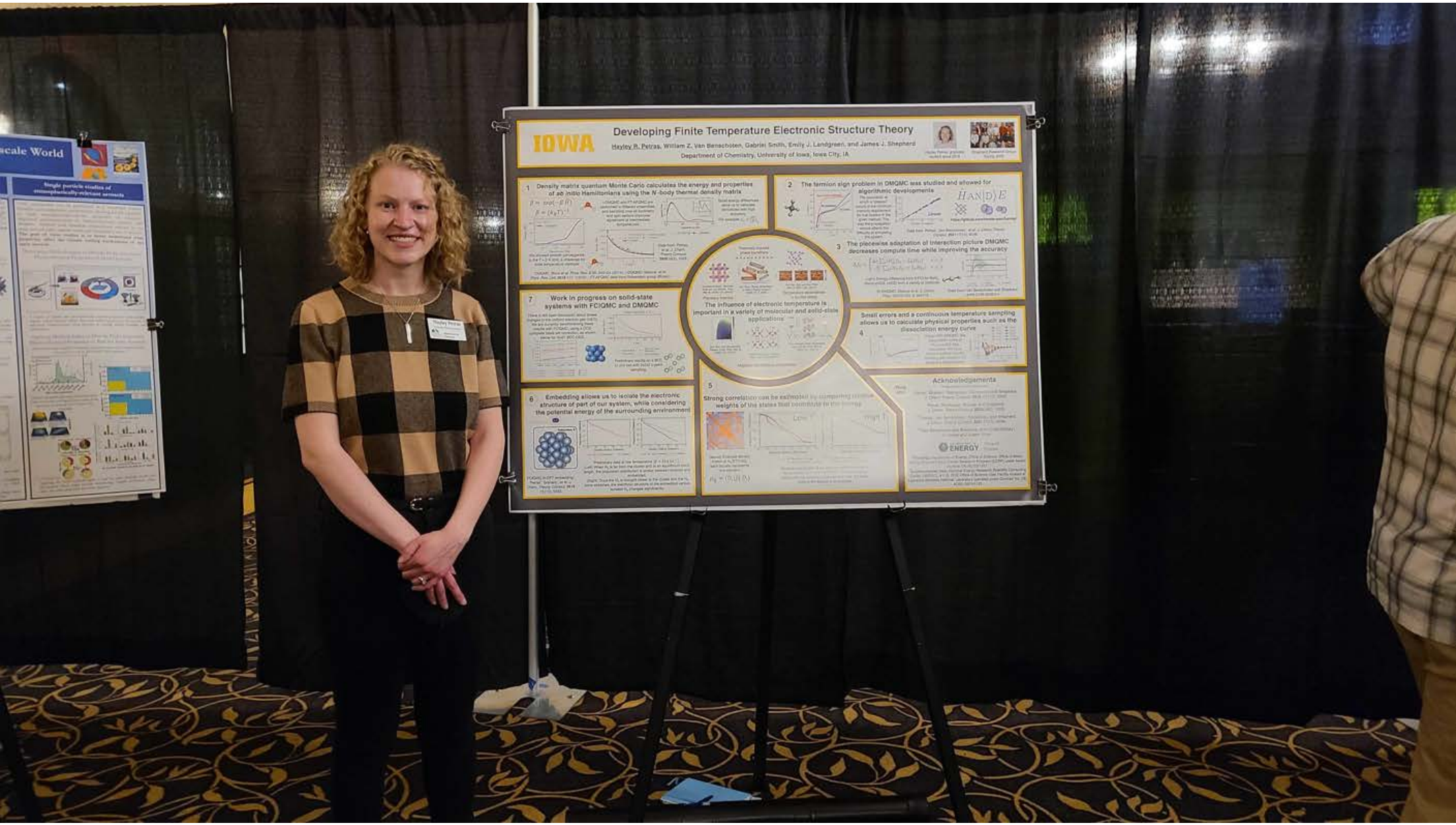
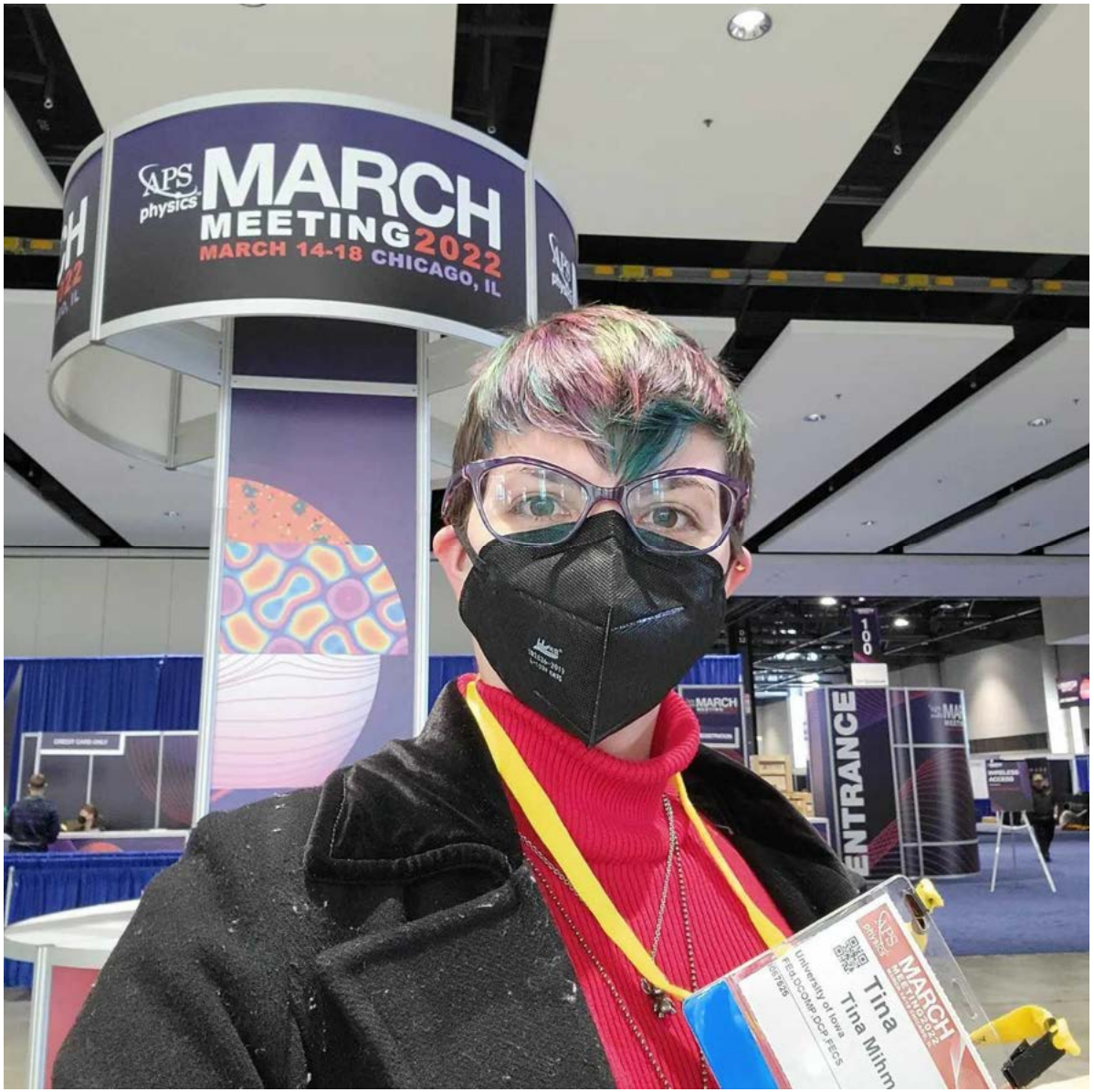

MARCH
MEETING 2019
BOSTON, MA
MARCH
MEETING 2020


IOWA
Developing Finite Temperature Electronic Structure Theory
Hayley R. Petras, William Z. Van Benschoten, Gabriel Smith, Emily J. Landgreen, and James J. Shepherd
Department of Chemistry, University of Iowa, Iowa City, IA
1 Density matrix quantum Monte Carlo calculates the energy and properties of ab initio Hamiltonians using the N-body thermal density matrix
2 The fermion sign problem in DMQMC was studied and allowed for algorithmic developments
3 The piecewise adaptation of interaction picture DMQMC decreases compute time while improving the accuracy
The influence of electronic temperature is important in a variety of molecular and solid-state applications
4 Small errors and a continuous temperature sampling allows us to calculate physical properties such as the dissociation energy curve
5 Strong correlation can be estimated by comparing relative weights of the states that contribute to the ground
6 Embedding allows us to isolate the electronic structure of part of our system, while considering the potential energy of the surrounding environment
7 Work in progress on solid-state systems with FCIQMC and DMQMC
Acknowledgements
ENERGY


MOUNTAYR
Raiders
20
21
GOLF


APS physics
MARCH MEETING 2022
MARCH 14-18 CHICAGO, IL
ENTRANCE
Tina
Tina Mihm
University of Iowa
FEB-DCOMP-DCP-FECS


GLASVIN


CHEMISTRY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HAWKEYES


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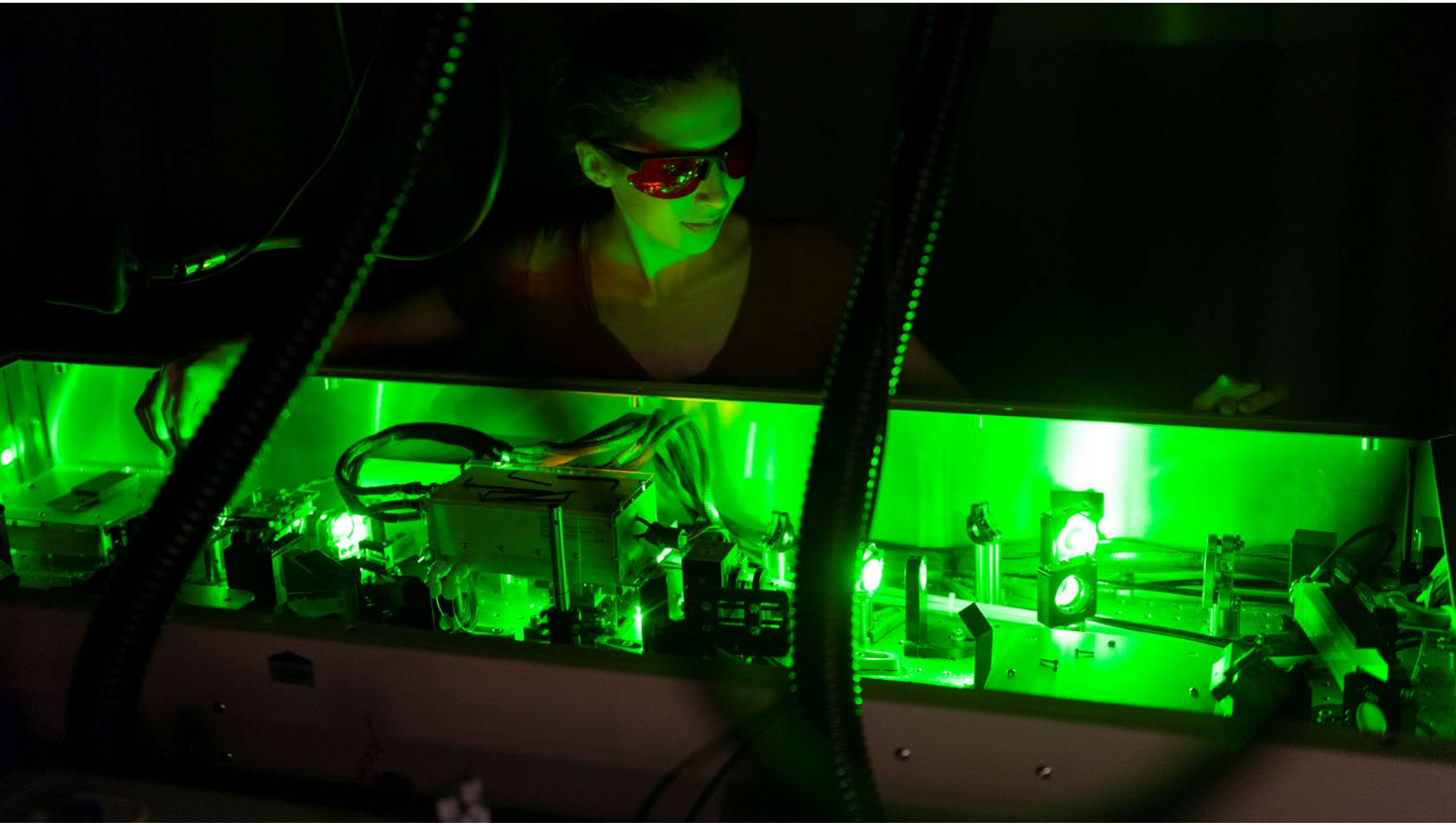
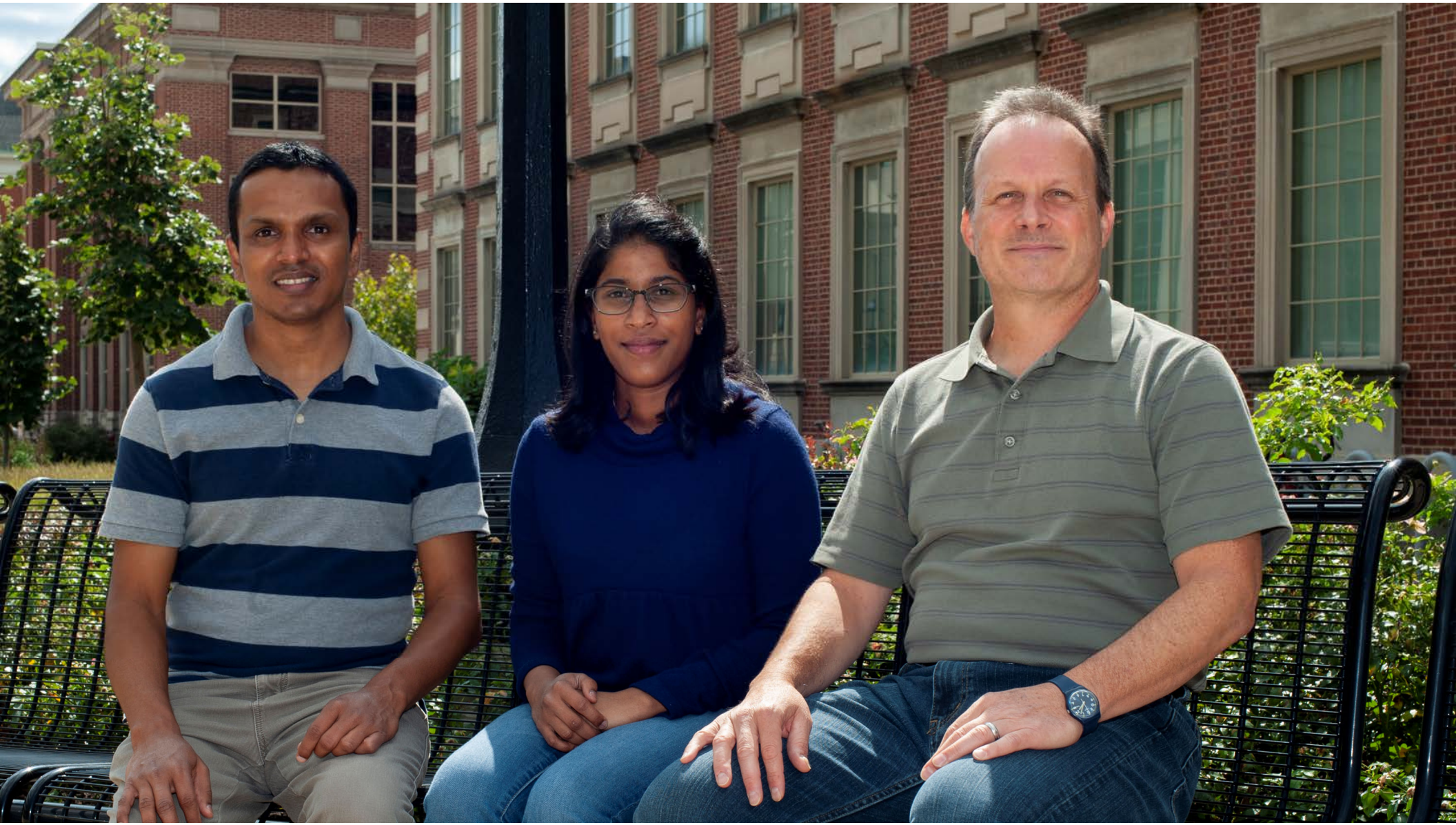
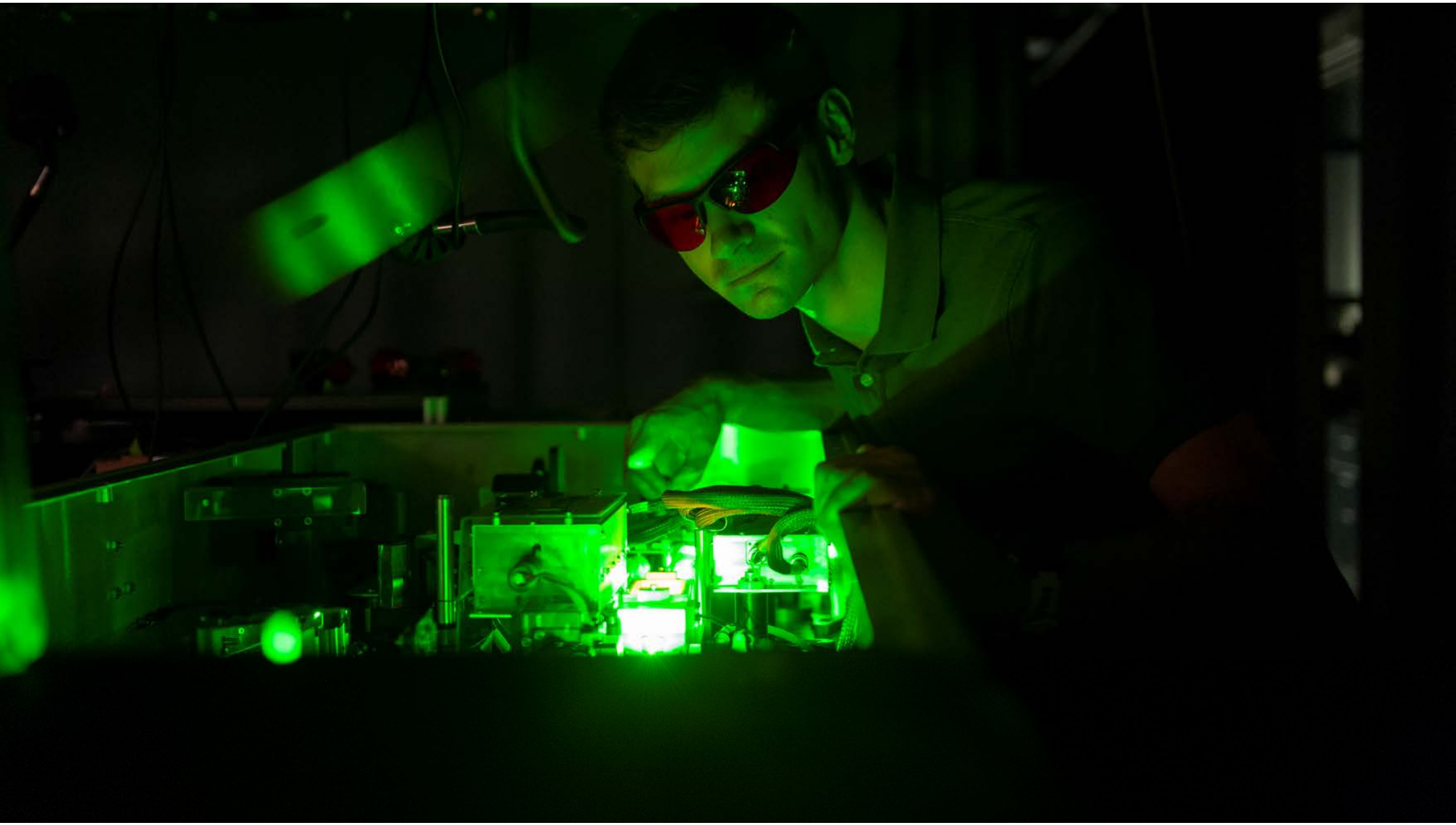



POLICE



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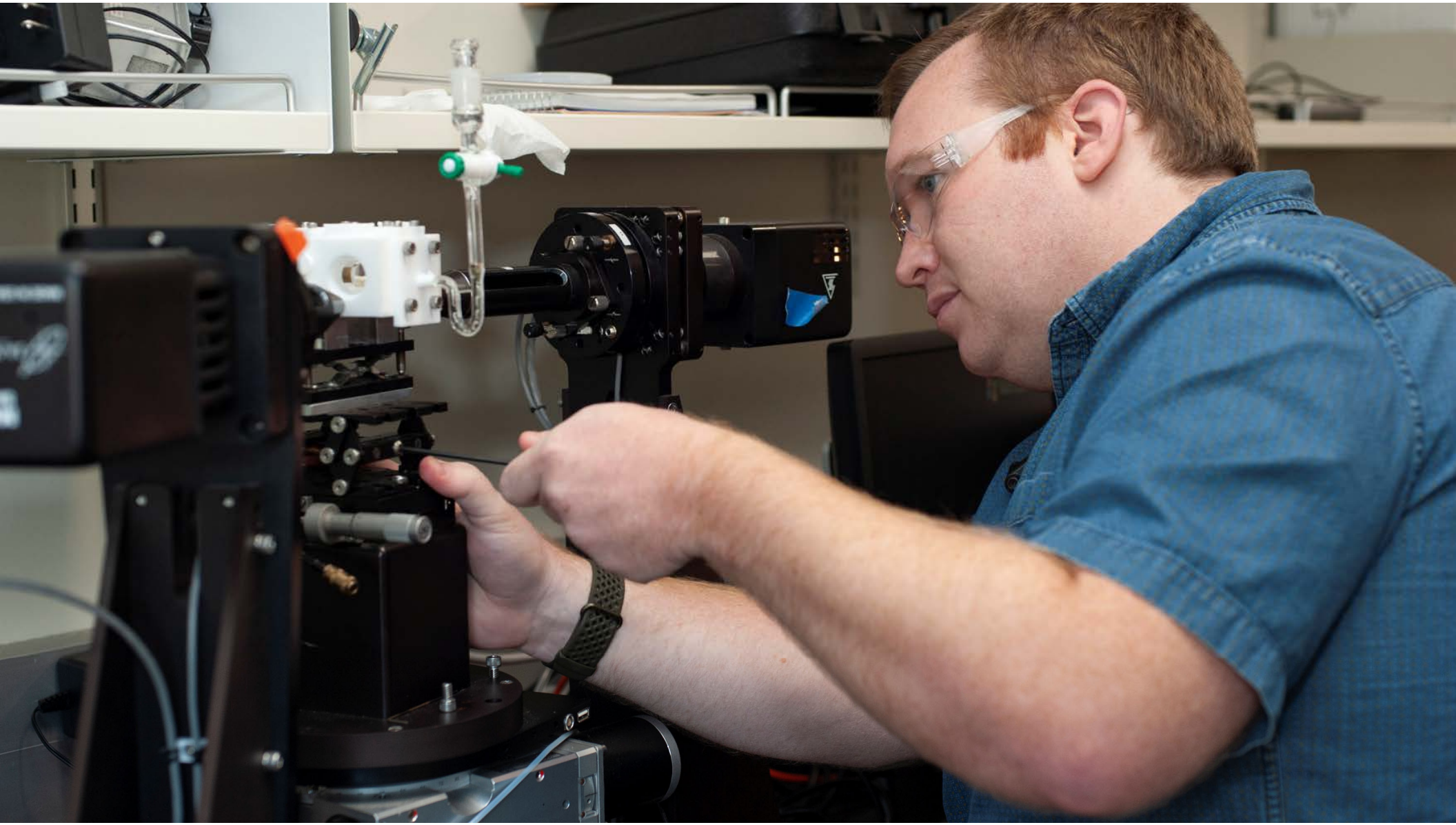

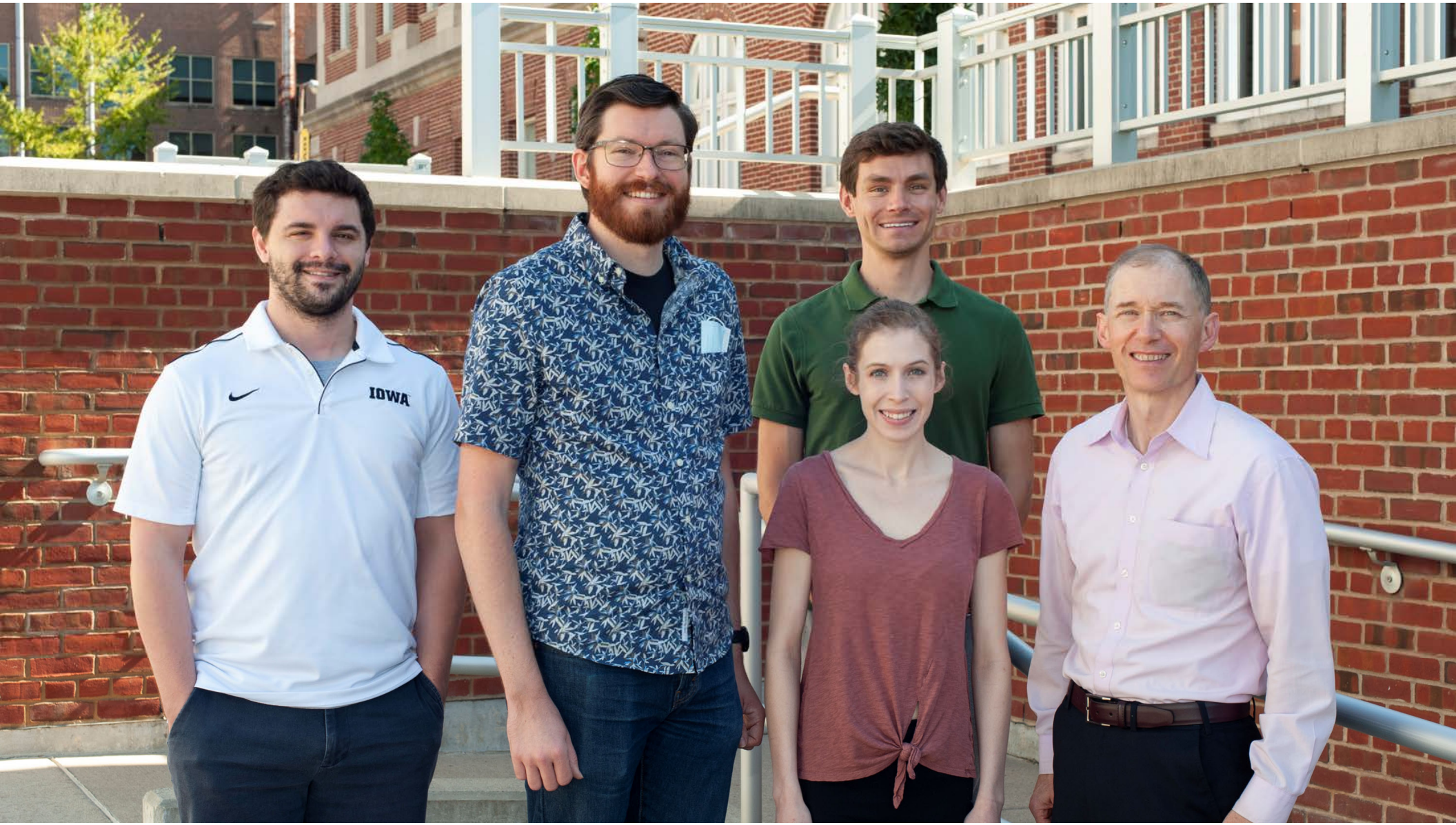
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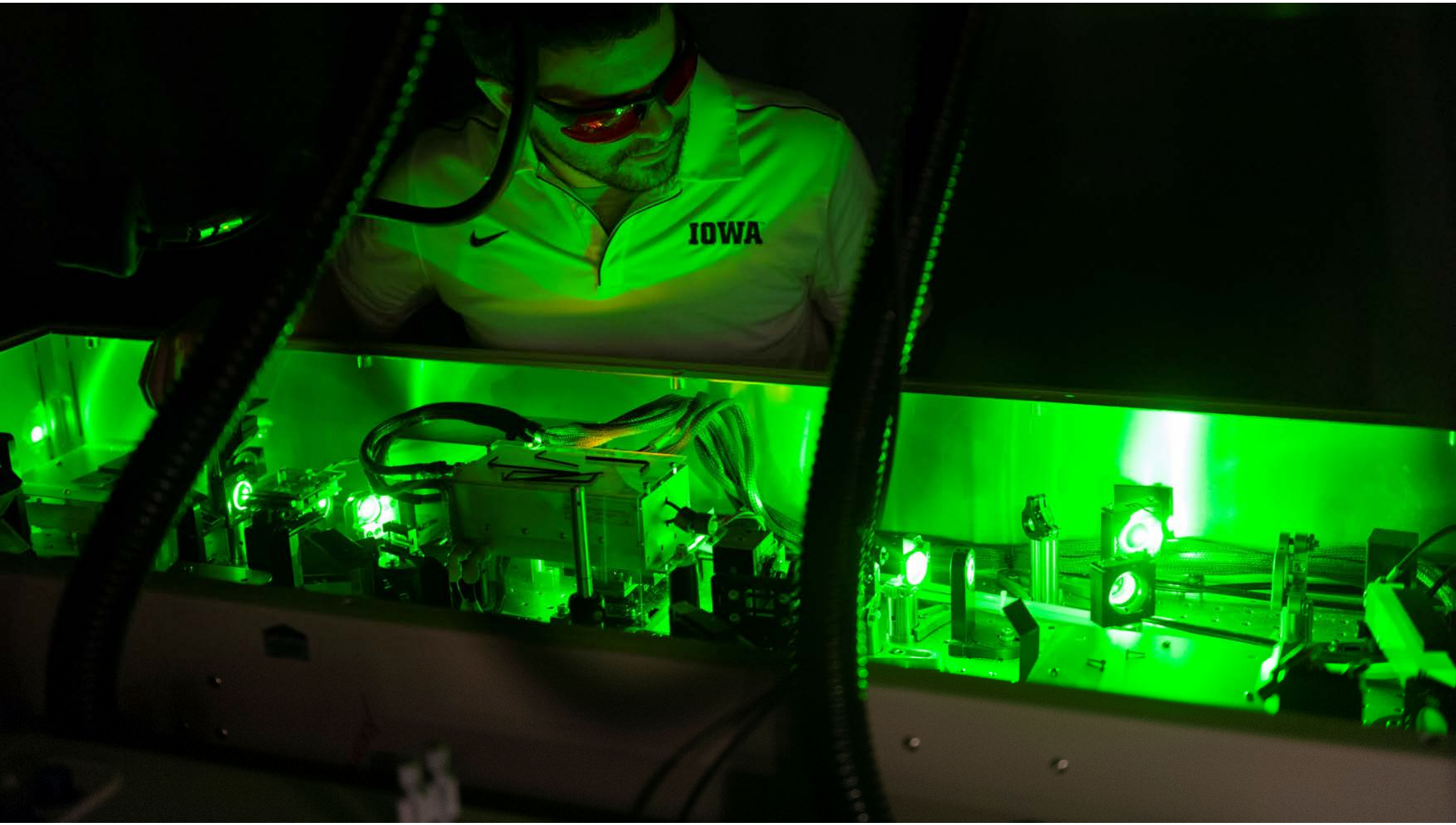
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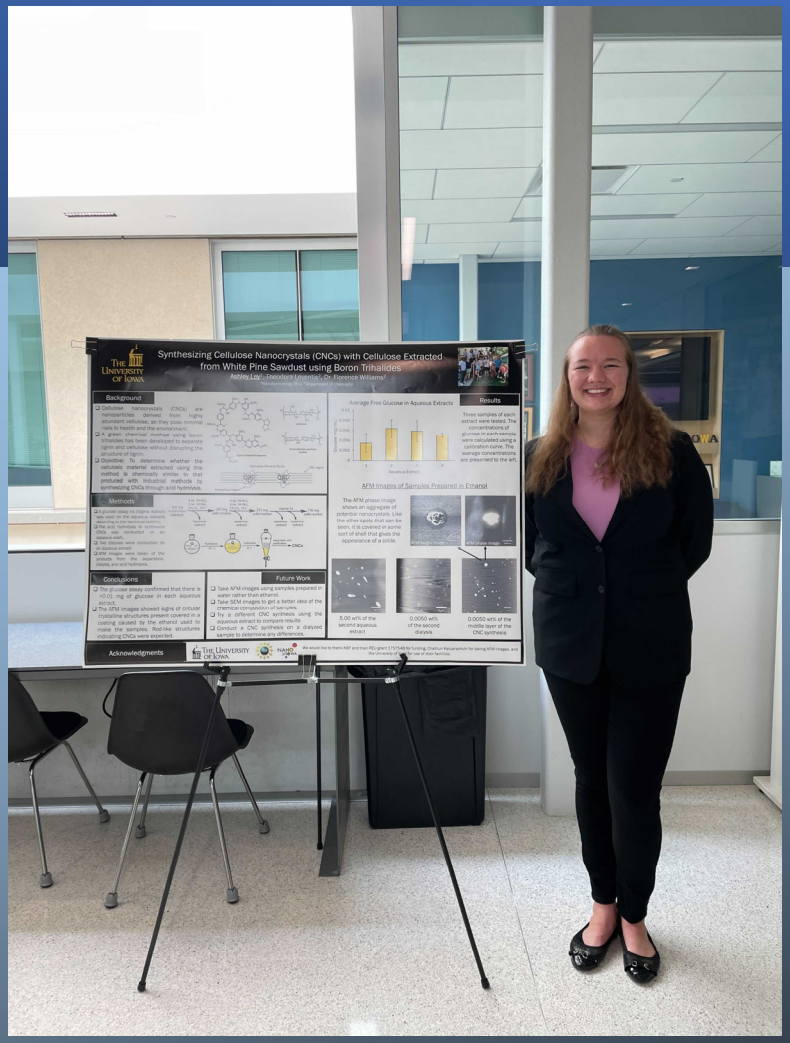
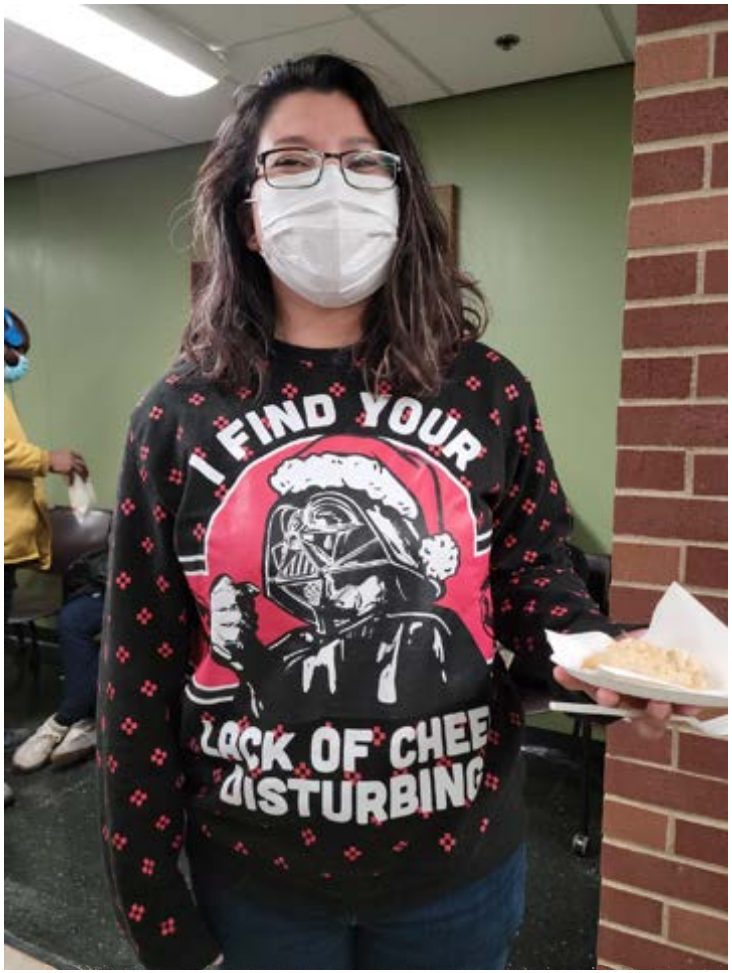
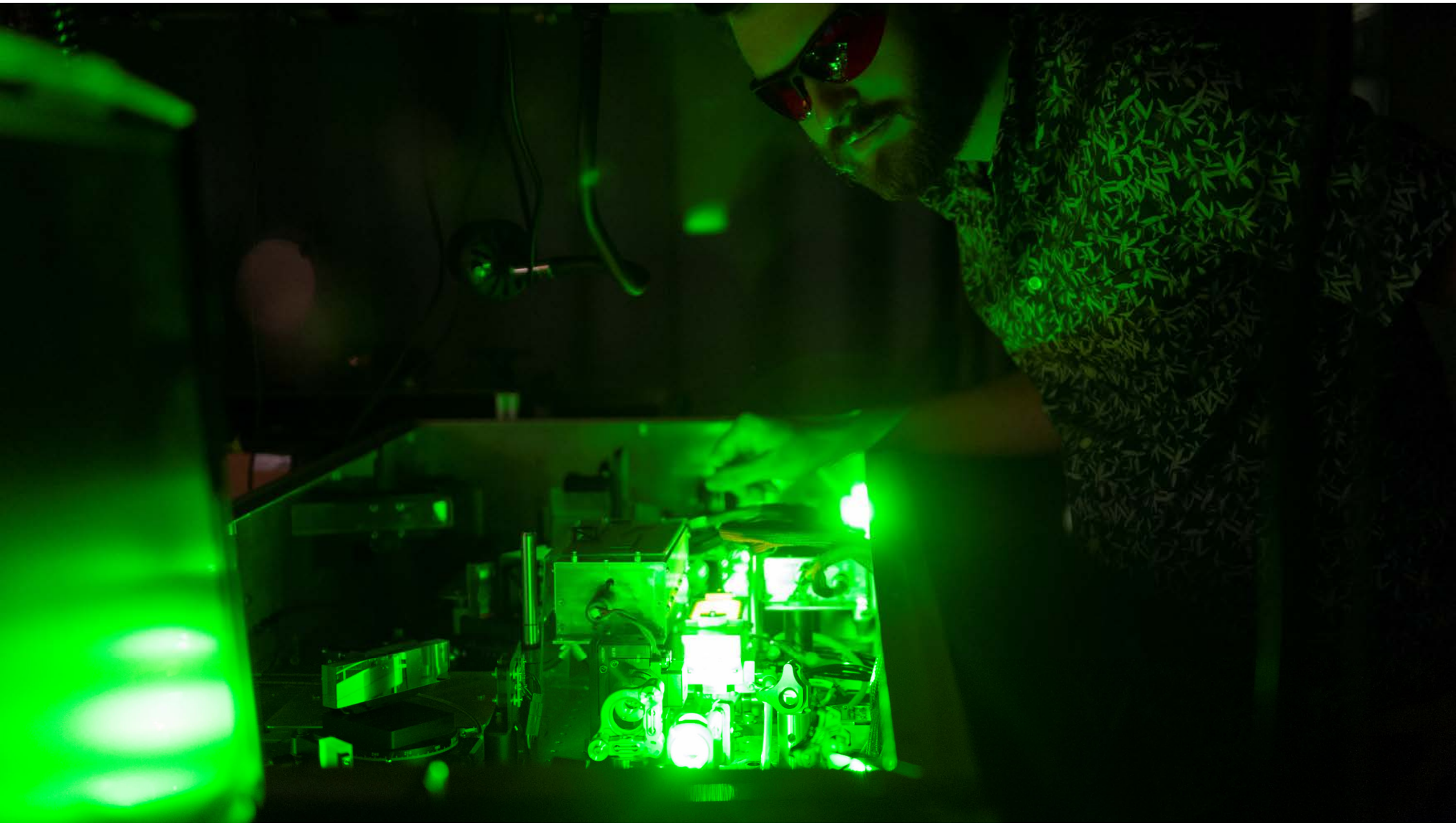

Synthesizing Cellulose Nanocrystals (CNCs) with Cellulose Extracted from White Pine Sawdust using Boron Trihalides
Ashley Loy[1], Hieodora Lovema[1], Dr. Florence Williams[1]
[1]Homecoming MU Researcher, University
Background
Methods
Conclusions
Future Work
Acknowledgments
Average Free Glucose in Aqueous Extracts
Results
AFM images of Samples Prepared in Ethanol
The AFM phase image shows an aggregate of potential nanocrystals. Like the other spots that can be seen, it is covered in some sort of shell that gives the appearance of a circle.
5.00 wt% of the second aqueous extract
0.0050 wt% of the second dialysis
0.0050 wt% of the middle layer of the CNC synthesis


I FIND YOUR
DISTURBING


richard
the whale
december 4
NASA
WEEK 14

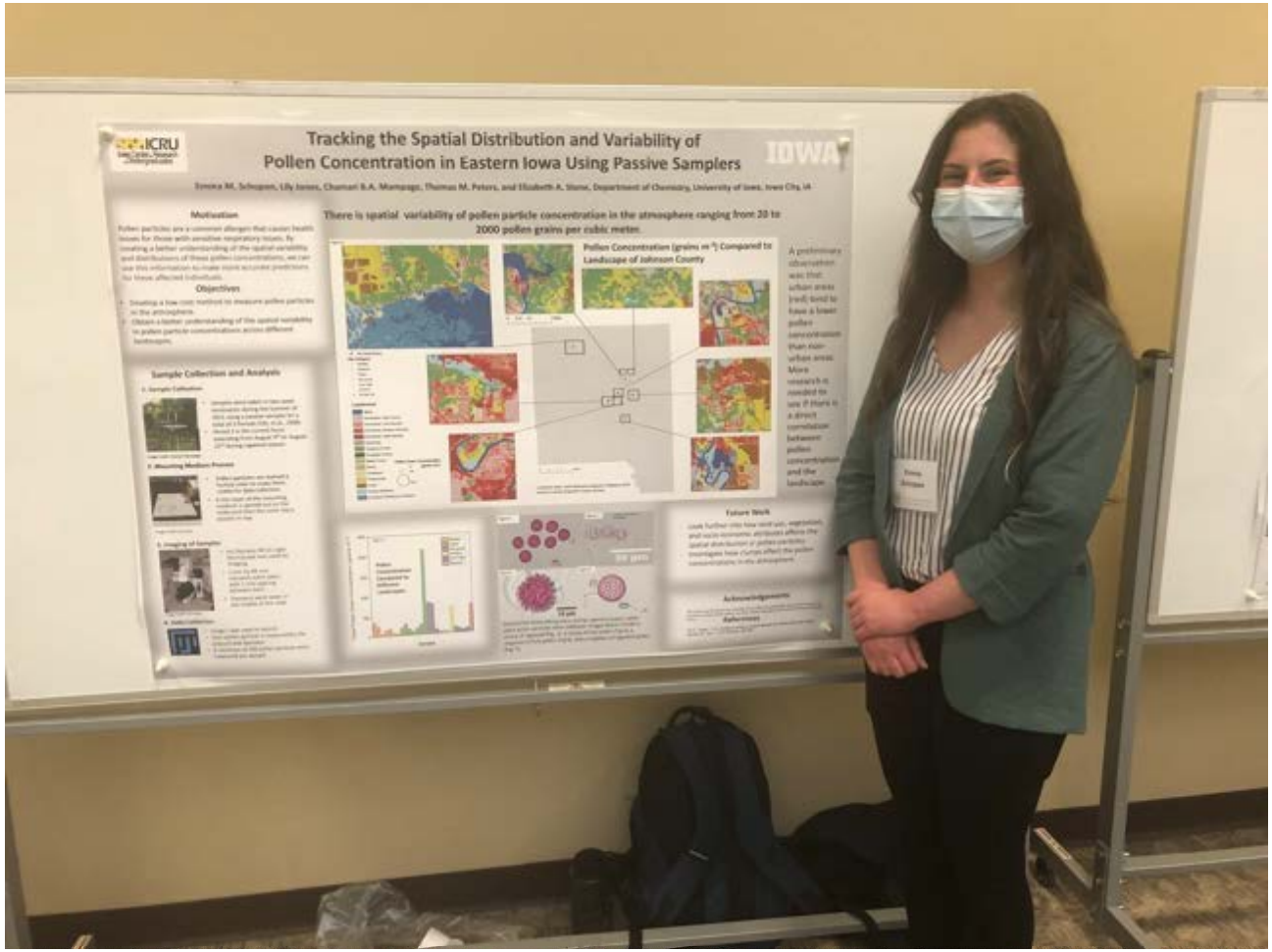

Steelers
Seagram's
Spiked

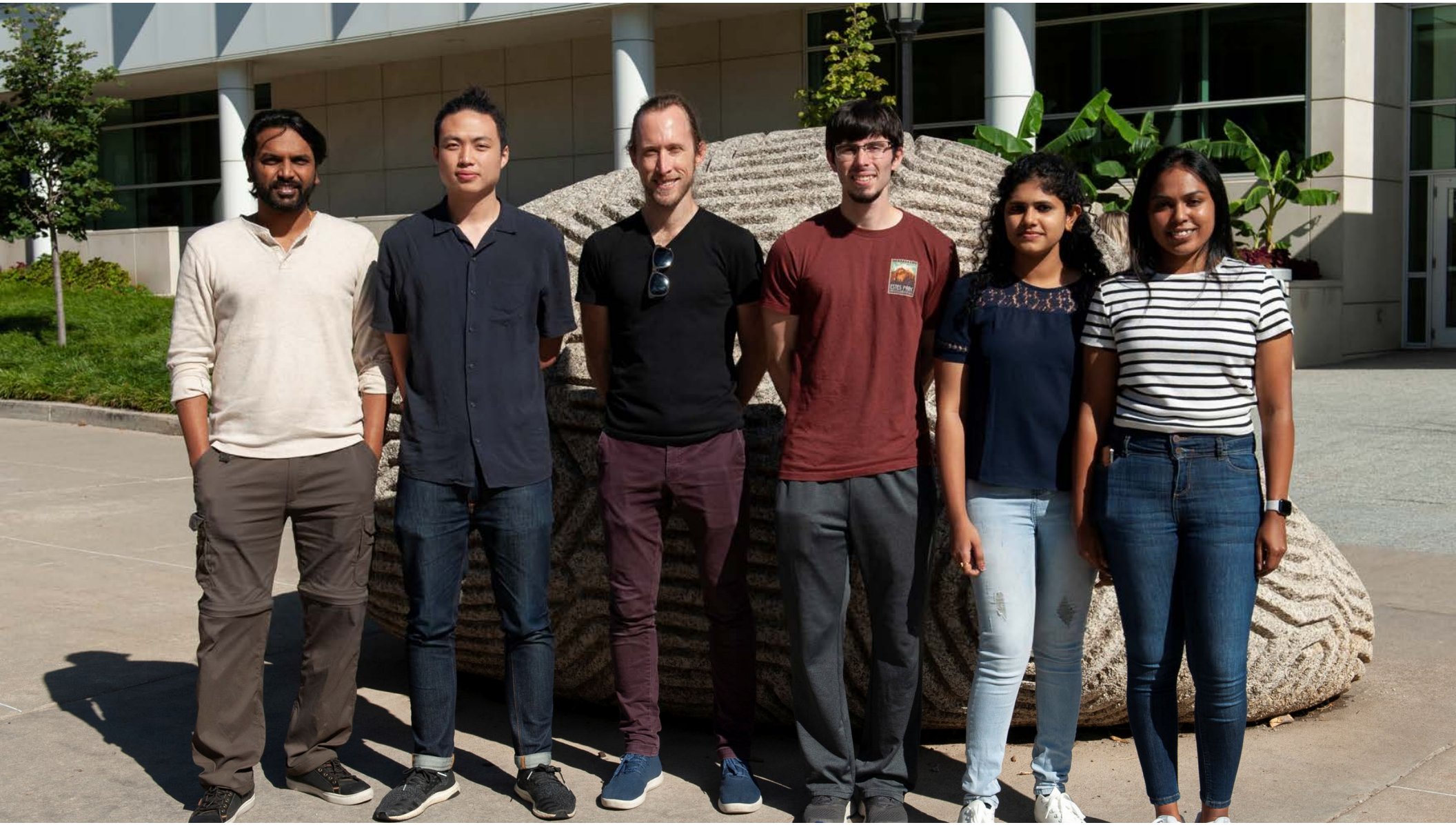


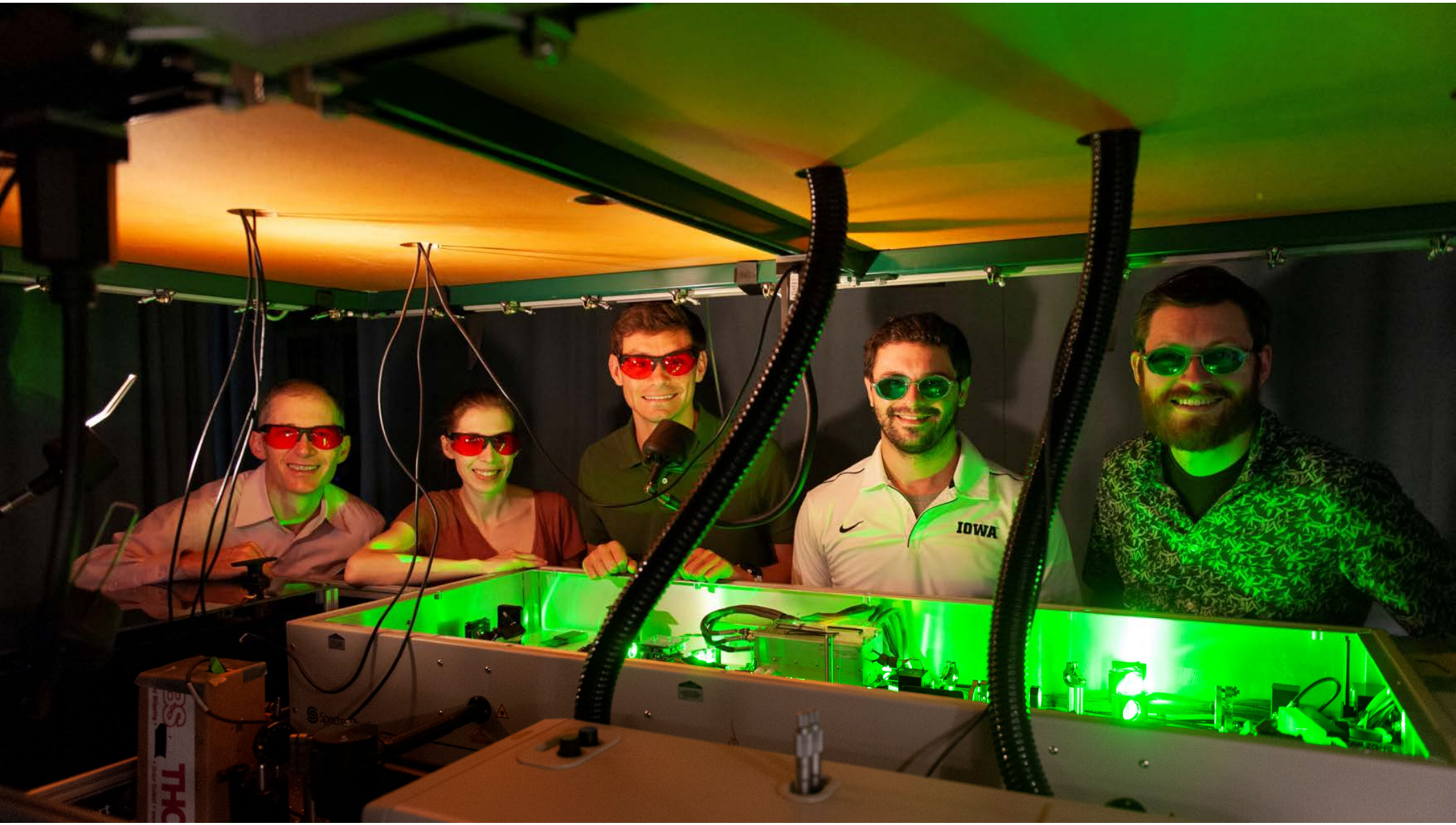

430


East
Elevator
EXIT
OH CHEMISTREE


H2O H2O H2O


Tracking the Spatial Distribution and Variability of
Pollen Concentration in Eastern Iowa Using Passive Samplers
IDWA
Motivation
Objectives
There is spatial variability of pollen particle concentration in the atmosphere ranging from 20 to 2000 pollen grains per cubic meter.
Pollen Concentration (grains m⁻³) Compared to Landscape of Johnson County
Sample Collection and Analysis
Future Work
Acknowledgements

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PAROLE


E 440
Chemistry
Teaching
Laboratory


OFFICE
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Faculty &
Staff
Commons


OH CHEMISTREE
OH CHEMISTREE!


Galaxy's
Greetings


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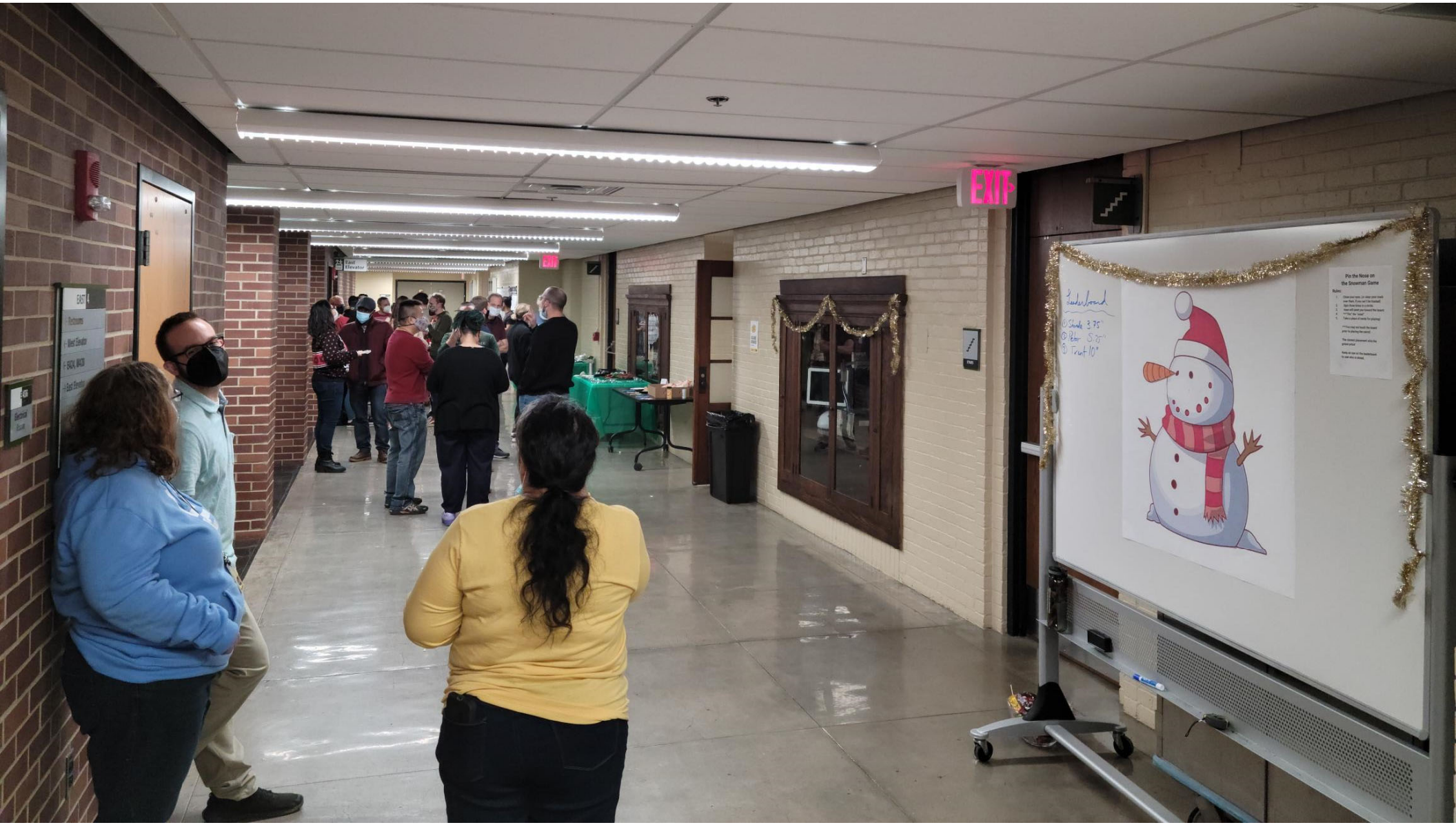
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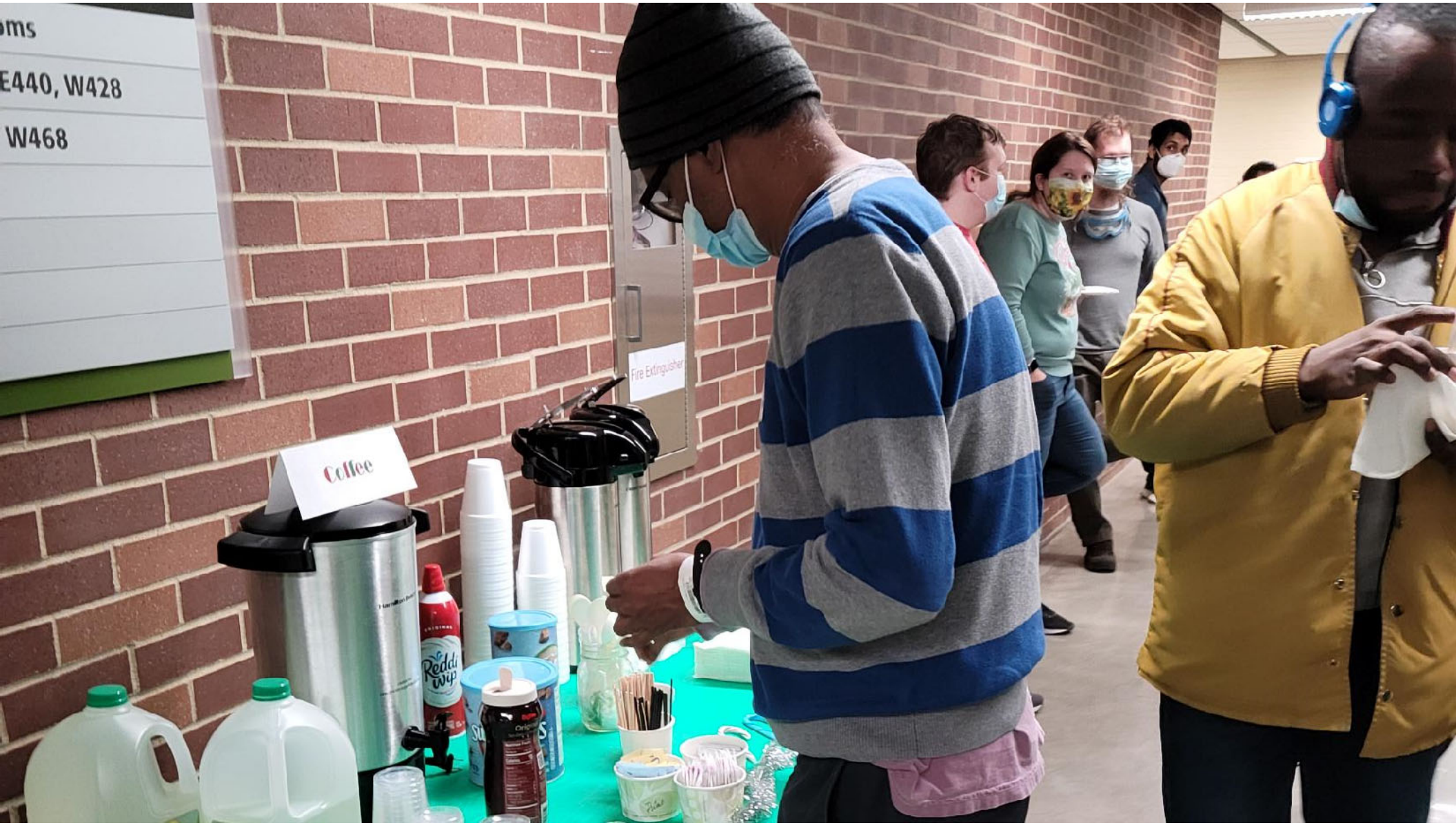
Pin the Nose on the Snowman Game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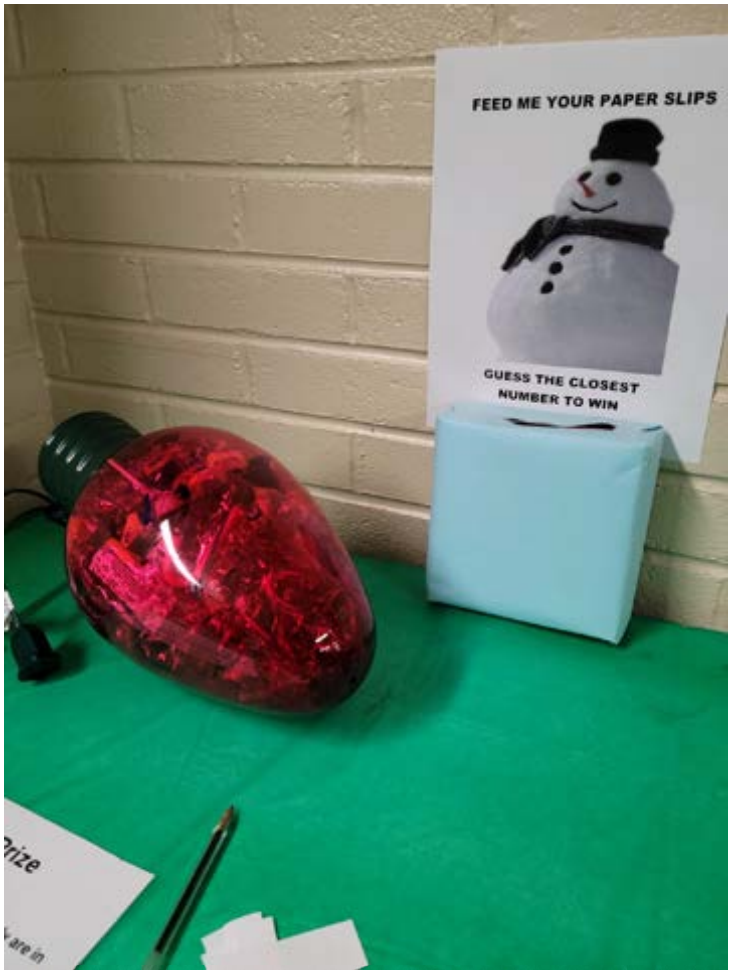
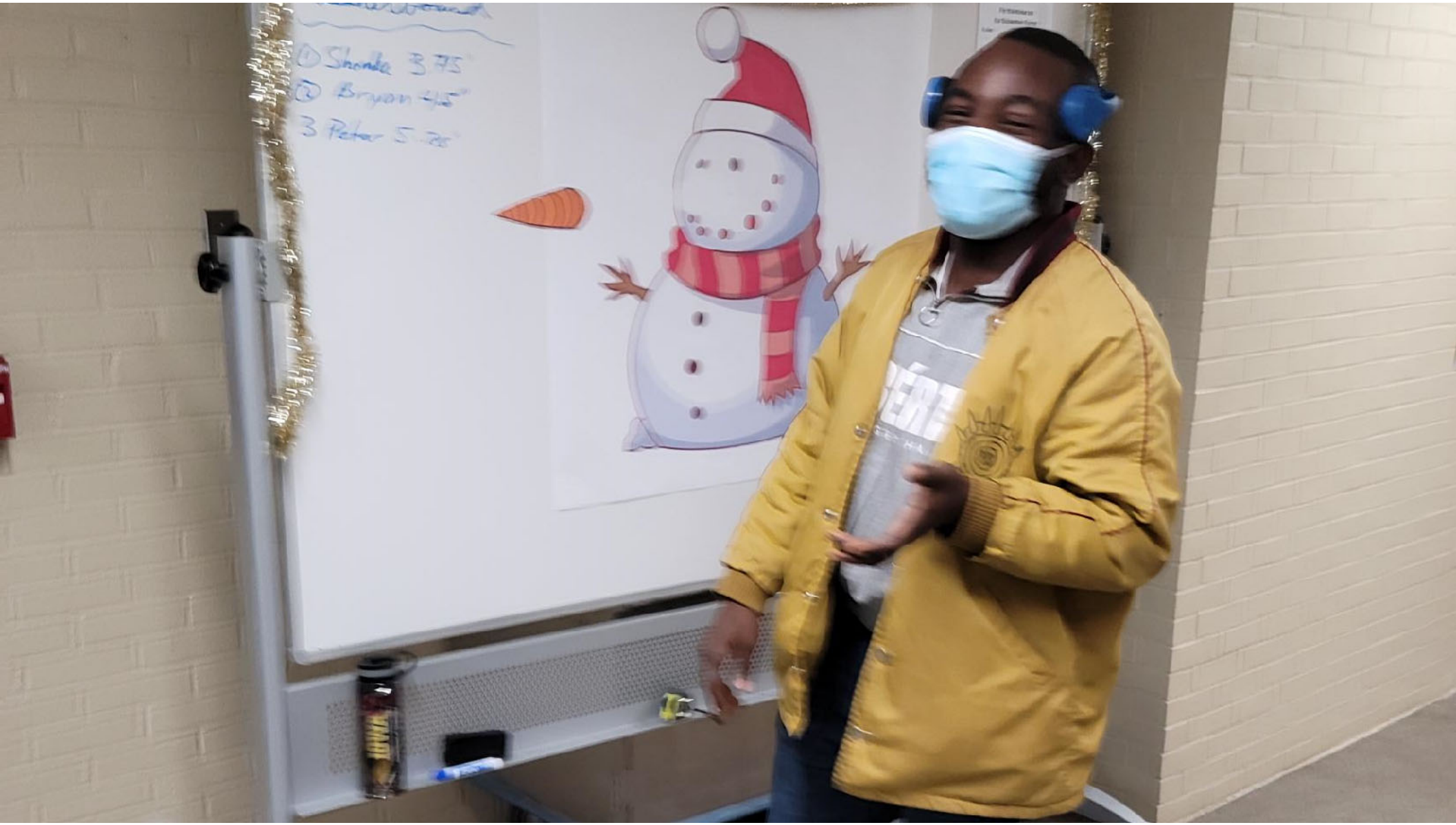
E440, W428
W468
Coffee
Fire Extinguisher
Reddi wip


FEED ME YOUR PAPER SLIPS
GUESS THE CLOSEST
NUMBER TO WIN


1 Shanda 375
2 Bryan 45
3 Peter 5


Joy
to the
Realm


9
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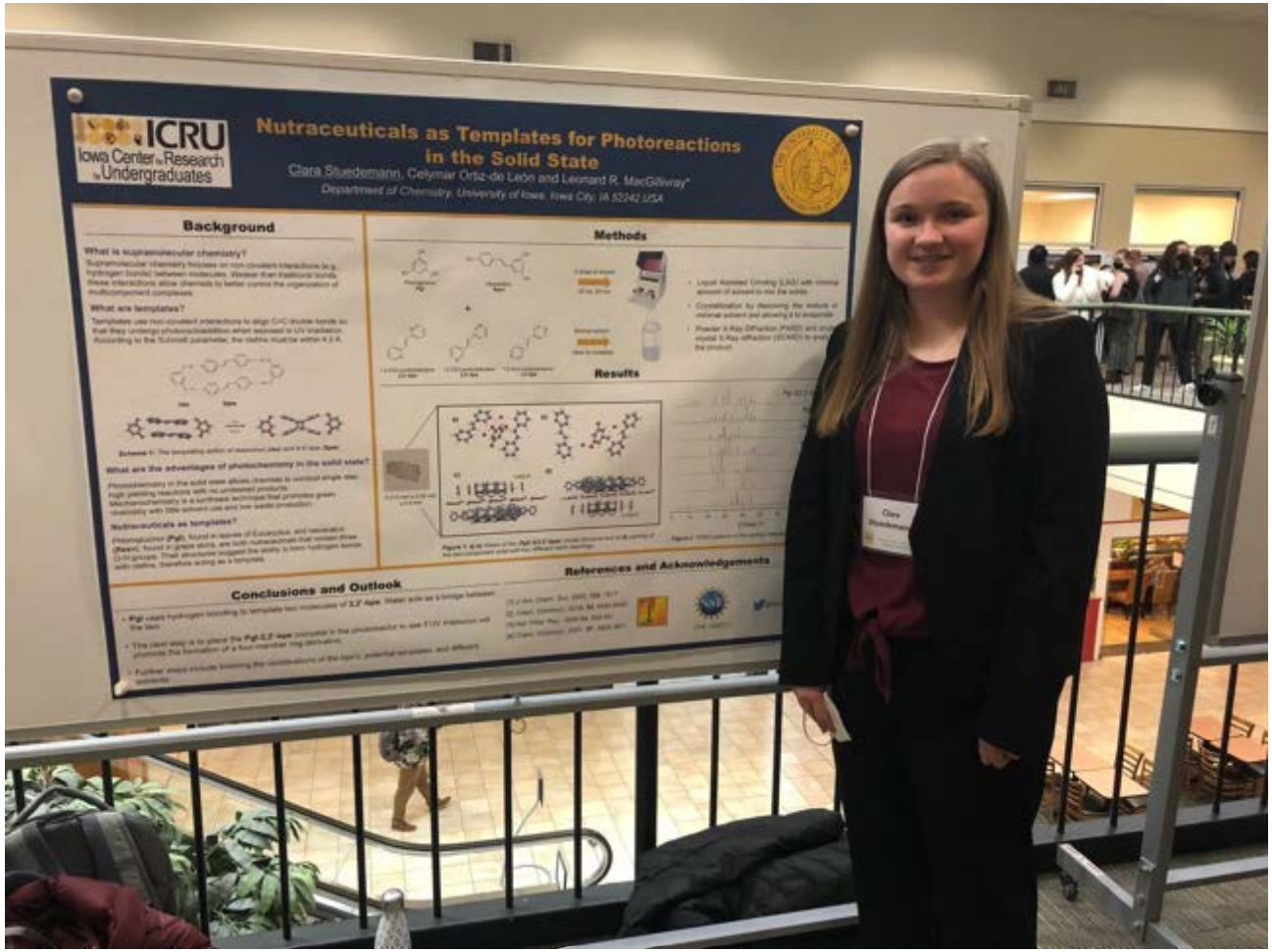
ICRU
Iowa Center for Research by Undergraduates
Nutraceuticals as Templates for Photoreactions in the Solid State
Clara Stuedemann, Gelymar Ortiz-de León and Leonard R. MacGillivray*
Department of Chemistry, University of Iowa, Iowa City, IA 52242 USA
Background
What is supramolecular chemistry?
What are templates?
What are the advantages of photochemistry in the solid state?
Nutraceuticals as templates?
Methods
Results
Conclusions and Outlook
References and Acknowledgements


It's A
FESTIVUS
For The
REST OF US


DESTINY
IOWA


FACE MASKS
ENCOURAGED
(but not required)
IOWA


East
Elevator
EXIT


East
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EXIT
TRUMAN
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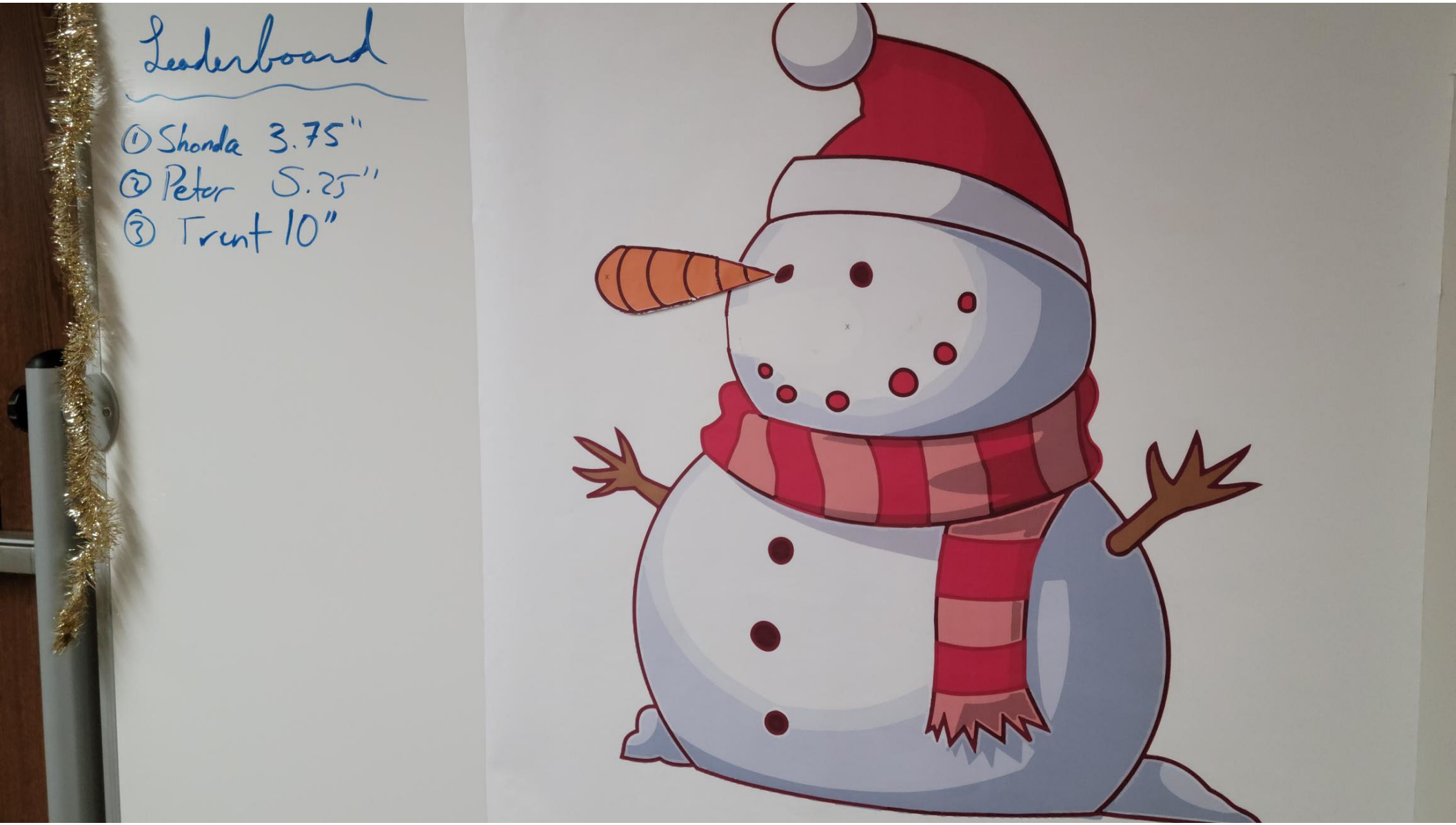
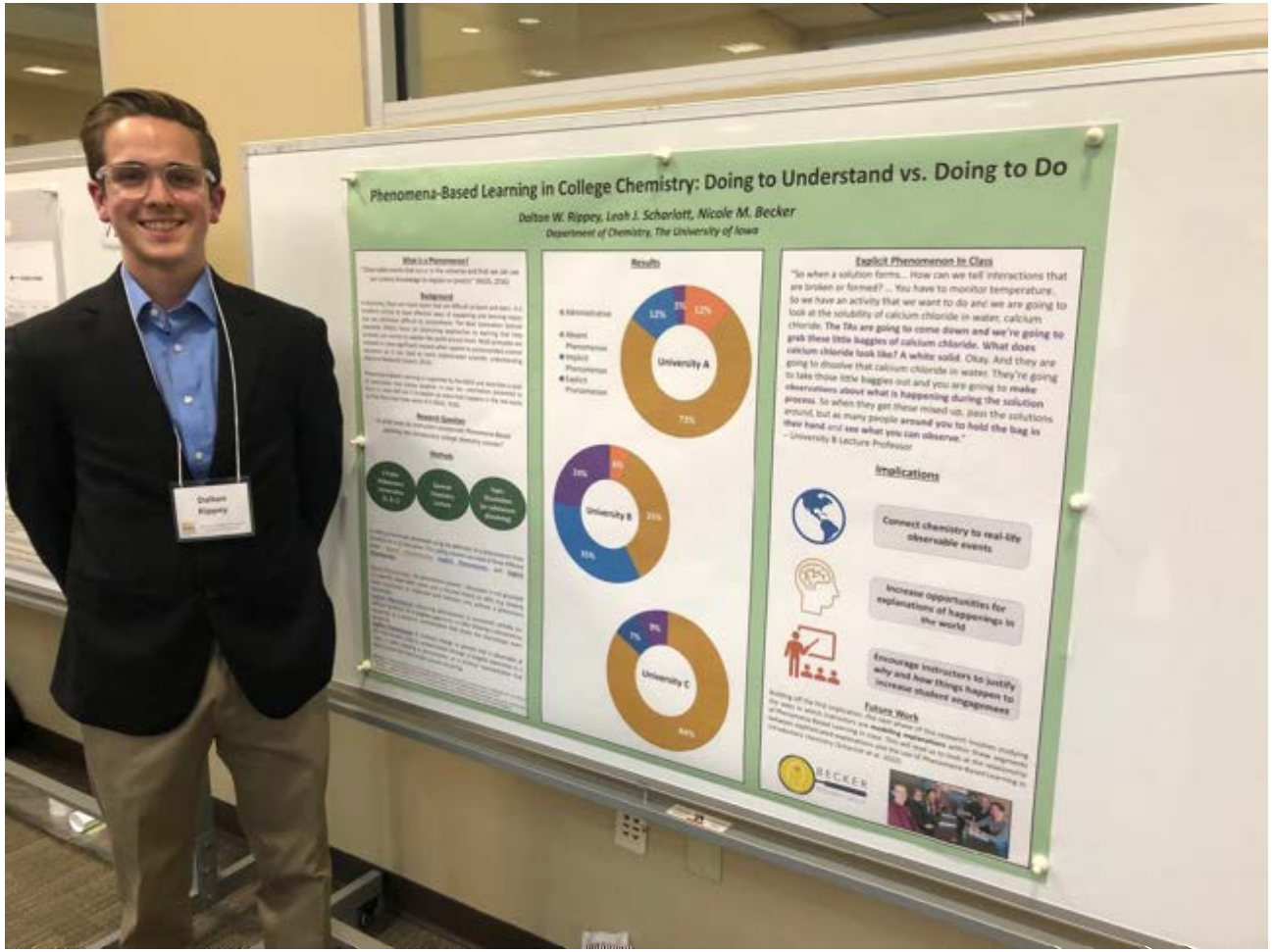
HI-REZ EXPO
HRX
2018


Leaderboard
① Shonda 3.75"
② Peter 5.25"
③ Trent 10"


Phenomena-Based Learning in College Chemistry: Doing to Understand vs. Doing to Do
Dalton W. Rippey, Leah J. Scharlott, Nicole M. Becker
Department of Chemistry, The University of Iowa
Results
University A
University B
University C
Explicit Phenomenon in Class
"So when a solution forms... How can we tell interactions that are broken or formed? ... You have to monitor temperature. So we have an activity that we want to do and we are going to look at the solubility of calcium chloride in water, calcium chloride. The TAs are going to come down and we're going to grab these little baggies of calcium chloride. What does calcium chloride look like? A white solid. Okay. And they are going to dissolve that calcium chloride in water. They're going to take those little baggies out and you are going to make observations about what is happening during the solution process. So when they get these mixed up, pass the solutions around, but as many people around you to hold the bag in their hand and see what you can observe."
– University B Lecture Professor
Implications
Connect chemistry to real-life observable events
Increase opportunities for explanations of happenings in the world
Encourage instructors to justify why and how things happen to increase student engagement
Future Work


HI-REZ EXPO
HRX
2018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Chemistry
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STOP
OH,

Exploring the Synthesis and Formation of Extended Uranyl Solid Materials Though a Mild Temperature Flux Reaction

Haley N. Lightfoot, Mikaela M. F. Pyrch, and Tori Z. Forbes

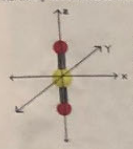
Department of Chemistry, The University of Iowa, Iowa City

Motivation

Uranium is a naturally occurring radioactive material that is toxic to living organisms when exposed in high concentrations. Understanding how uranium interacts within the environment can improve our ability to predict of the mobility and enhance our detection of uranium species. Reactions involving uranium are of interest as they can impact a variety of scientific fields such as the nuclear energy cycle and environmental sciences.

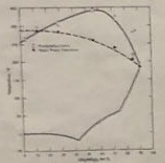
The Uranyl Cation $(UO_2)^{2+}$

The uranyl cation is a common form of uranium found in environmentally relevant conditions.



Two axial oxygen atoms bind with the uranium metal center to form a linear triatomic cation with a 2+ charge. Further coordination with the uranyl cation occurs in the equatorial plane which can affect the strength of the uranium-oxygen bonds, and impact the overall structure.

Figure 1. The uranyl cation shown with 3D axes.



The phase diagram shows us the percent of solid uranyl nitrate (by weight) which will change phases at specific temperatures, allows us to predict when the solid uranyl nitrate may be able to act as a solvent

Figure 2. Phase diagram of aqueous Uranyl Nitrate Hexahydrate (ref 1)

Synthesis and Bomb Calorimetry

Figure 3. Components of an acid digestion parr bomb.

Hydrothermal synthesis is a method of synthesizing crystals that depends on the solubility of the materials involved in high temperatures and pressures. These reactions take place in a metal pressure vessel that is specifically designed to contain high pressure reactions. Parr bombs are the reaction vessels we utilized to run a reaction at consistent pressure and temperature

Solid State Chemistry and Flux Reactions

Solid-state chemistry explores the structure, synthesis, and properties of solid-state materials. There are various pathways that can be utilized to synthesize solid materials, an emerging pathway involves solid-state synthesizes that do not utilize a solvent to aid the reaction mechanism. Solventless reactions often require the reaction to overcome an energy barrier. Temperature and pressure variables can be manipulated to overcome these energy barriers to allow the reactions to proceed. Flux reactions occur when two solids are heated past one of their melting points which allows for this compound to act as the solvent.

Experimental Reactions

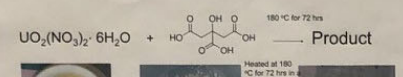


Figure 5. Solid Uranyl Nitrate Hexahydrate

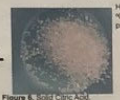


Figure 6. Solid Citric Acid.

Heated at 180 °C for 72 hrs in a parrbomb

Figure 7. Crystalline product for prep U-64 synthesized via hydrothermal synthesis

Crystalline Structure of U64

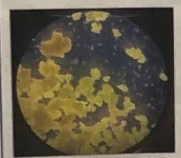


Figure 10. Crystalline product as viewed under the lens of a compound microscope

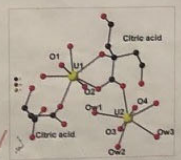


Figure 9. Unit Cell of Uranyl Citrate which packs to form 2 small pores.

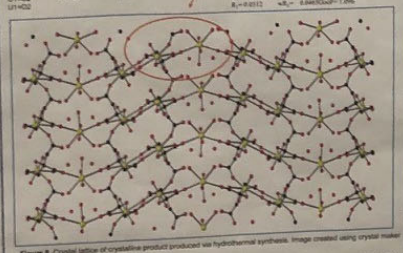
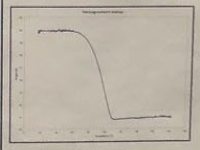


Figure 8. Crystal lattice of crystalline product produced via hydrothermal synthesis. Image created using crystal maker

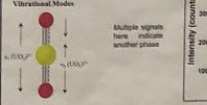
The 3D nature of this metal-organic framework(MOF) is of high interest to the community since MOFs have high surface areas and unique properties, allowing for gas sorption, gas storage, and heightened catalytic reactivity.

Characterization

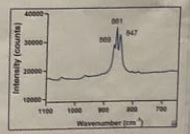


The TGA, P-XRD, and Raman spectra, when compared to the literature values, confirm the identity of the crystalline material synthesized. And tells us about the behavior of the material.

Figure 11. TGA spectrum taken for U64



Multiple signals here indicate another phase



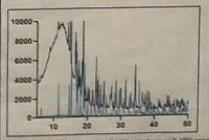


Figure 12. Overlay of the predicted P-XRD and observed P-XRD spectrum for U64

The broad shape of the spectra from 0-20 2theta is representative of an amorphous phase, while the blue predicted pattern matches the experimental for U64

Future Works/ Conclusions

Known products can be synthesized using mild temperatures and pressures to melt the solids.

Synthesis of crystalline products without the use of solvent offers new pathways to well known products with wanted topologies and structural characteristics.

Future experiments look to explore the additional by-products of hydrothermal synthesis without the use of a solvent.

Various other ligand systems and metal centers will be mixed with the uranyl nitrate to determine the methodologies of this synthesis at elevated temperatures and pressures.

Acknowledgments

The authors would like to acknowledge the funding from the Department of Energy (grant number) and the fellowship given by Iowa Center for Research by Undergraduates (ICRU) that supports this research. We would also like to acknowledge the Fedes research group who assisted in various ways to this project.

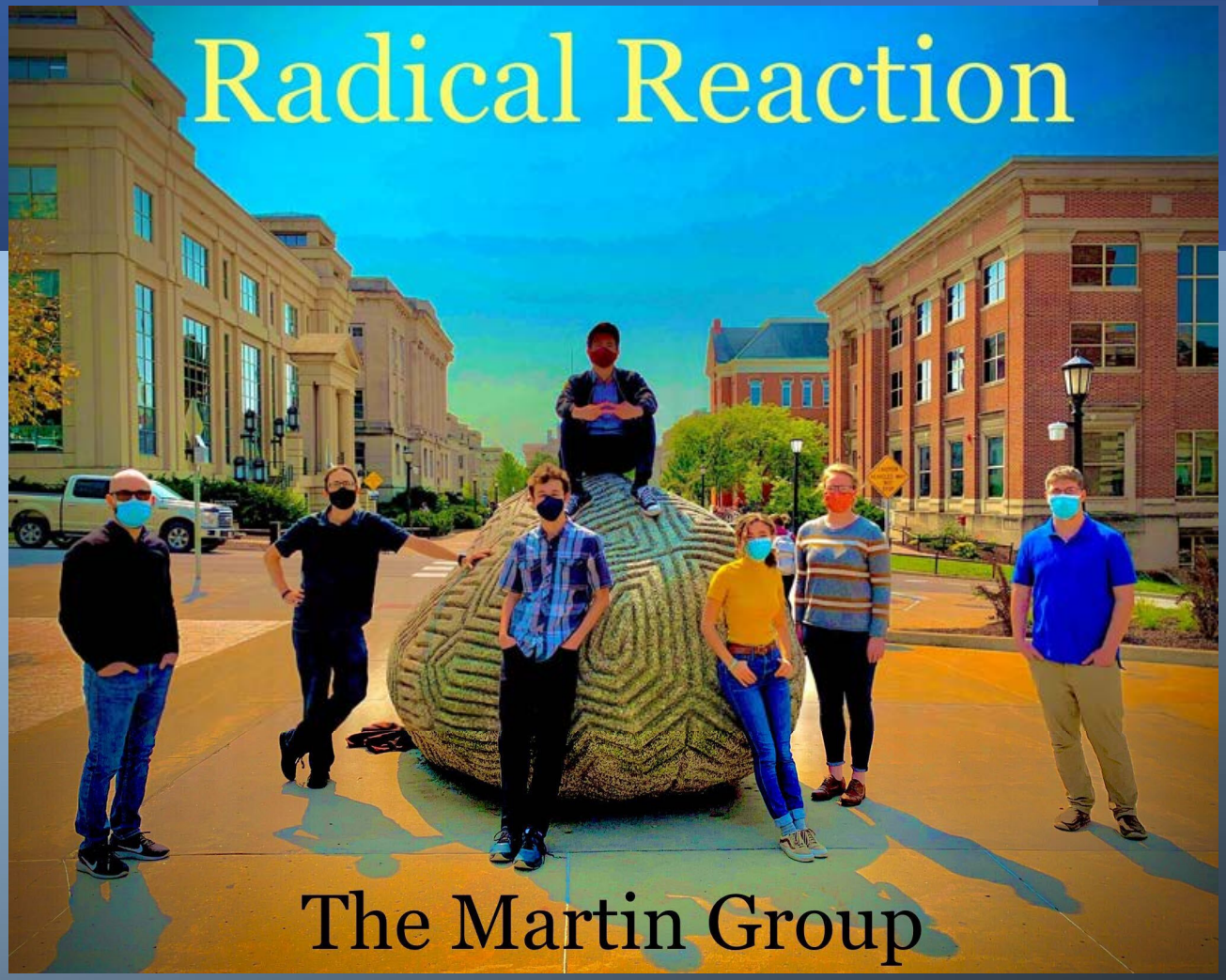
References

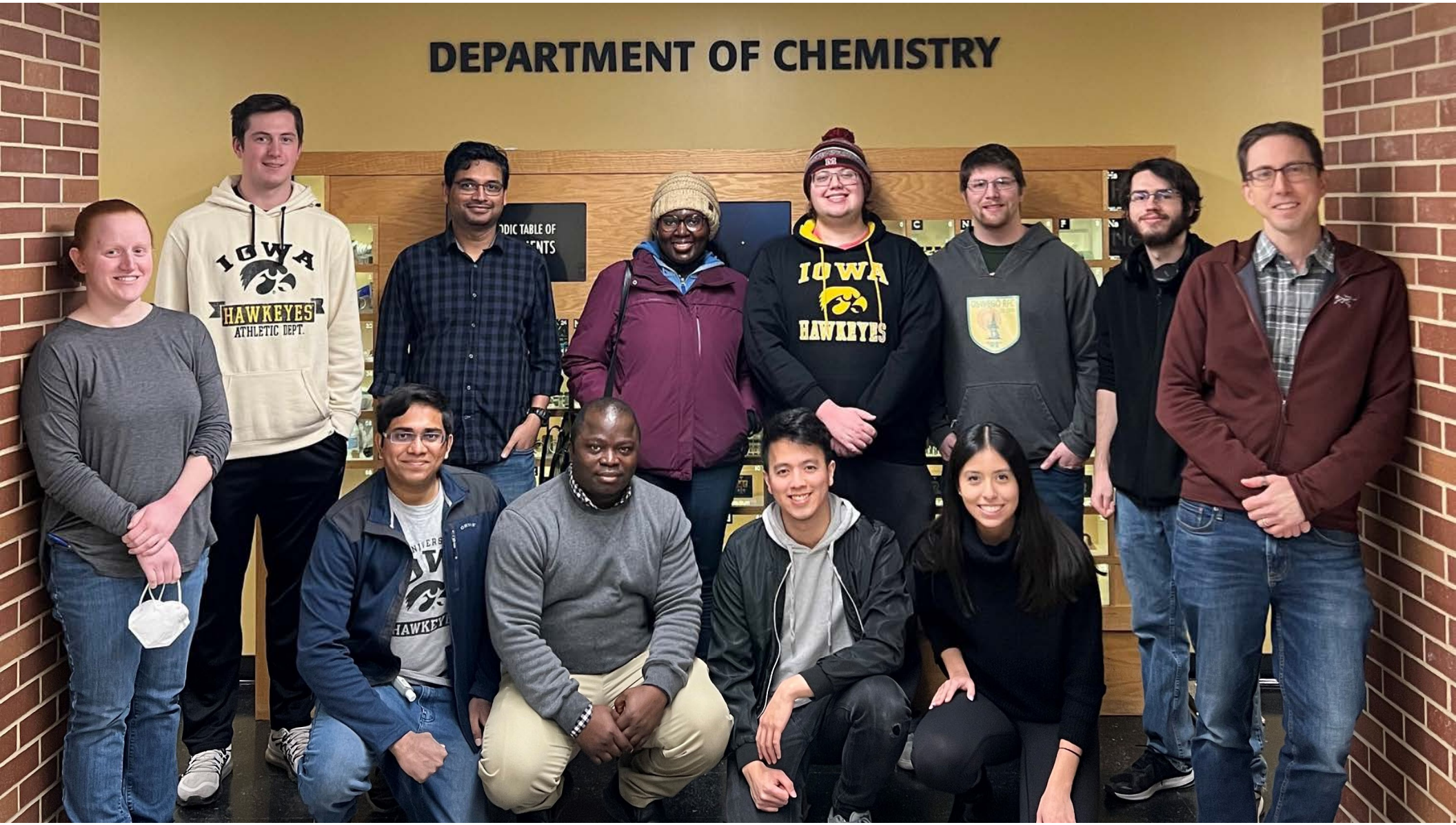
1. Chapter 2 Properties of Aqueous Fuel Solutions [n.d.]. Retrieved October 15, 2021, from http://moltensalt.org/references/static/downloads/pdf/ORNL-chap02.pdf.
2. Pierre Thuéry Chem Comm, **2008** 853-855 DOI: DOI https://doi.org/10.1039/B818181F

Haley Lightfoot


East
Elevator


CARDLE
DID IT


Radical Reaction
The Martin Group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richard
the whale
december 4
NASA
WEEK 14