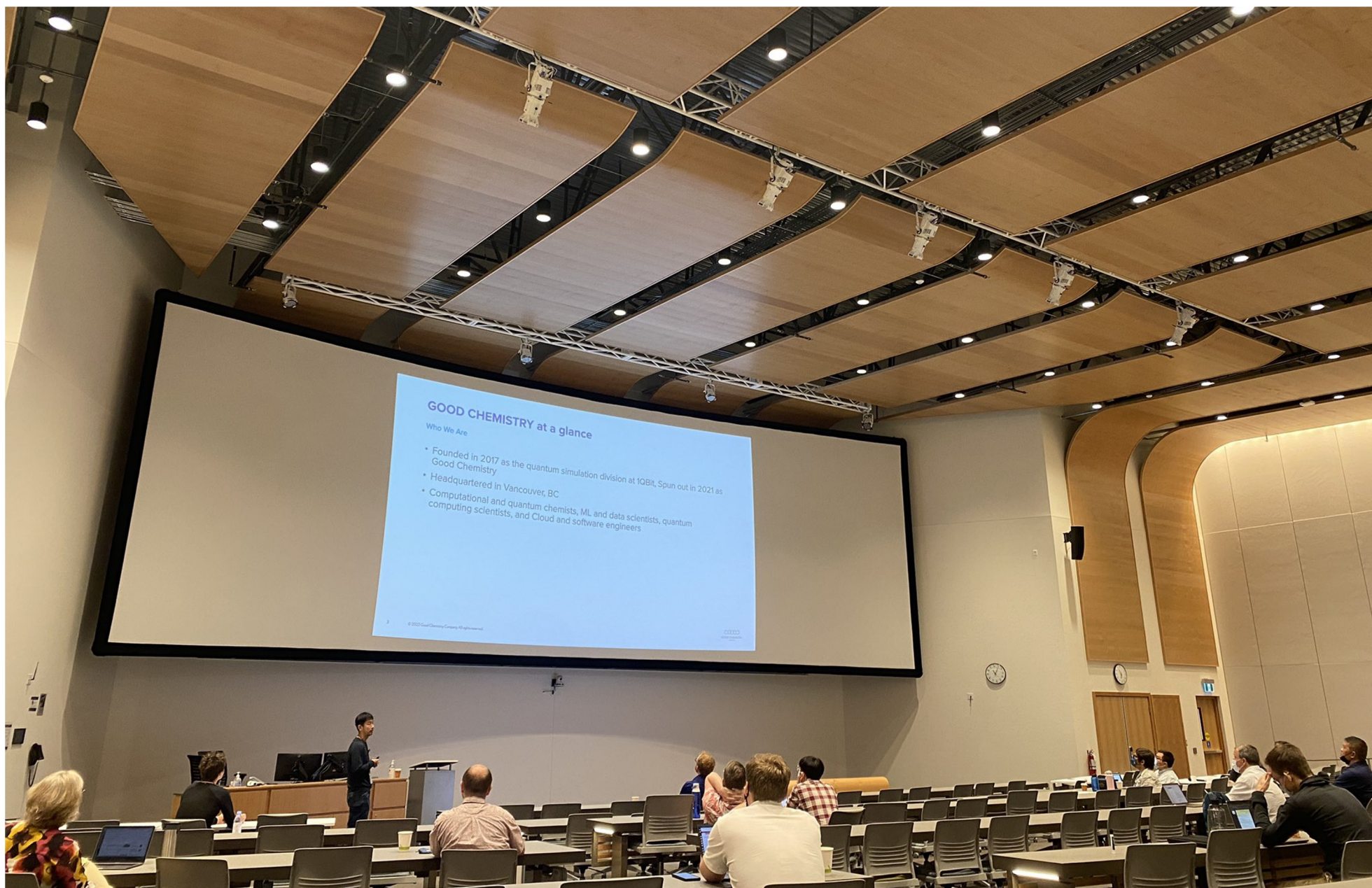
Farnaz Heidar-Zadeh



Paul Ayers



Thomas Baker



GOOD CHEMISTRY at a glance

Who We Are

- Founded in 2017 as the quantum simulation division at IQBit. Spun out in 2021 as Good Chemistry
- Headquartered in Vancouver, BC
- Computational and quantum chemists, ML and data scientists, quantum computing scientists, and Cloud and software engineers

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Takeshi Yamazaki

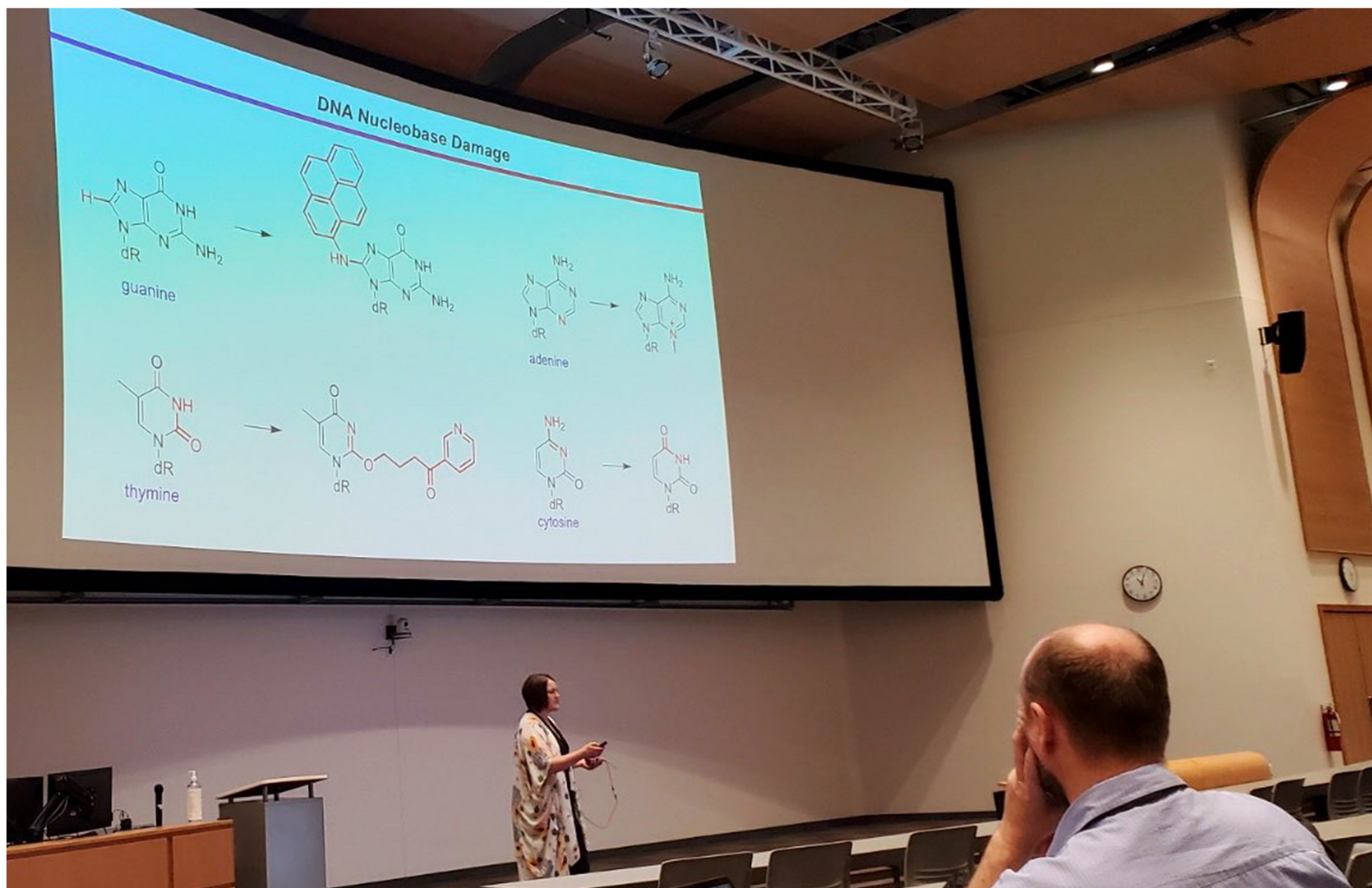
Question

- Question: What makes a good ice nucleus (IN)?
- Experiments: cannot probe the small length (nm) and short (ns) timescales on which ice nucleation occurs
- Molecular Dynamics Simulations: "Experiments" with realistic molecular models can reveal ice nucleation mechanisms.

8



Robert Szilagy



Stacey Wetmore

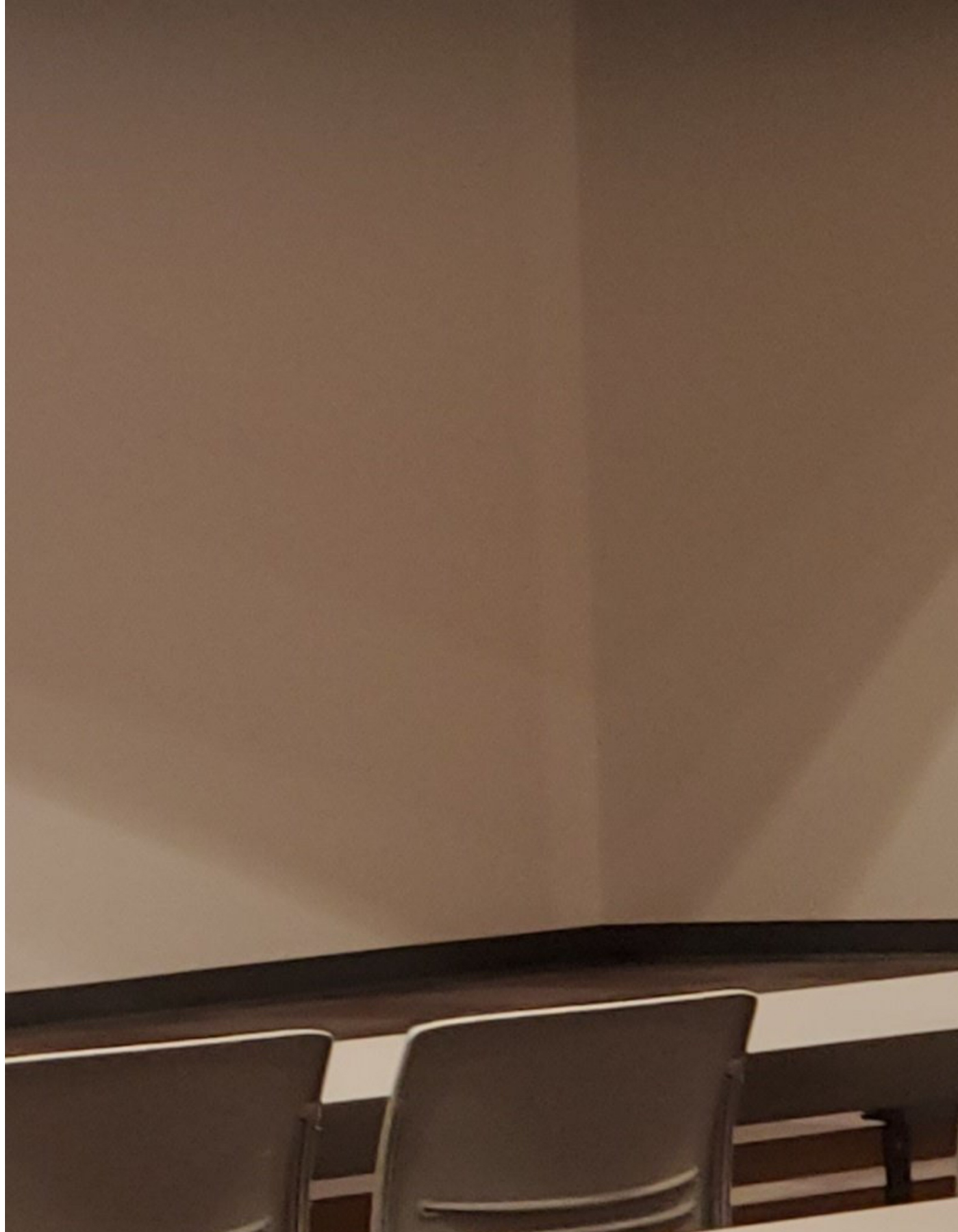


PES Fitting & QD: Why?

- Assign IR spectra (3-7+ atoms = 3-15+ vibrational DOF)
 - "High"-resolution (1-10 cm^{-1} accuracy)
 - From fundamentals to high energy overtones/combinations
 - Beyond harmonic/VPT2
- Explore Intramolecular Vibrational Redistribution
- Examine dynamical processes
 - Cis-trans isomerisation
 - Proton exchange
- Laser control of molecular dynamics

Alex Brown

Gino DiLabio giving the
concluding remarks









Paci Group Adventures







Selfies with Alán









All minors must be accompanied by an adult

MORE
CANADIAN
SOMERSBY
Cider
AROMATIC & TANGY
MORE
4.5% alc./vol. 473 mL
FARMHOUSE
CROISSANT RAFFINOSITY

BLACKBERRY
CANADIAN
SOMERSBY
BLACKBERRY
FLAVOURED
Cider
4.5% alc./vol. 473 mL
MADE IN CANADA
REFRESHINGLY CRISP





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Design:

@CompChemGuelph