29th Canadian Symposium on Theoretical and Computational Chemistry

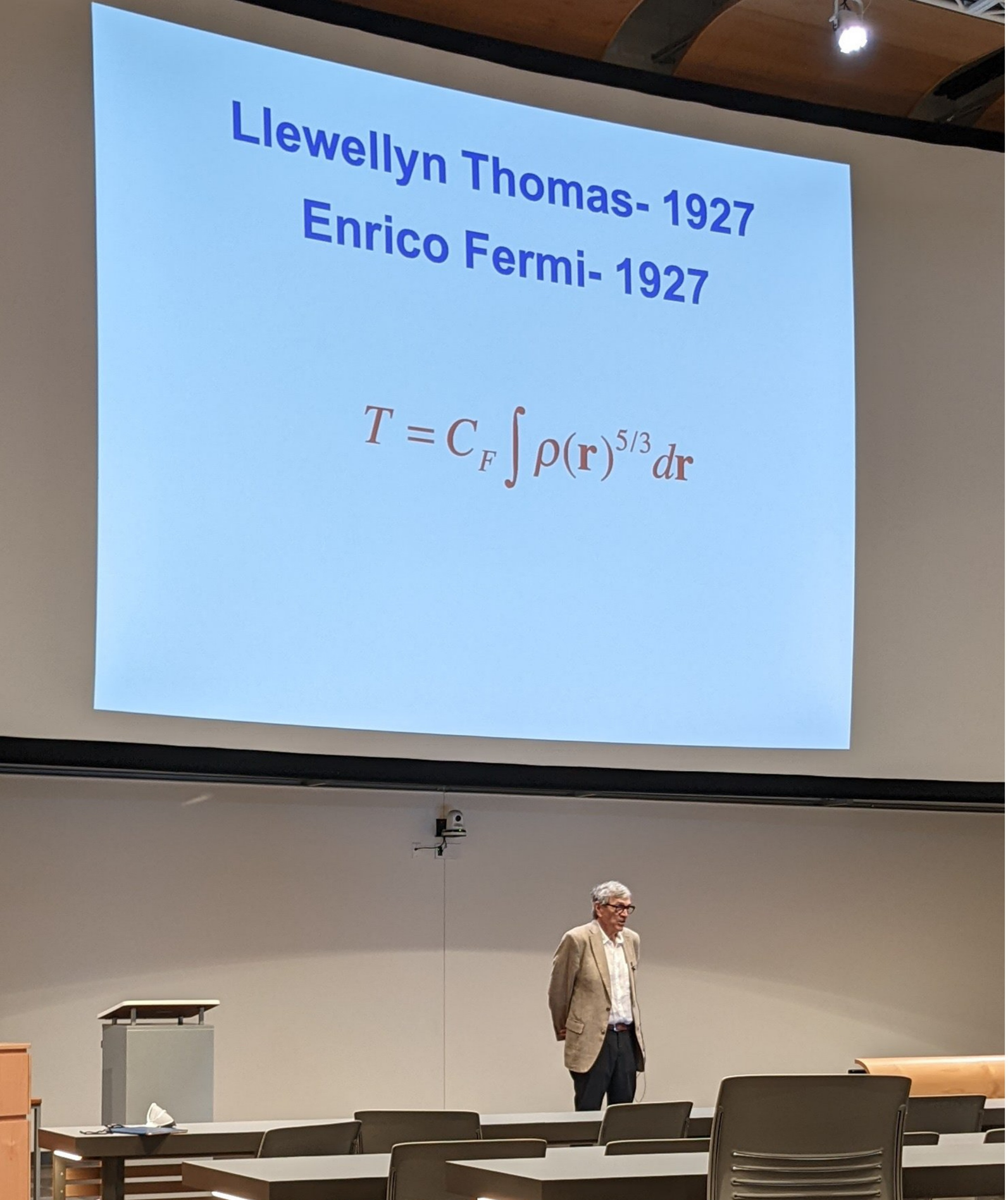
CSTCC 2022

Canadian Association of Theoretical Chemists

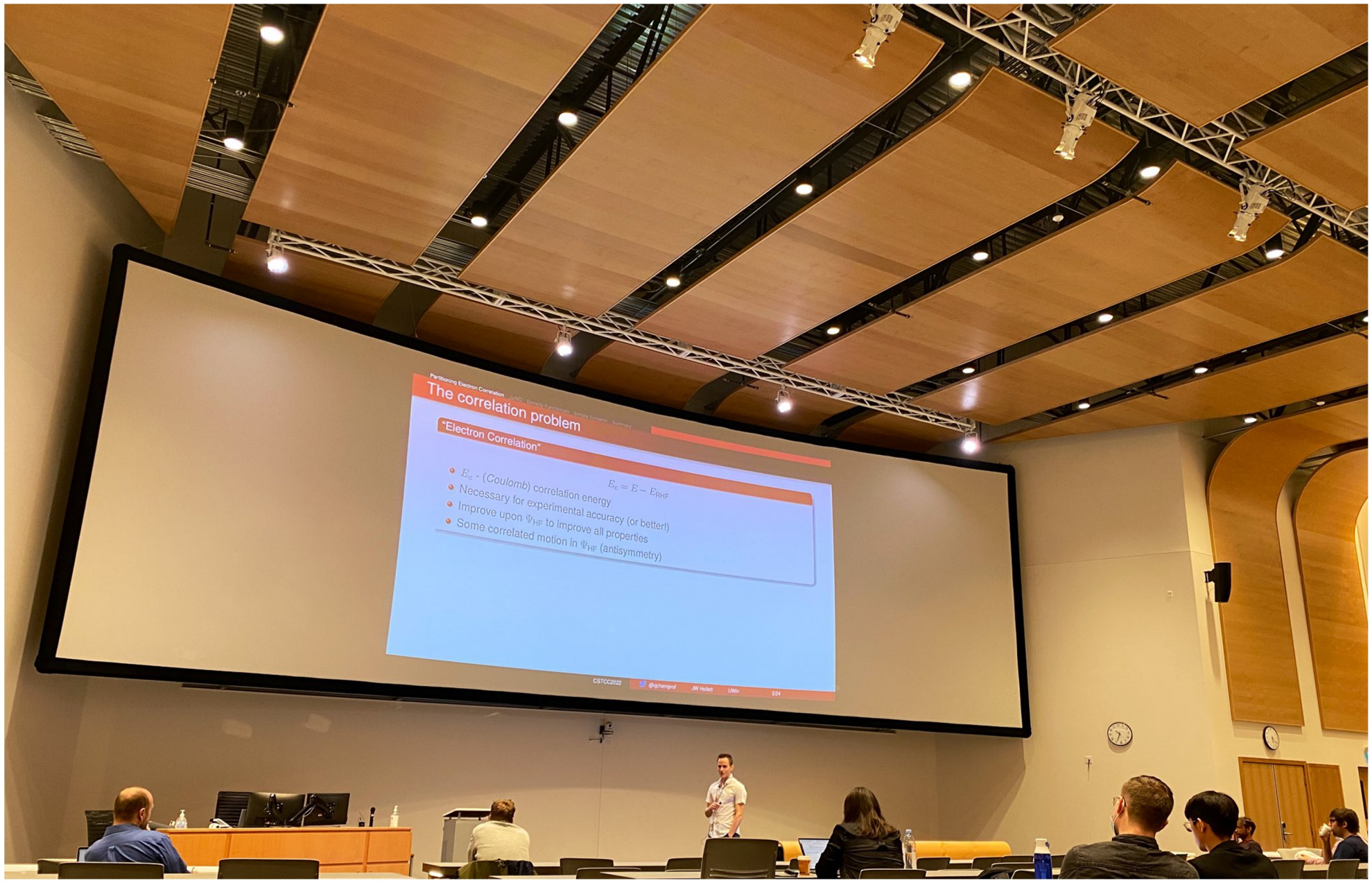
29th Canadian Symposium on Theoretical and Computational Chemistry

CSTCC 2022

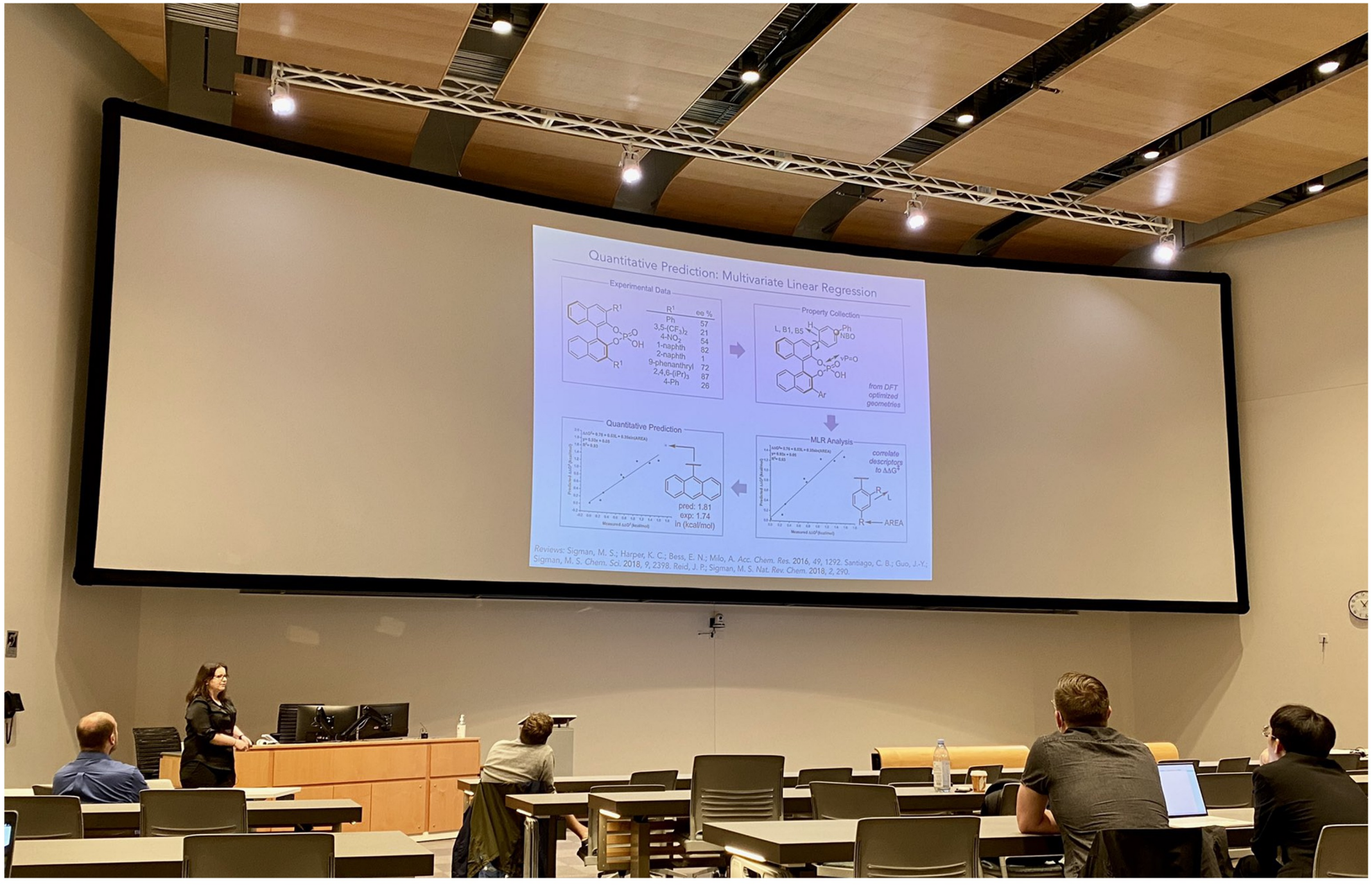
Canadian Association of Theoretical Chemists



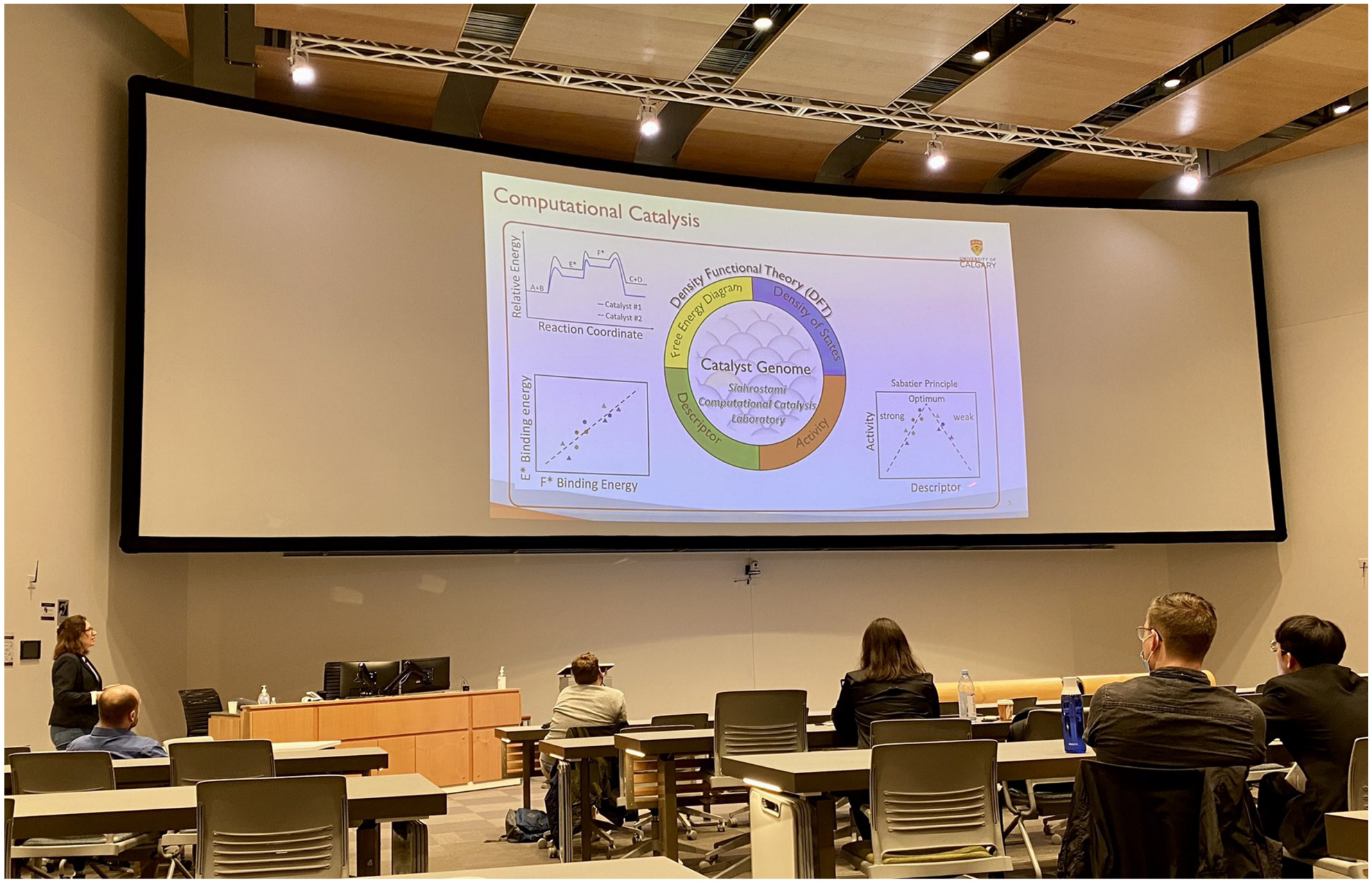
Dennis Salahub



Joshua Hollett


Quantitative Prediction: Multivariate Linear Regression
Experimental Data
R1
R1
O
P
O
OH
R1 ee %
Ph 57
3,5-(CF3)2 21
4-NO2 54
1-naphth 82
2-naphth 1
9-phenanthryl 72
2,4,6-(iPr)3 87
4-Ph 26
Property Collection
L, B1, B5
H
Ph
NBO
vP=O
Ar
from DFT optimized geometries
MLR Analysis
correlate descriptors to ΔΔG‡
R
L
R
AREA
Quantitative Prediction
pred: 1.81
exp: 1.74
in (kcal/mol)
Reviews: Sigman, M. S.; Harper, K. C.; Bess, E. N.; Milo, A. Acc. Chem. Res. 2016, 49, 1292. Santiago, C. B.; Guo, J.-Y.; Sigman, M. S. Chem. Sci. 2018, 9, 2398. Reid, J. P.; Sigman, M. S. Nat. Rev. Chem. 2018, 2, 290.

Jolene Reid



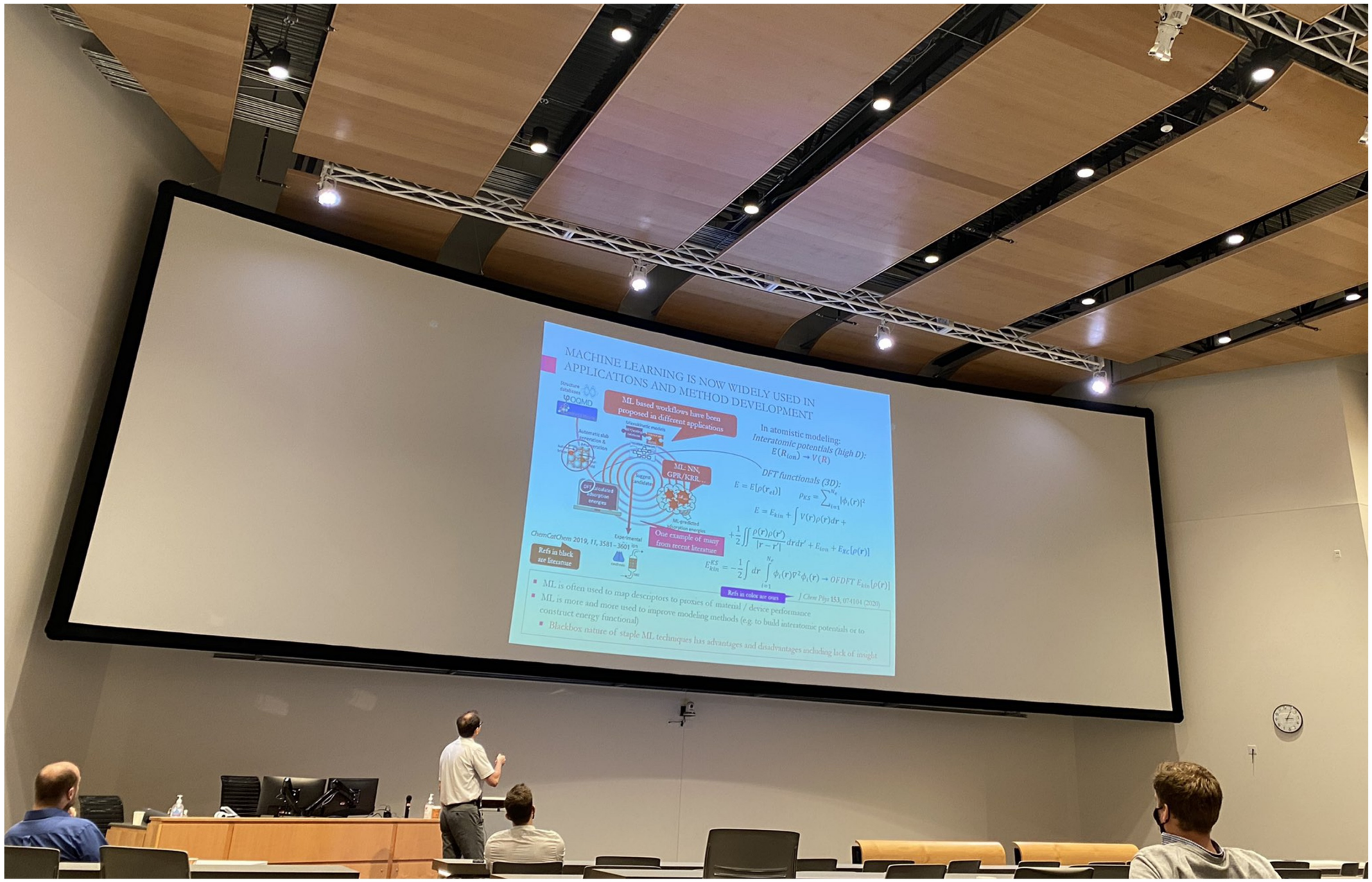
Samira Siahrostami


Theory + Experiment
Characterization
Synthesis
Test
Theory
H_2O
CO_2
N_2
H_2
$C_3H_8O_2$
NH_3
mechanistic understanding
↓
stable, active, and selective electrocatalysts
Seh, Z. W.; Kibsgaard, J.; Dickens, C. F.; Chorkendorff, I.; Jaramillo, T. F. Science 2017, 355, eaad4998.
UNIVERSITY of GUELPH
8

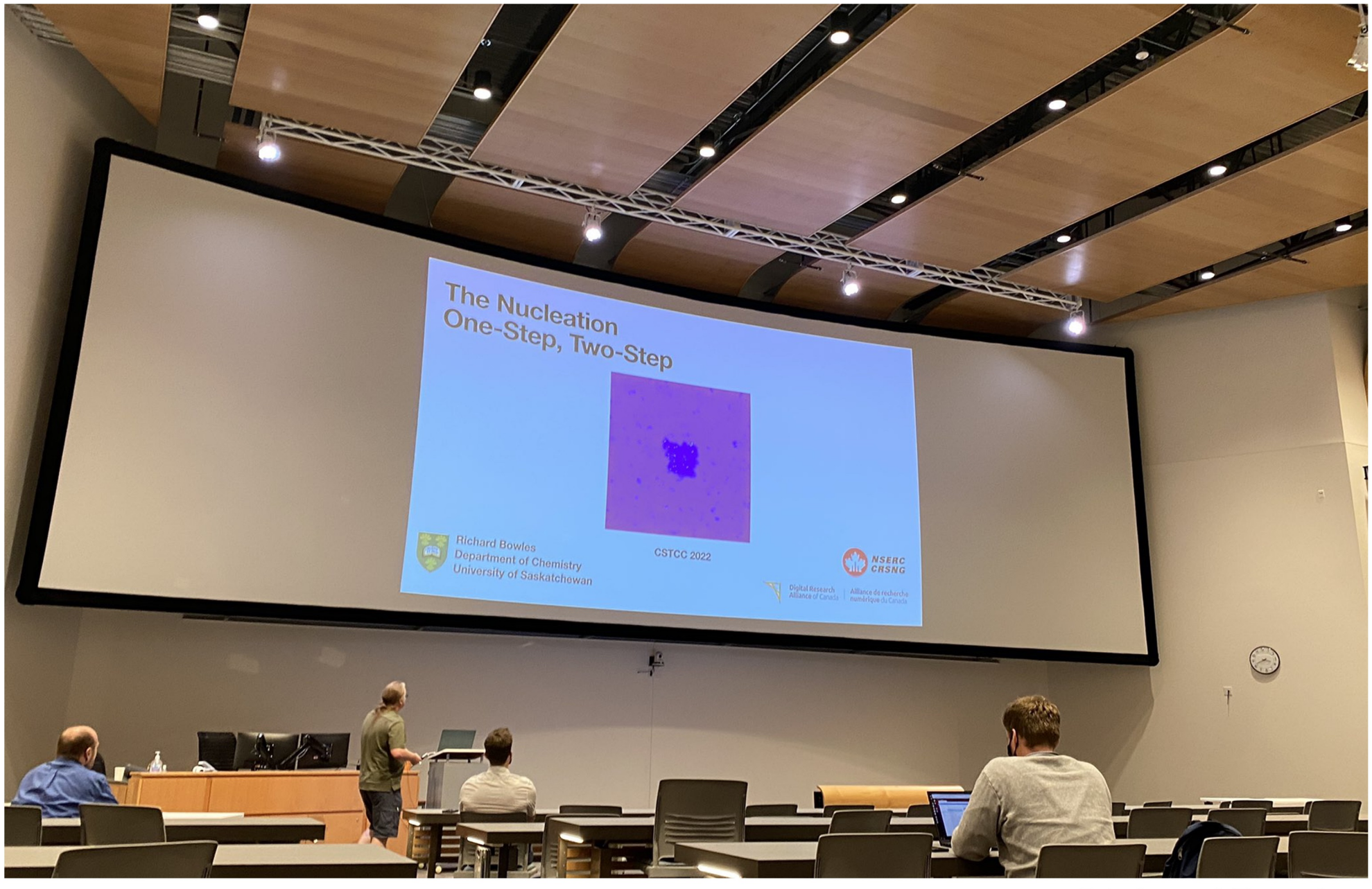
Leanne Chen

Albert Poater

Rachel Otero Crespo

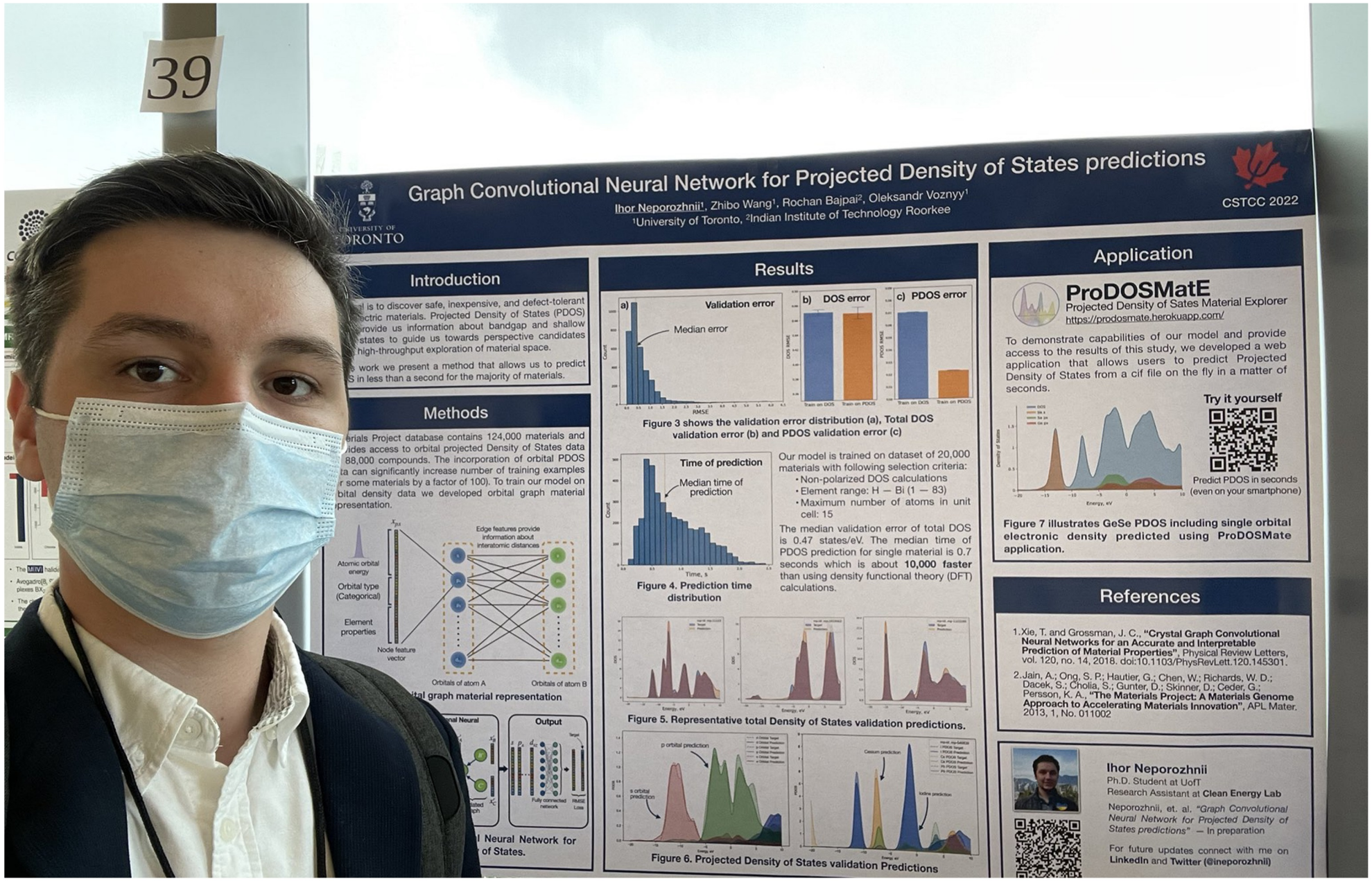


Sergei Manzhos

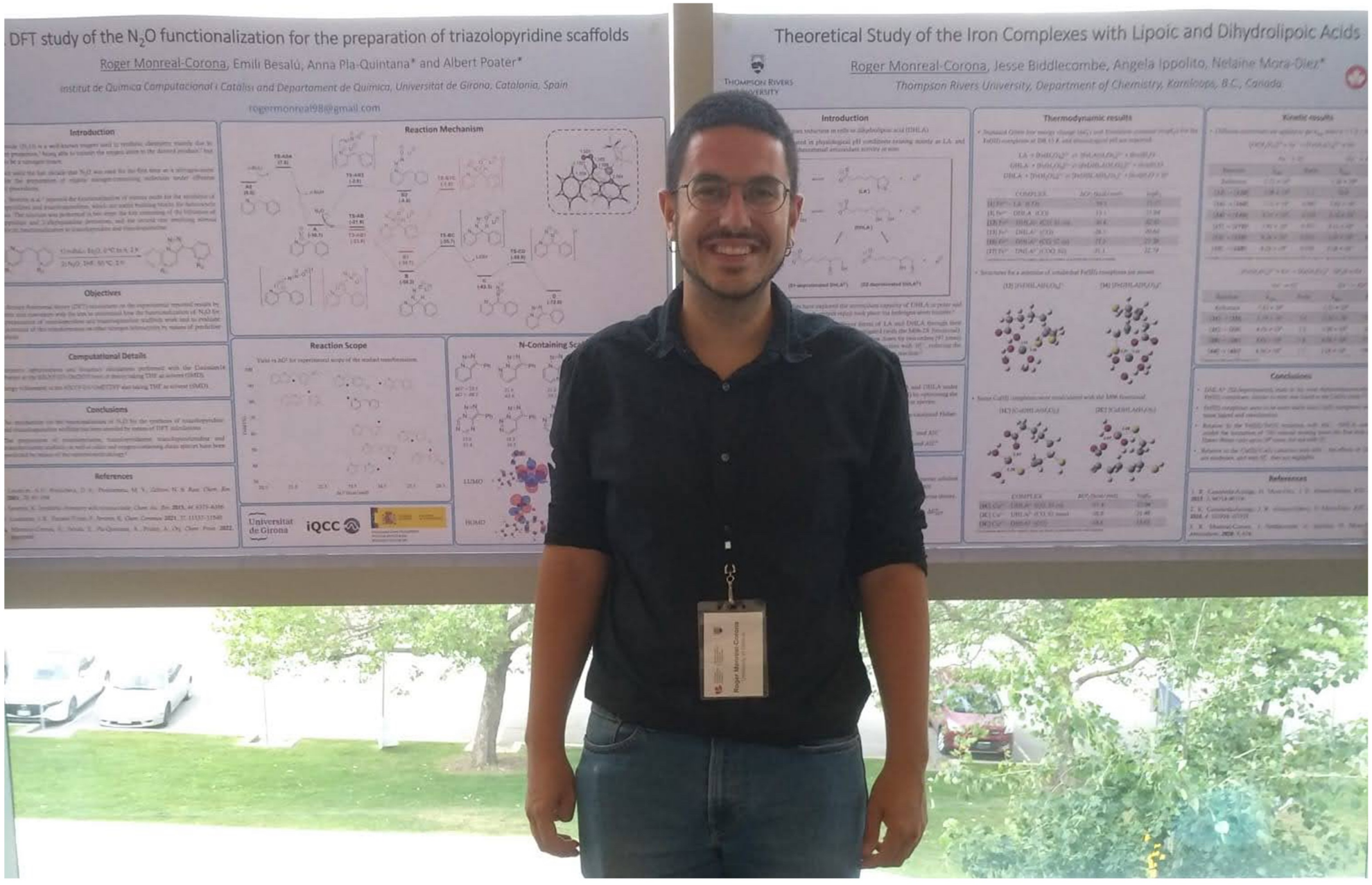


Richard Bowles

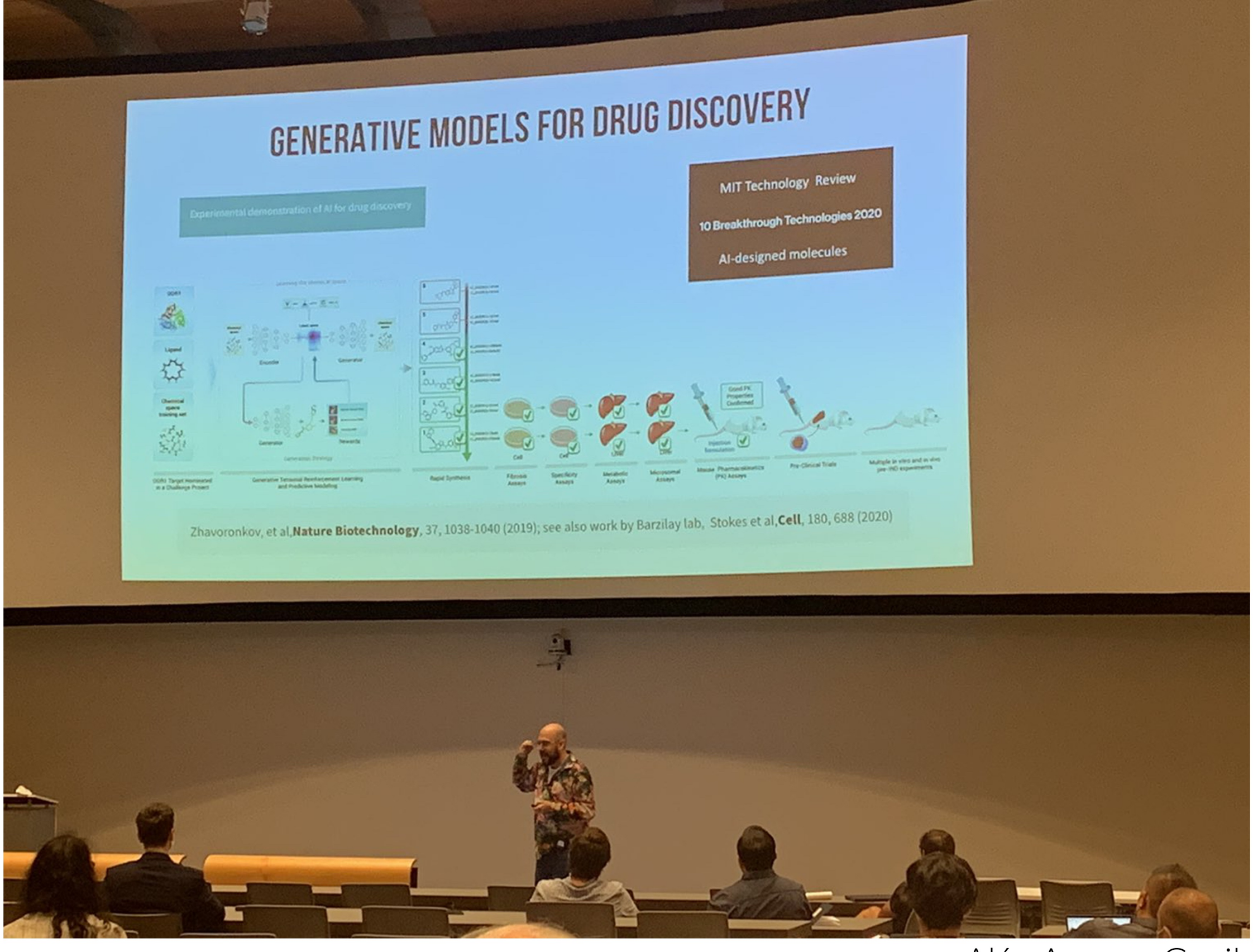
Poster Session



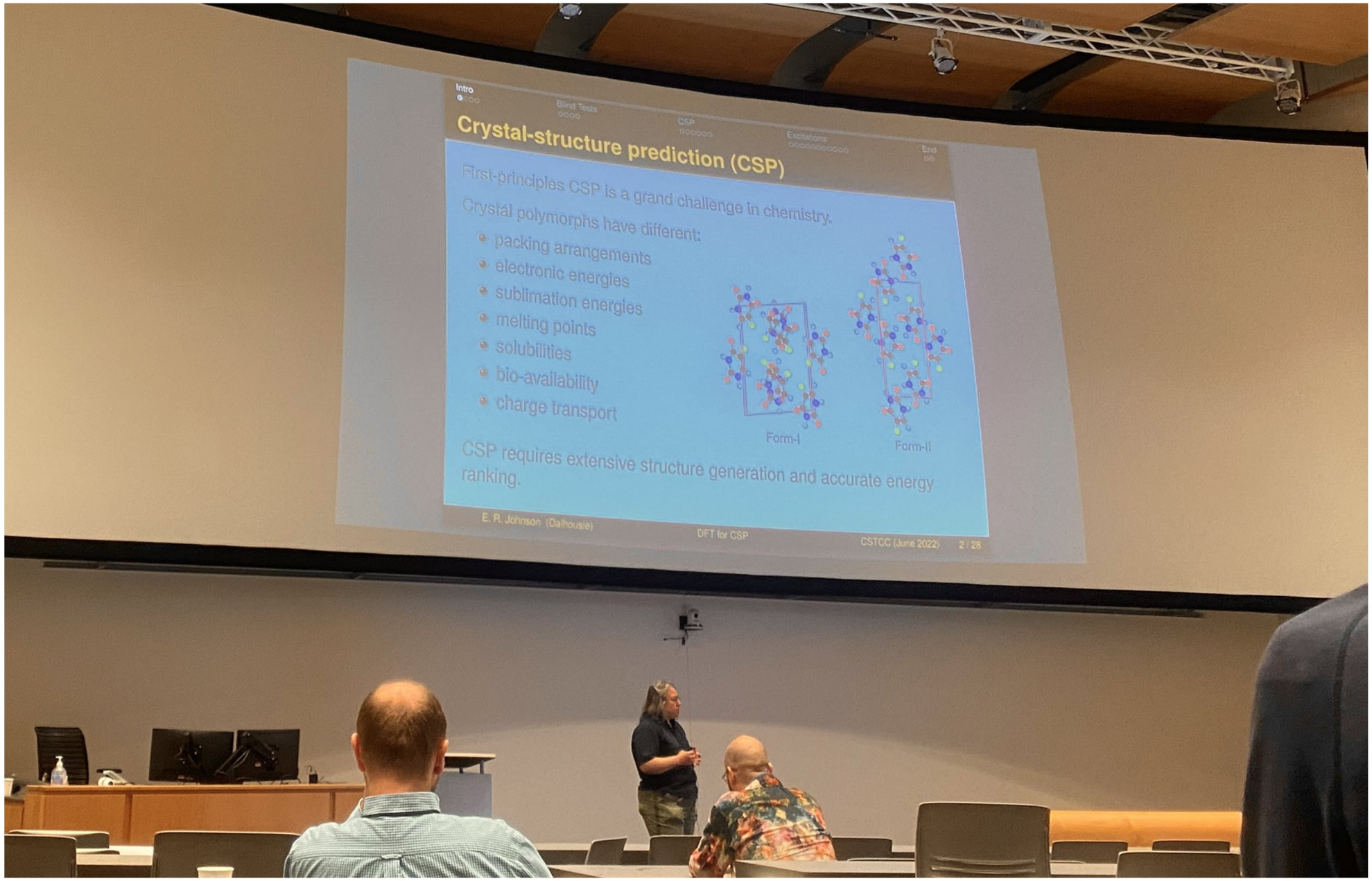
Ihor Neporozhnii



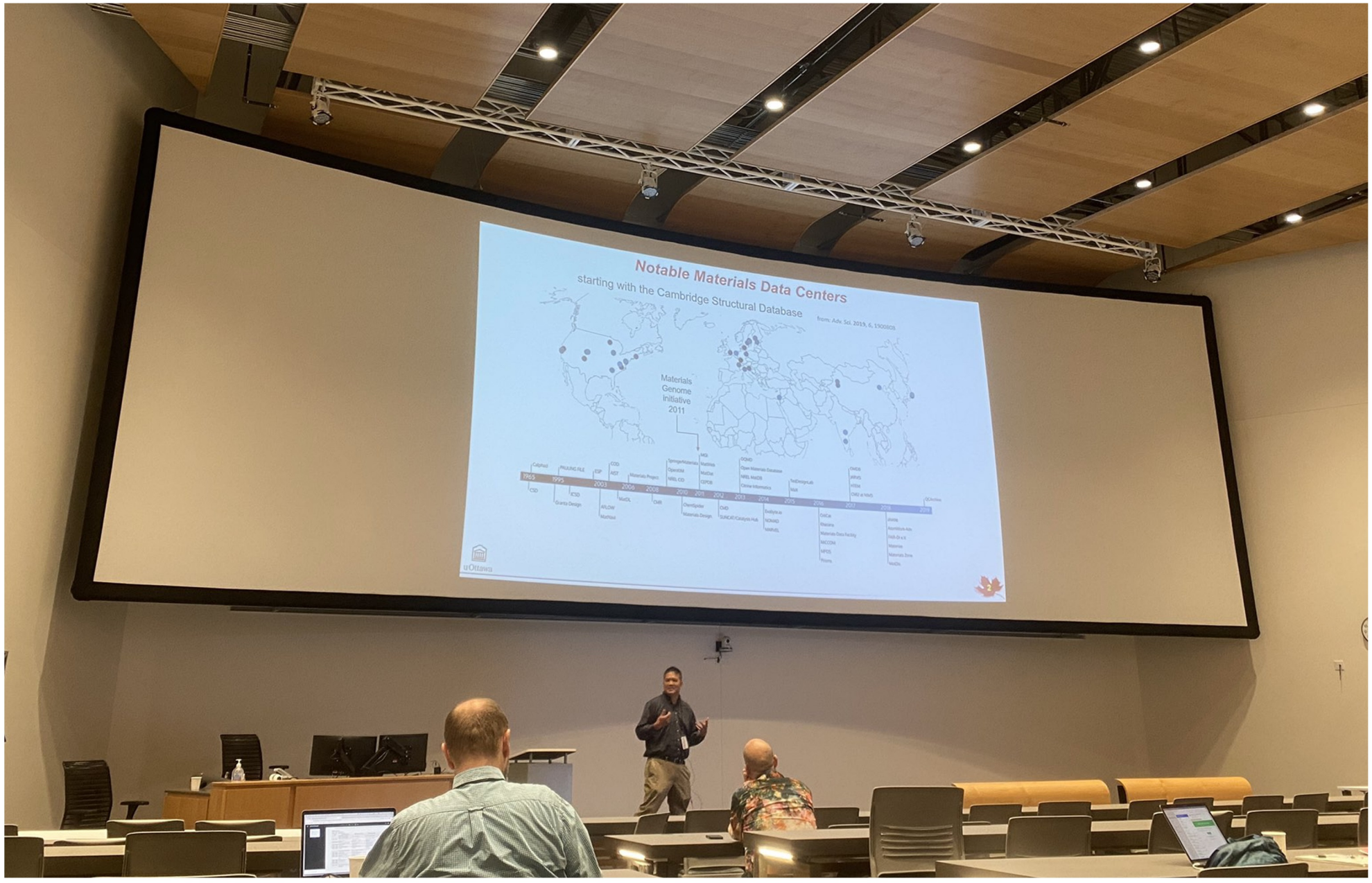
Roger Monreal-Corona with dual posters



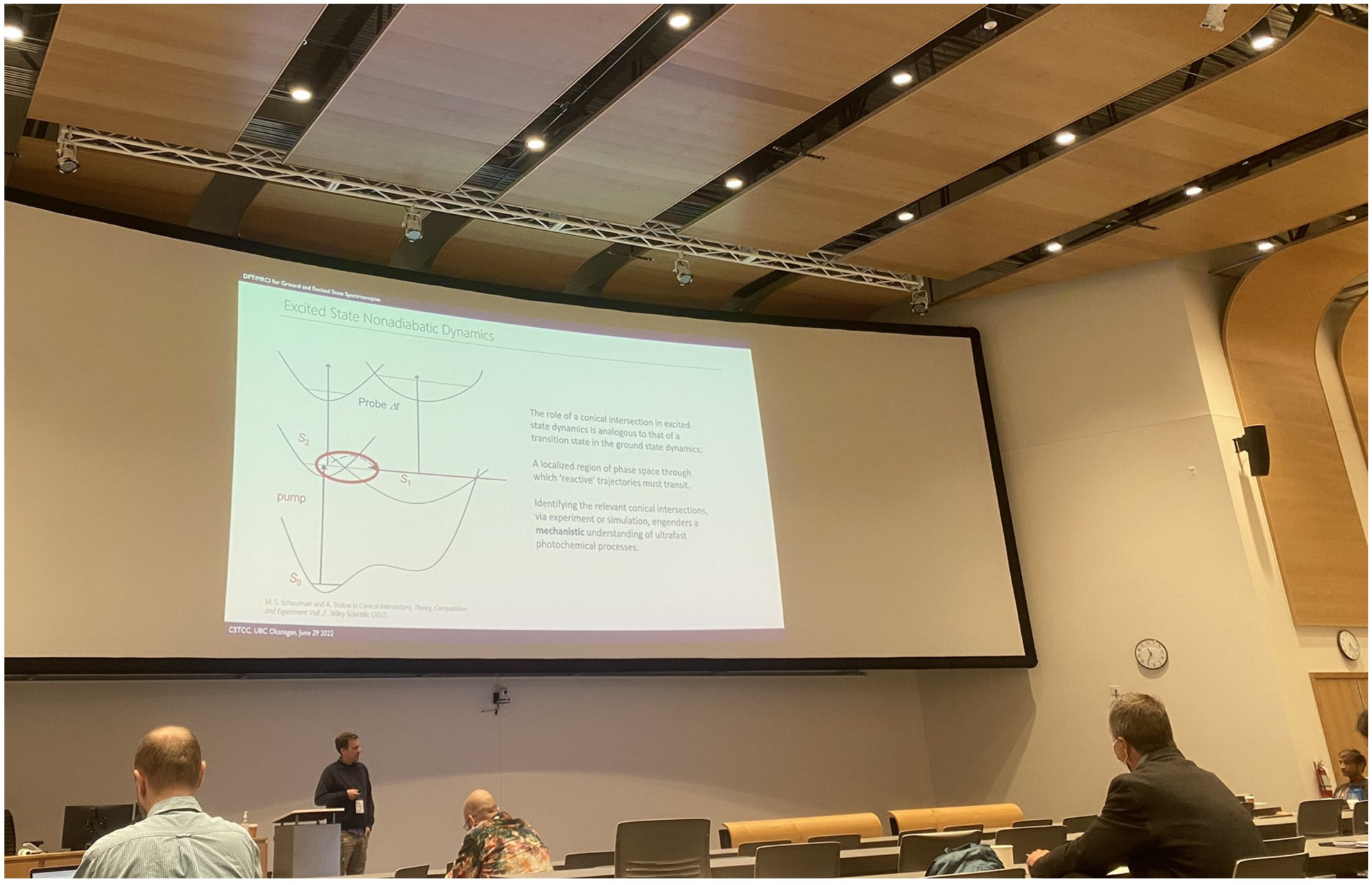
Alán Aspuru-Guzik



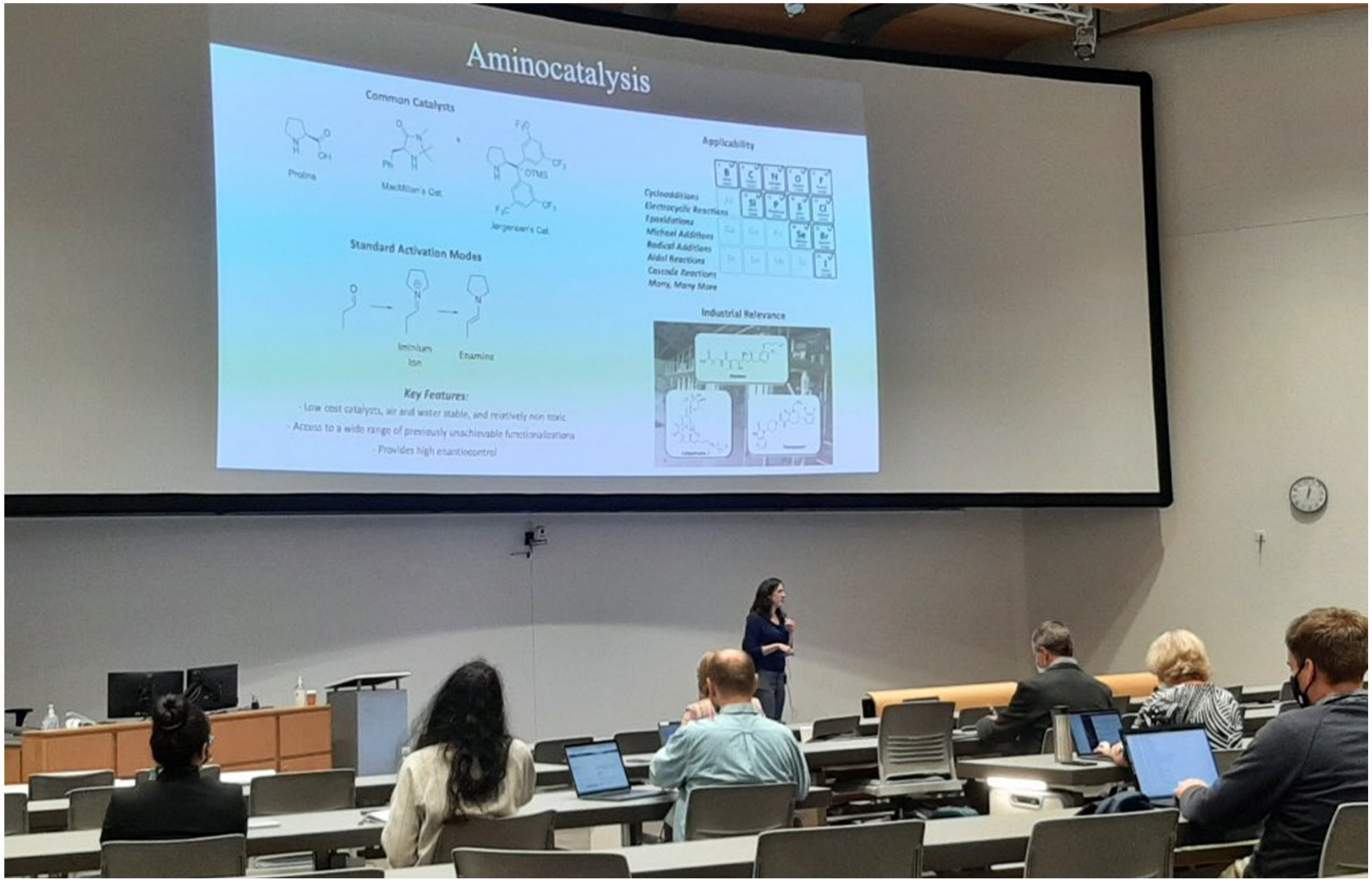
Erin Johnson


Notable Materials Data Centers
starting with the Cambridge Structural Database
from: Adv. Sci. 2019, 6, 1900808
Materials Genome Initiative 2011
1965
1995
2003
2006
2008
2010
2011
2012
2013
2014
2015
2016
2017
2018
2019
uOttawa

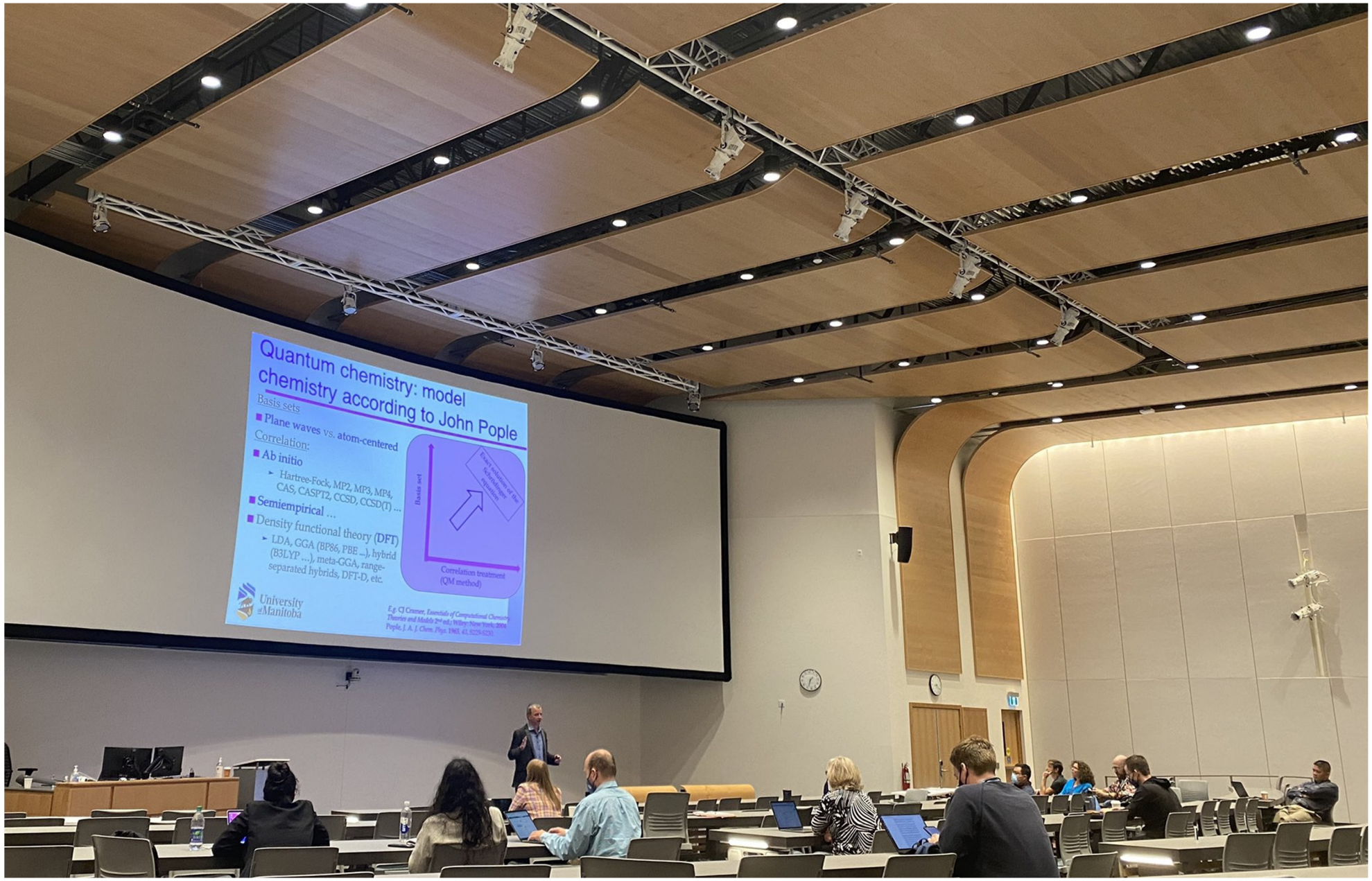
Tom Woo



Michael Schuurman



Rebecca Davis

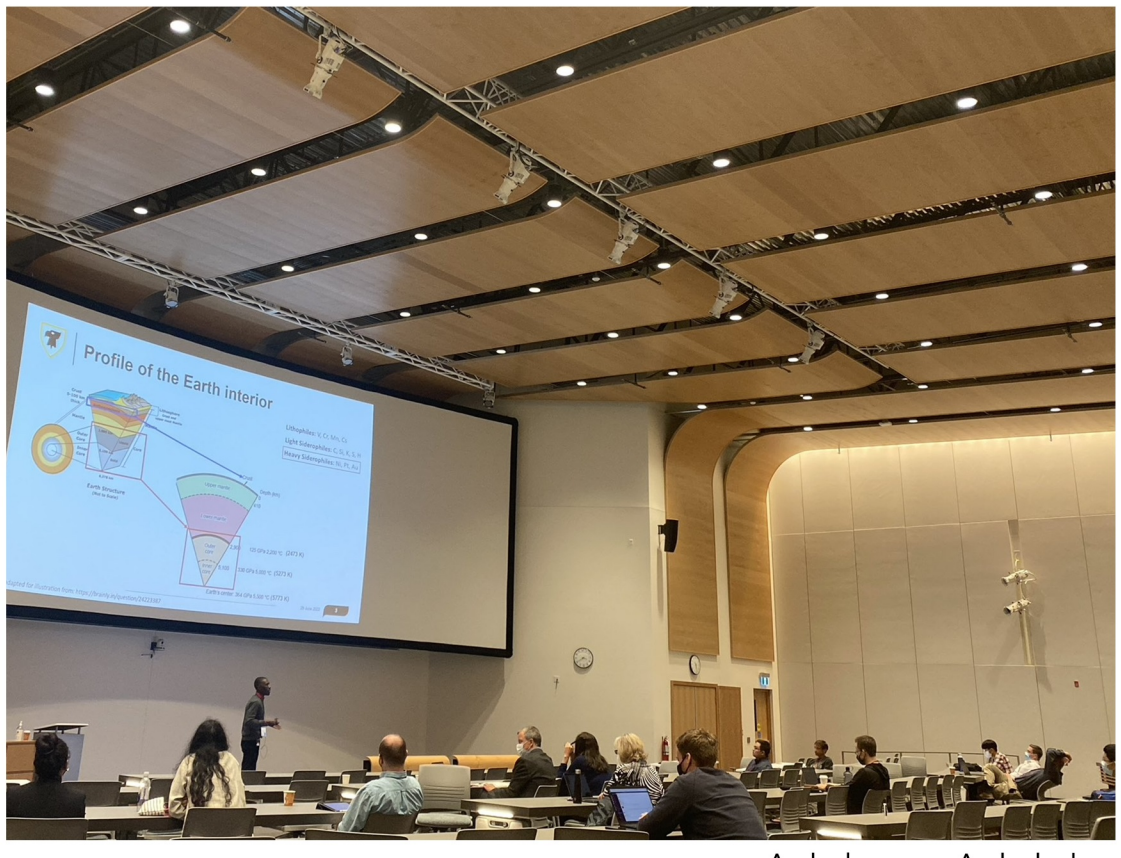


Georg Schreckenbach

Heather Wiebe

Rachelle Choueiri

Lizandra Barrios Herrera



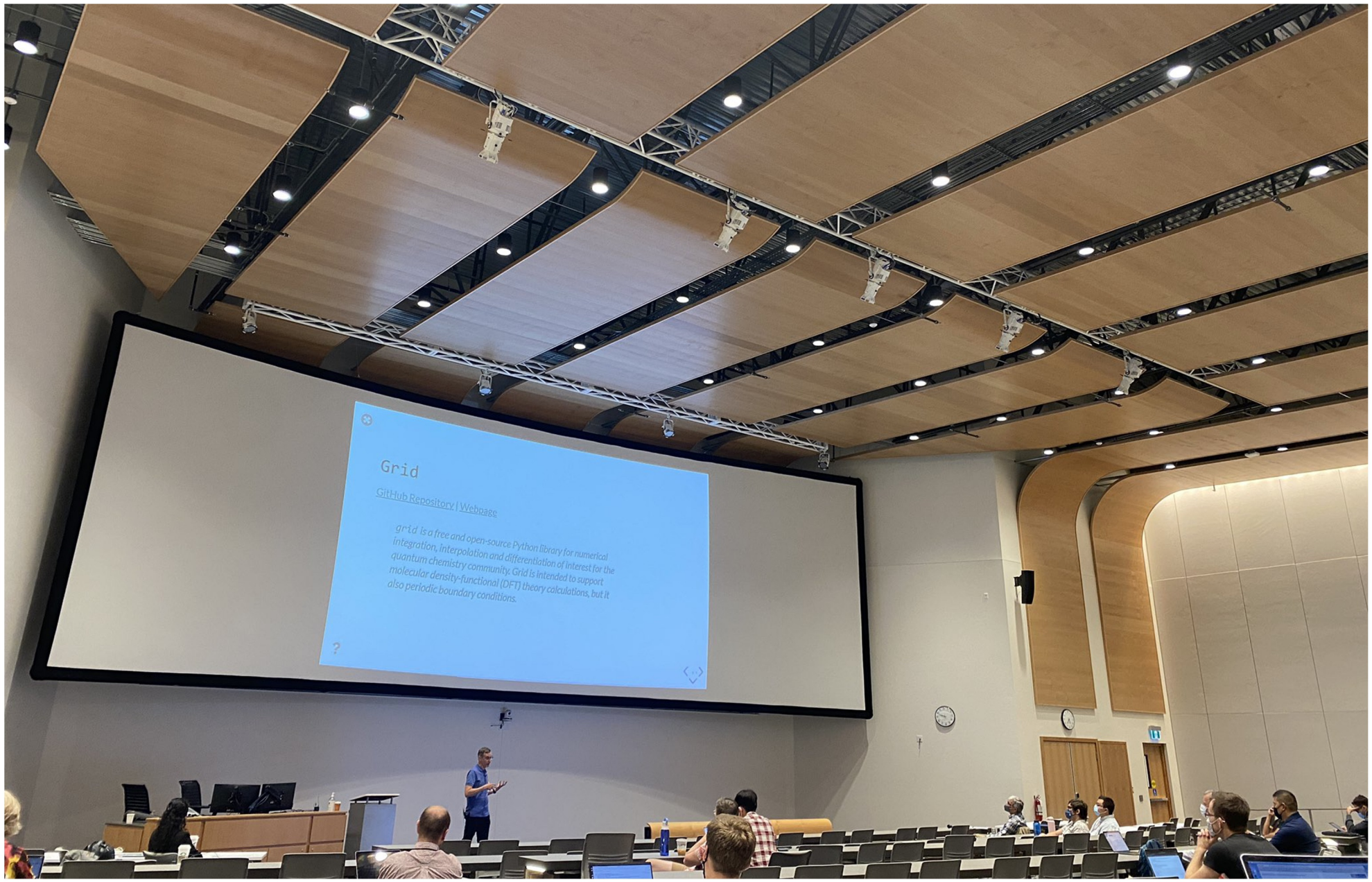
Adebayo Adeleke

Eduardo Romero-Montalvo

Alex Brown and Gino DiLabio in conversation

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

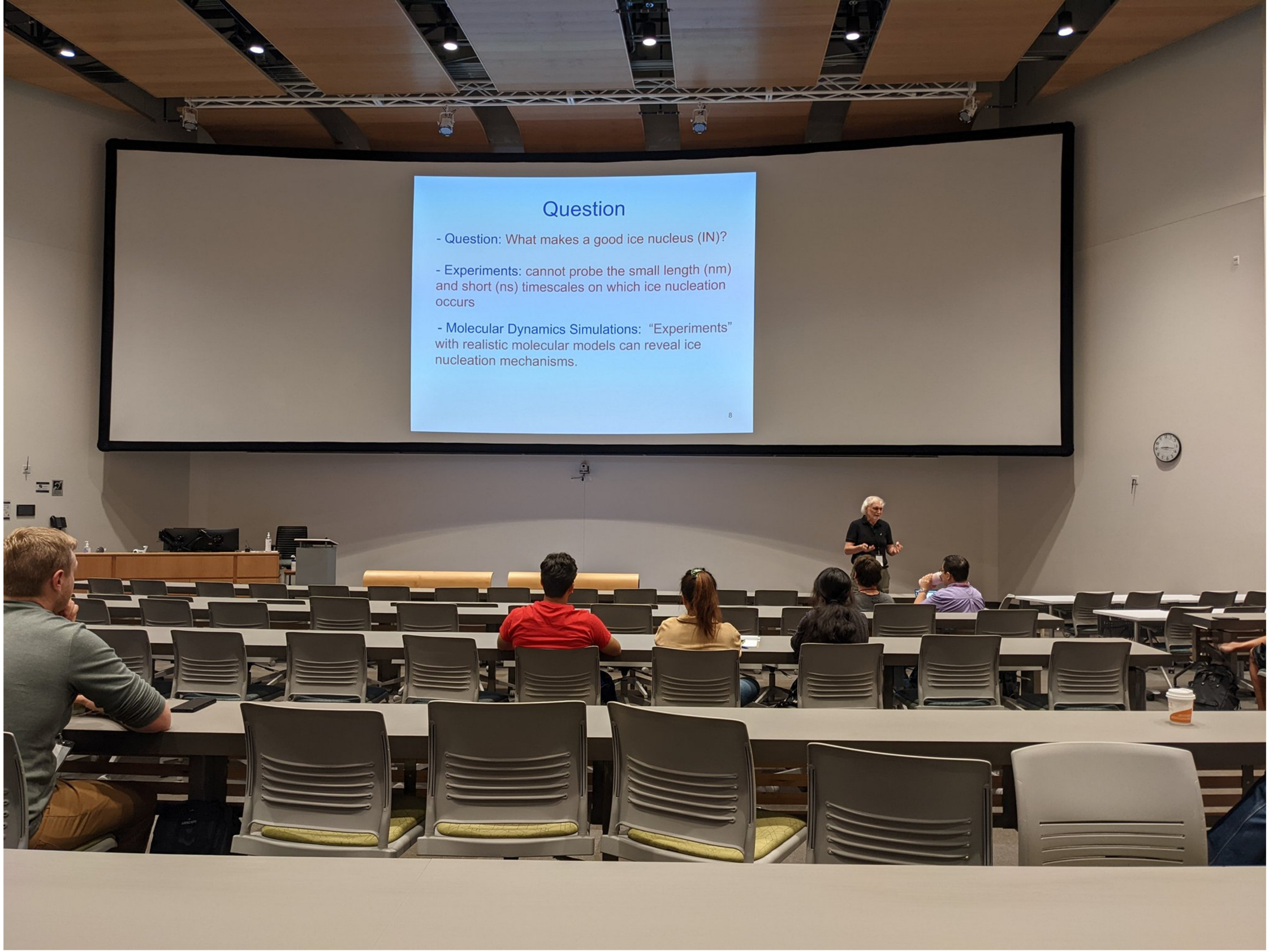
Farnaz Heidar-Zadeh


Grid
GitHub Repository | Webpage
grid is a free and open-source Python library for numerical integration, interpolation and differentiation of interest for the quantum chemistry community. Grid is intended to support molecular density-functional (DFT) theory calculations, but it also periodic boundary conditions.
?

Paul Ayers

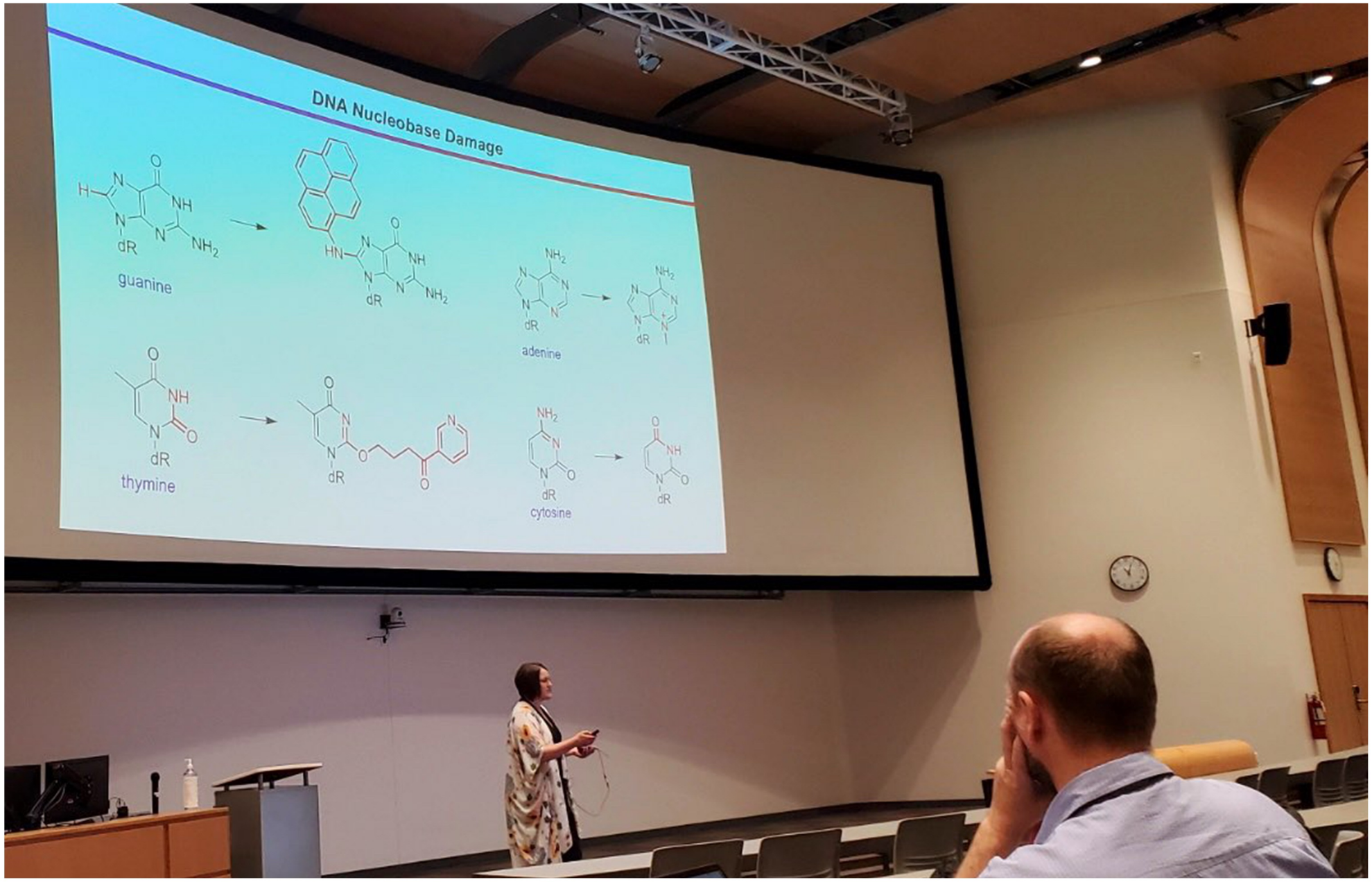
Thomas Baker

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

Gren Patey

Robert Szilagyi

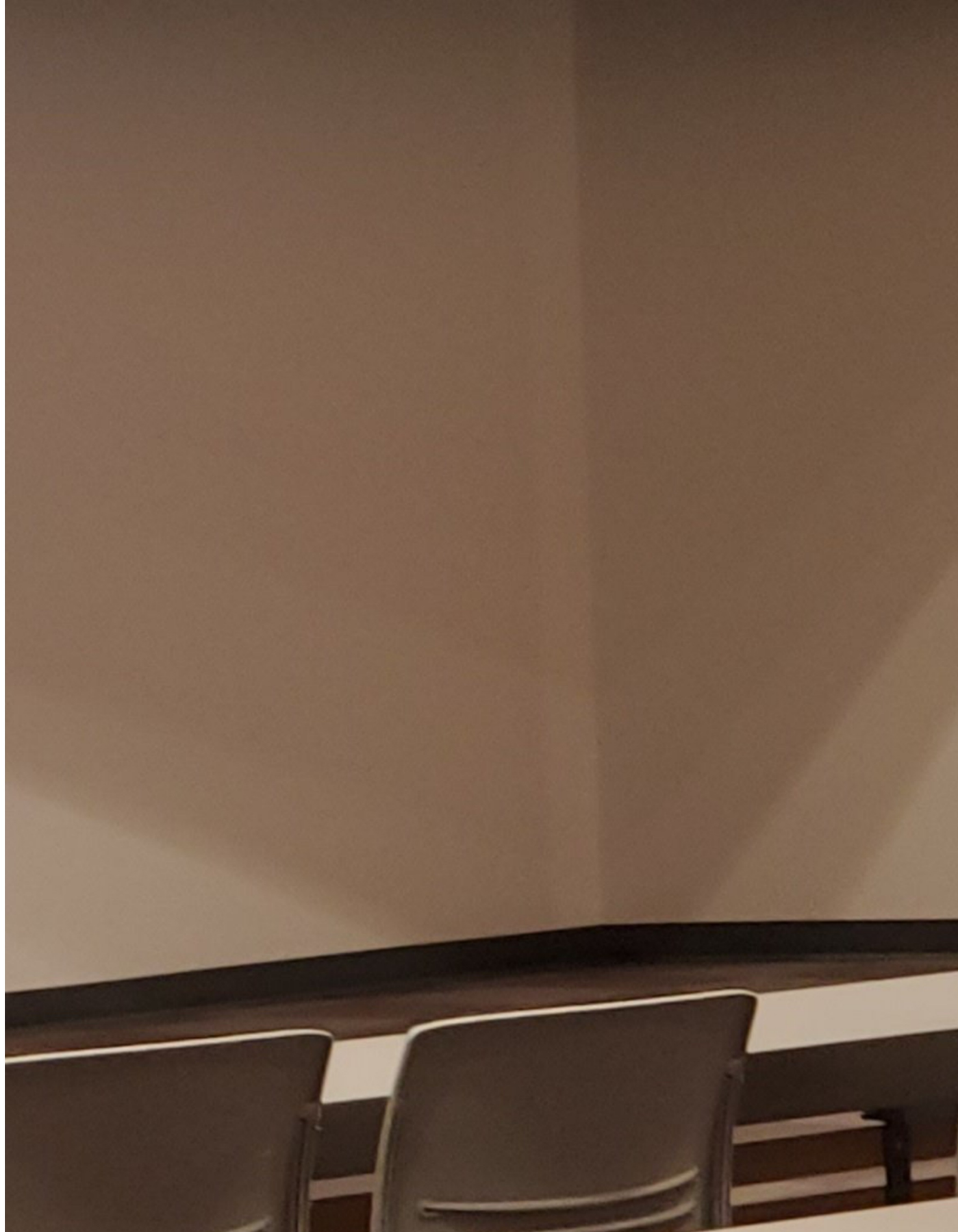


Stacey Wetmore


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


GROWLERS
VALVOLINE
HEARTBEAT
RUN & WALK
KELOWNA BREWING COMPANY


13


AJANI


All minors must be accompanied by an adult
MÛRE
SOMERSBY
BLACKBERRY
FLAVOURED
Cider
4.5% alc./vol. 473mL
MADE IN CANADA
REFRESHINGLY CRISP

Image Credits:

@A_Aspuru_Guzik
@abrown_uofa
@Albd90
@CompChemGuelph
@CSTCC2022
@DIMOCAT_iqcc
@i_paci
@ineporozhnii
@qchemprof
@SofiaDonnecke
@wetmorelab

Design:

@CompChemGuelph