UW Board of Trustees Research and Economic Development Committee Agenda January 22, 2025, at 1:00 pm – 3:00 pm

 Research Excellence Presentation: Wyoming Research Scholars – Dr. Jamie Crait Isabelle Burky^{1,2} – Mentors: Drs. Meredith Journey^{1,2}, Amy Krist², Katie Wagner³, and Annika Walters ^{4,1,2} - ¹Wyoming Cooperative Fish and Wildlife Research Unit, ²Department of Zoology and Physiology, ³Department of Botany, ⁴U.S. Geological Survey <i>Title: "Effects of Season and Competition on Trout Diets in Alpine Lakes"</i> Brody Greene – Mentor: Dr. Xiang Zhang - Computations for Advance Materials and Manufacturing Laboratory, Department of Mechanical Engineering 	2 6 7
 Wyoming Research Scholars – Dr. Jamie Crait Isabelle Burky^{1,2} – Mentors: Drs. Meredith Journey^{1,2}, Amy Krist², Katie Wagner³, and Annika Walters ^{4,1,2} - ¹Wyoming Cooperative Fish and Wildlife Research Unit, ²Department of Zoology and Physiology, ³Department of Botany, ⁴U.S. Geological Survey <i>Title: "Effects of Season and Competition on Trout Diets in Alpine Lakes"</i> Brody Greene – Mentor: Dr. Xiang Zhang - Computations for Advance Materials and Manufacturing Laboratory, Department of Mechanical Engineering 	6
 Isabelle Burky^{1,2} – Mentors: Drs. Meredith Journey^{1,2}, Amy Krist², Katie Wagner³, and Annika Walters ^{4,1,2} - ¹Wyoming Cooperative Fish and Wildlife Research Unit, ²Department of Zoology and Physiology, ³Department of Botany, ⁴U.S. Geological Survey <i>Title: "Effects of Season and Competition on Trout Diets in Alpine Lakes"</i> Brody Greene – Mentor: Dr. Xiang Zhang - Computations for Advance Materials and Manufacturing Laboratory, Department of Mechanical Engineering 	6
• Brody Greene – Mentor: Dr. Xiang Zhang - Computations for Advance Materials and Manufacturing Laboratory, Department of Mechanical Engineering	7
Title: "Multiphysics Modeling on Frontal Polymerization in 3d-Printed Resin"	
 Ty Hults¹ – Mentors: Drs. Rachel Smiley², Brittany Wagler², Kevin Monteith², ¹Department of Zoology and Physiology, ²Wyoming Cooperative Fish and Wildlife Research Unit <i>Title: "Diet Comparison of Greater Yellowstone Rocky Mountain Bighorn</i> <i>Sheep (Ovis canadensis)"</i> 	8
• Alison Jensen – Mentor: Laura Sousa de Oliveira	11
Title: "Atomistic Modelling of Nuclear Fuels and Fission Products"	
• Jack Leever – Mentors: Dr. Riley Bernad Department of Zoology and Physiology, Ellen Whittle, Wyoming Natural Diversity Database <i>Title: "Methods of Recording Acoustic Reference Calls from Hand-Released Bats"</i>	20
• Nikiphoros Vlastos – Mentor: Dr. Laura de Sousa Oliveira, Department of Physics, Department of Chemistry	24
Title: "Probing Light-Induced Isomerization Dynamics of Azobenzene Confirmed within Metal-Organic Frameworks: A Time Dependent Density Functional Theory Investigation"	
 Lucas Wall – Department of Molecular Biology Title: "Protecting Teeth with Viruses?" 	31
REDD Updates	41
	 Title: "Multiphysics Modeling on Frontal Polymerization in 3d-Printed Resin" Ty Hults¹ – Mentors: Drs. Rachel Smiley², Brittany Wagler², Kevin Monteith², ¹Department of Zoology and Physiology, ²Wyoming Cooperative Fish and Wildlife Research Unit Title: "Diet Comparison of Greater Yellowstone Rocky Mountain Bighorn Sheep (Ovis canadensis)" Alison Jensen – Mentor: Laura Sousa de Oliveira Title: "Atomistic Modelling of Nuclear Fuels and Fission Products" Jack Leever – Mentors: Dr. Riley Bernad Department of Zoology and Physiology, Ellen Whittle, Wyoming Natural Diversity Database Title: "Methods of Recording Acoustic Reference Calls from Hand-Released Bats" Nikiphoros Vlastos – Mentor: Dr. Laura de Sousa Oliveira, Department of Physics, Department of Chemistry Title: "Probing Light-Induced Isomerization Dynamics of Azobenzene Confirmed within Metal-Organic Frameworks: A Time Dependent Density Functional Theory Investigation" Lucas Wall – Department of Molecular Biology Title: "Protecting Teeth with Viruses?"

Research and Economic Development COMMITTEE MEETING MATERIALS

AGENDA ITEM TITLE: <u>Wyoming Research Scholars Student Presentations</u> – Crait

 \boxtimes OPEN SESSION

 \Box CLOSED SESSION

PREVIOUSLY DISCUSSED BY COMMITTEE:

□ Yes

🛛 No

FOR FULL BOARD CONSIDERATION:

□ Yes [Note: If yes, materials will also be included in the full UW Board of Trustee report.]
 ☑ No

Attachments/materials are provided in advance of the meeting.

EXECUTIVE SUMMARY: Wyoming Research Scholars - Student Presentations

The Wyoming Research Scholars Program is a university-wide <u>UW Science Initiative</u> program that pairs undergraduate students with faculty mentors to participate in cutting-edge research starting as early as their freshman year. The majority of practicing scientists, as well as corporate and civic leaders, credit an early research opportunity in college as having a profound effect on affirming their career path and on their personal growth. Research internships demonstrably build confidence and competence in young scholars at a formative stage in their training. Program Goals include:

- Attract top high school graduates from Wyoming to the University of Wyoming
- Retain promising students in the sciences at UW through early involvement in science research, department seminars, and public outreach events
- Pair talented college students with a faculty mentor who can model the scholarship, teaching, service, and outreach activities of a professional scientist
- Teach science writing and presentation skills to undergraduates via regular participation in UW's Annual Undergraduate Research Day and public outreach events (e.g., UW Planetarium, Biodiversity Institute, State Science Fair, Women in Science).

Today you will hear from the following students:

1. Student name: Isabelle Burky

Title: Effects of Season and Competition on Trout Diets in Alpine Lakes

Advisors: Annika Walters, Amy Krist, Meredith Journey

Summary: The Wind River Mountain Range has over 1,300 glacially formed lakes that are naturally fishless. Beginning in the early 1900s, some lakes were stocked with native and nonnative trout. Now over 500 lakes contain various trout species. Alpine lakes are ideal study sites for diet studies given their simplistic food webs. In this study we seek to explore the effects of seasonality on trout diets and how competition might drive diet specialization in these sensitive ecosystems.

2. Student name: Brody Greene

Title: Multiphysics Modeling of Frontal Polymerization in 3D-Printed Resins Advisor: Xiang Zhang

Summary: We are working to examine the behavior of advanced composite materials in solid modeling software. Simultaneously, we are studying how to produce these materials via experimental 3D printing.

3. Student name: Ty Hults

Title: Diet Comparison of Greater Yellowstone Rocky Mountain Bighorn Sheep (*Ovis anadensis*) Advisors: Kevin Monteith, Rachel Smiley, Brittany Wagler

Summary: Rocky Mountain bighorn sheep (*Ovis canadensis*) may be declining due to nutritionrelated factors such as habitat loss and disease. Current research in the Greater Yellowstone Ecosystem (GYE) highlights varying nutritional availability, but key plant species in their diets remain unidentified. Understanding their diet selection and availability within populations can inform management strategies and help guide habitat restoration, but current identification methods have limitations. Modern camera collars may offer a more accurate way to study dietary selection, advancing our ability to support bighorn sheep.

4. Student name: Alison Jensen

Title: Atomistic Modelling of Nuclear Fuels and Fission Products

Advisor: Laura de Sousa Oliviera

Summary: This presentation describes foundational work for a proposed multiscale engineering thermodynamics code, focused on modeling electron and phonon thermal transport using *ab initio*, semi-empirical, and classical simulation methods. Our materials of interest are the common nuclear fuel uranium dioxide (UO2), a common surrogate fuel cerium(IV) oxide (CeO2), and Xenon (Xe) a fission gas often found in reactors. Through computation, we find thermodynamic properties of these materials. Our future work will focus on thermal transport across fuel matrix/fission product boundaries and analysis of fuels containing structural defects and impurities.

5. Student name: Jack Leever

Title: Methods of Recording Acoustic Reference Calls for Hand-Released Bats Advisors: Riley Bernard, Ellen Whittle

Summary: Bat populations face growing threats from habitat loss and disease, making acoustic monitoring of bat populations critical. However, standardized methods for obtaining high-quality calls from hand-released bats are lacking. On top of this, bats alter their echolocation calls depending on the environmental conditions, making acoustic monitoring unreliable in understudied regions. Using three detectors and various methodologies, we recorded 520 calls from 192 hand-released bats across 11 species in the Northern Great Plains and Wyoming. We documented the environmental conditions for each bat recording. Recordings were then evaluated for quality based on environmental noise, call duration, and more. This will allow us to identify what recording methods and environmental conditions produced the highest-quality recordings of bats. Ultimately, we want to create a more standardized methodology for recording bats from hand releases and use our recordings to improve auto-ID software.

6. Student name: Nikiphoros Vlastos

Title: Probing Light-Induced Isomerization Dynamics of Azobenzene Confined within Metal-Organic Frameworks: A Time-Dependent Density Functional Theory Investigation Advisor: Laura de Sousa Oliviera

Summary: Metal-Organic Frameworks (MOFs) are gaining attention for their tunable structures and broad applications. Metal-Organic Responsive Frameworks (MORFs) offer further potential by using light-triggered behavior in sensing, catalysis, drug delivery, and carbon capture. This research examines azobenzene, a photoisomerizing molecule, confined within MOFs. Using Time-Dependent Density Functional Theory (TD-DFT) and Time-Dependent Density Functional Tight Binding (TD-DFTB), we explore the trans-to-cis and cis-to-trans isomerization dynamics of azobenzene under confinement. Our study aims to understand how factors like wavelength, electronic excitations, and steric effects influence this process, offering insights to enhance MORFs for real-world applications.

7. Student name: Lucas Wall

Title: Protecting Teeth with Viruses? Advisor: Dan Wall Summary: We are working with a bacteriophage that infects a type of bacteria called Streptococcus mutans. These bacteria are the leading microorganism responsible for dental decay.

PRIOR RELATED COMMITTEE DISCUSSIONS/ACTIONS: Information only

WHY THIS ITEM IS BEFORE THE COMMITTEE: Information only

ACTION REQUIRED AT THIS COMMITTEE MEETING: None

PROPOSED MOTION: N/A

Wyoming Research Scholars Program



Jamie Crait, Isabelle Burky, Brody Greene, Ty Hults, Alison Jensen, Jack Leever, Nikiphoros Vlastos, and Lucas Wall

University of Wyoming Board of Trustees Research & Economic Development Committee January 22, 2025

Effects of Season and Competition on Trout Diets in Alpine Lakes

Isabelle Burky^{1,2}, Meredith Journey^{1,2}, Amy Krist², Katie Wagner³, and Annika Walters^{4,1,2} ¹Wyoming Cooperative Fish and Wildlife Research Unit, ²Department of Zoology and Physiology, University of Wyoming, Laramie, WY 82071, USA, ³Department of Botany, University of Wyoming, Laramie, WY 82071, USA. ⁴U.S. Geological Survey

INTRODUCTION

The Wind River Mountain Range has over 1,300 glacially formed lakes that are naturally fishless. Beginning in the early 1900s, some lakes were stocked with native and nonnative trout. Now over 500 lakes contain various trout species. Alpine lakes are ideal study sites for diet studies given their simplistic food webs (Thompson et al., 2005). In this study we seek to explore the effects of seasonality on trout diets and how competition might drive diet specialization in these sensitive ecosystems.

STUDY SITE



Our study area is glacially formed lakes in the Wind River Mountain Range from 3 primary basins: Stough Basin and Bear Basin (August 2023 only) and Big Sandy Basin (July-Sept 2024).





Golden Trout Oncorhynchus aguabonita

Brook Trout

Salvelinus fontinalis





Cutthroat Trout Oncorhynchus virginalis

RESEARCH QUESTIONS

- \gg 1. How does trout diet composition vary across multiple species (Rainbow, Golden, Cutthroat, and Brook Trout) in alpine lakes?
- ≥ 2. How do Brook Trout and Cutthroat Trout diet compositions vary seasonally?
- > 3. Does the presence of Cutthroat Trout alter Brook Trout diet composition in lakes with both species.

METHODS

Field

- Gill netting via pack raft.
- Measuring length and weight.
- Extracting and preserve stomachs.



ACKNOWLEDGEMENTS



PRELIMINARY RESULTS (August 2023)



Across all trout species, aquatic prey by count (blue) comprises most of the diet, and terrestrial prey by count (green) is present but in smaller proportions.

Large Fish Typically Have More Stomach Contents



Larger fish have higher variation in stomach content weight

- Next Steps Analyze 2024 samples and look at seasonal variation between Cutthroat and Brook Trout.
- Determine if the presence of Cutthroat Trout alters Brook Trout diet composition in lakes where both species occur.

Thompson, R., Kamenik, C., & Schmidt, R. (2005). Ultra-sensitive Alpine lakes and climate change. Journal of Limnology, 64(2), 139 enthal, W. C., Boyle, L. J., Rick, J. A., Mandeville, E. G., Krist, A. C., ... & Wagner, C. E. (2023). Parallel shifts in trout feeding morphology suggest rapid adaptation to alpine lake environments. Evolution, 77(7), 1522-1538



removed, weighed, and identified. • Contents are analyzed using a dissecting





Multiphysics Modeling of Frontal Polymerization in 3D-Printed Resins



Brody Greene, Xiang Zhang

Computations for Advanced Materials and Manufacturing Laboratory

Dept. of Mechanical Engineering, University of Wyoming

Background

Frontal polymerization (FP) is a manufacturing process where a 3D printer deposits a liquid monomer that cures into a solid polymer. The reaction front is the leading exothermic reaction that sets the pace of the curing process.



Motivation

We sought to improve the printing process by discovering the optimal printing parameters. Printing conditions can be modeled in multiphysics capable software to avoid expensive trial and error test prints.

Fully Coupled Thermo-Chemical PDEs

$$\begin{cases} \kappa \frac{\partial^2 T}{\partial x^2} + \rho H_r \frac{\partial \alpha}{\partial t} = \rho C_p \frac{\partial T}{\partial t} \\\\ \frac{\partial \alpha}{\partial t} = k(T) f(\alpha) = A_0 \exp(-\frac{E}{RT}) f(\alpha) \end{cases}$$

Experimental Setup and Methodology

We developed the source code to model the curing process in the Multiphysics Object-Oriented Simulation Environment (MOOSE), an open-source finite element solver. The simulation data was then processed to create the visual aids in Paraview and MATLAB.





) 50 100 150 200 260 Temperature (°C)



Conclusion

We have successfully matched experimental curing data with simulation data using MOOSE. The reaction front should closely follow the nozzle of the printer to maintain the accuracy of the print; with the conditions of this printer, fewer than 7mm is optimal. Further, higher printing velocities (0.8-1.5 mm/s in this case) tend to produce higher degrees of the cure, which decreases the time needed for prints. With such simulation data, we now have a better idea of the optimal printing parameters.

Reference

Chen, Z., Ziaee, M., Yourdkhani, M., & Zhang, X. (2022). Multiphysics modeling of frontal polymerization-assisted layer-by-layer additive manufacturing of thermoset polymer components. *Additive Manufacturing*, 59, 103182. 10.1016/j.addma.2022.103182



Diet Analysis of Rocky Mountain Bighorn Sheep (*Ovis canadensis*)

Ty Hults





- Rocky Mountain bighorn sheep (Ovis canadensis) may be declining due to nutrition-related factors such as habitat loss and disease.
- Current research in the Greater Yellowstone Ecosystem (GYE) highlights varying nutritional availability, but key plant species in their diets remain unidentified.
- Modern camera collars may offer a more accurate way to study dietary selection, advancing our ability to support bighorn sheep.

9



•Dubois: Consumed many grasses, avoided shrub and trees entirely, and under-consumed many forbs.
•Jackson: Consumed some shrubs, avoided trees, and consumed many forbs and grasses.
•Cody: Consumed more forbs than grasses, but occasionally consumed shrubs and trees.

Consumption patterns differ in direction (over or under consumption) from plant availability. Significant dietary differences suggest that factors other than availability are at play and may be shaped unique preferences, such as feeding locations, forage quality, or herd-specific behaviors. Further research will examine how nutritional content differs among plants consumed, possible remote sensing of habitat features, and further data collection across seasons.

Atomistic modelling of nuclear fuels and fission products

Presented by Alison Jensen for the WRSP Advisor Dr. Laura de Sousa Oliveira Computational Design of Inorganic Materials Lab January 22, 2025 University of Wyoming

1/22/2025

Goal:



Investigate engineering-scale thermodynamic behavior using atomistic parameters in collaboration with Idaho National Laboratory (INL).

rials of Inte Mater

Uranium Dioxide (UO2)



Cerium IV Oxide (CeO2)



1/22/2025

3

Electronic Band Structure and Density of States Plot for Uranium Dioxide (UO2)



1/22/2025

Electronic **Band Structure** and Density of States Plot for Cerium IV Oxide (CeO2)



1/22/2025

5

Electronic **Band** Structure and Density of States Plot for Xenon (Xe)



1/22/2025

Phonon Band Structure and Density of States Plots for Xenon (Xe)



1/22/2025

7

Calculating Thermal Properties

$$\mathbf{J} = rac{1}{V} \Bigg[\sum_i e_i \mathbf{v}_i + rac{1}{2} \sum_{i < j} ig(\mathbf{F}_{ij} \cdot (\mathbf{v}_i + \mathbf{v}_j) ig) \mathbf{r}_{ij} \Bigg]$$

- Green Kubo Theorem
- Molecular Dynamics (MD)

 $\kappa = \frac{V}{k_B T^2} \int_0^\infty \langle J_x(0) J_x(t) \rangle \, \mathrm{d}t = \frac{V}{3k_B T^2} \int_0^\infty \langle \mathbf{J}(0) \cdot \mathbf{J}(t) \rangle \, \mathrm{d}t$

• Python and C

Questions?

Thank you to the WRSP for their support, the ARCC for their resources, my group for their guidance, and thank you for your attention!







1/22/2025





Methods of Recording Acoustic Reference Calls from Hand-Released Bats

Researcher: Jack Leever Mentors: Dr. Riley Bernard (Dept of Zoology & Physiology) Ellen Whittle (Wyoming Natural Diversity Database)





Background

- Determining the presence of bat species is crucial for conservation efforts and new development projects
 - Ultrasonic detectors
 - Auto-ID software

Challenges

- Bats alter their echolocation depending on environmental conditions
- Auto-ID software is primarily trained on bat recordings from eastern acoustic studies
- There is no stardardized method for recording hand-released bats







Goals

- Develop a optimized and standardized methodology for recording hand-released bats
- Use our high-quality recordings to help train auto-ID software to be more accurate for western acoustic studies











College of Engineering and Physical Sciences



Probing Light-Induced Isomerization Dynamics of Azobenzene Confined within Metal-Organic Frameworks: A Time-Dependent Density Functional Theory Investigation

Nikiphoros Vlastos & Laura de Sousa Oliveira University of Wyoming, Department of Physics & Department of Chemistry

Background

Metal-Organic Frameworks (MOFs) are materials known for their tunable structures and diverse applications in chemistry, physics, and materials science. Metal-Organic Responsive Frameworks (MORFs) leverage light-actuated properties for enhanced applications in sensing, catalysis, drug delivery, carbon capture, etc.



Azobenzene

Azobenzene as a Photoisomerizing

Molecule undergoes reversible trans-tocis and cis-to-trans isomerization upon light excitation, making it a key molecule for photonics and molecular switches. The large variations in shape, size, and polarity during isomerization make it a promising candidate for integration into smart materials.

Integrating azobenzene into

MOFs aims to create MORFs, which can alter their properties in response to light. Isomerization behavior is influenced by confinement within MOFs, leading to changes in its intrinsic properties.





Methods & Preliminary Results

Time-Dependent Density Functional Theory (TD-DFT) and **Time-Dependent Density Functional Tight Binding (TD-DFTB)** are used to model azobenzene's light-induced trans-to-cis and cis-to-trans isomerization. TD-DFT with B3LYP and 6-31G* & 6-31G are used for excited-state calculations, while TD-DFTB simulates the time evolution.



Preliminary Results











Research Goal

This research aims to uncover design principles that optimize the performance of light-responsive MORFs for practical applications, leading to more efficient materials for a wide range of uses.



(Rojas, Sara, et al. CrystEngComm 15.45 (2013): 9364-9367)



(Wu, Shuangyan, et al. Advanced Materials(2019): 1805871)



Cui, Wen-Gang, et al. Coordination Chemistry Reviews 387 (2019): 79-120

Gas storage



(Image: Luping Han)

Thanks To



Computational Design of Inorganic Materials Lab

Dr. Laura de Sousa Oliveira

Masoumeh Gahrouei

Kolbe Chavez

Dr. Adrian E. Roitberg Frank - University of Florida

Denis Jacquemin - Université de Nantes

UW Advanced Research Computing Center

Wyoming Research Scholars Program





Protecting Teeth with Viruses?

Lucas Wall

Department of Molecular Biology

College of Agriculture, Life Sciences, & Natural Resources



Cavity Causing Bacteria = Streptococcus mutans





Lucas Wall



Bacterial Killing Viruses (phage)

- <u>Specifically</u> binds and kills the target bacteria.
- Does not target human cells or even other species of bacteria
- How does this virus identify the cavity causing bacteria?
- How may these bacteria develop immunity to the virus?



Immunity Mechanisms:

- Adaptive Immunity, Crisper: Bacteria can remember and destroy invading virus DNA
- Prevent Binding: Bacteria can alter the receptor the virus binds to

Isolated mutants that gained immunity to the virus







Cell Morphology Phenotype



WT

RgpF

RgpX



Biofilm Assay



What Next?

Present at National Dental Conference:
 American Association for Dental, Oral and
 Craniofacial Research



- Publish a Scientifically Reviewed Paper:



Acknowledgements:



🐐 UNIVERSITY of WYOMING





College of Agriculture, Life Sciences and Natural Resources



Research and Economic Development COMMITTEE MEETING MATERIALS

AGENDA ITEM TITLE: <u>REDD Updates</u>- Chitnis

 \boxtimes OPEN SESSION

 \Box CLOSED SESSION

PREVIOUSLY DISCUSSED BY COMMITTEE:

□ Yes

🛛 No

FOR FULL BOARD CONSIDERATION:

□ Yes [Note: If yes, materials will also be included in the full UW Board of Trustee report.] ⊠ No

Attachments/materials are provided in advance of the meeting.

EXECUTIVE SUMMARY:

Vice President Chitnis and others will provide brief update on activities within the division. REDD Annual Report presented in Full Board on January 23, 2025.

PRIOR RELATED COMMITTEE DISCUSSIONS/ACTIONS: Information only

WHY THIS ITEM IS BEFORE THE COMMITTEE: Information only

ACTION REQUIRED AT THIS COMMITTEE MEETING: None

PROPOSED MOTION: N/A