Monthly Newsletter Edition #2 March 2025 WELCOME TO EARTH **Environmentally Applied Refrigerant Technology Hub** stay fresh on upcoming events, surveys, publications, and more! **OUR DIRECTORS OUR PILLARS** Innovation Convergent Research Ecosystem Engineering Impact and Workforce Belonging Mark B. Shiflett Jennifer L. Schaefer Development **Deputy Director Center Director** U. Kansas U. Notre Dame The News, Distilled **Biannual Team** Internship **Member** Achievements Meeting Opportunities Funding Meet **Read More! Opportunities Crosscut 3** happy spring!

**Environmentally Applied** COMMUNITIES, the HVACR industry, and society!

## 📥 Member Achievements 🖌 🍃



Congratulations to **Professor Damena Agonafer** for receiving the Presidential Early Career Award for Scientists and Engineers (PECASE), the highest honor bestowed by the U.S. government for scientists and engineers!

Click <u>here</u> for the news story from The White House and <u>here</u> for the UMD news story.



Congratulations to **Professor Mark Shiflett** on being featured on the cover of the first 2025 KU Alumni Magazine!

Click <u>here</u> to read the article mentioning ERC EARTH, The Wonderful Institute for Sustainable Engineering (WISE-KU), and Icorium Engineering Company.

Separation and recycling of hydrofluorocarbon refrigerant mixtures with fluoropolymer-coated hollow fiber membranes

Harders, A.N.; Wallisch, L.; Lundin, M. D.; Le, C.; Zaher, G.; Atchison, E.; White, W.; Shiflett, M. B. *Sci. Adv.* **2025**, *11*, eadp7414, DOI:<u>10.1126/sciadv.adp7414</u>.

Lead author **Dr. Abby Harders** earned her doctorate in chemical and petroleum engineering at the University of Kansas and now serves as head of research and development at **Icorium Engineering Company**, one of our industry members! View the corresponding news story <u>here</u>.

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## Member Achievements



Congratulations to KU graduate student **Claire Sabolay** (Prof. Mark Shiflett's group) for receiving the prestigious Madison and Lila Self Graduate Fellowship!

Click here to learn more about the fellowship at KU.



Congratulations to ND graduate student **Krishnendu Mukherjee** on defending his dissertation! If you are at Notre Dame, check out the event on March 20th! *Details below.* 



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On March 13-14, The University of Kansas hosted our Biannual Team Meeting! There were over 100 total attendees who traveled from all over the country. Thank you all for attending and engaging in our pillars: convergent research, impact & belonging, innovation ecosystem, and engineering workforce development. We look forward to hosting you again for our NSF Evaluation Meeting on October 21-23, 2025.



# Internship, Co-Op, and Fellowship Opportunities

<u>Check out our website for opportunities with our industry members,</u> professional organizations, and national labs!

#### University of Notre Dame Provost's Postdoctoral Fellowships in Engineering Program

Fellowships are supported institutionally for 24 months, with a renewal at 12 months, carry a \$75,000/year stipend, and include a \$15,000 allowance to cover expenses related to independent research endeavors, training, and professional development.





Faculty: Click here for our complete list of opportunities!

Mathematical Foundations of Digital Twins (MATH-DT)

Defense University Research Instrumentation Program (DURIP)

Materials Innovation Platforms (MIP)

Social Psychology

Human-Environment and Geographical Sciences Program (HEGS)

**Economics** 

Materials Research Science and Engineering Centers (MRSEC)

Behavioral and Social Sciences

## Computation and Experimentation Are Complementary!

Meet Modeling & Analysis Crosscut #3

Start









































### DAMENA AGONAFER



#### Associate Professor of Mechanical Engineering & Clark Faculty Fellow University of Maryland; agonafer@umd.edu



Professor Damena Agonafer's research interest is at the intersection of thermal-fluid sciences, interfacial transport phenomena, and renewable energy. He is focused on developing novel materials and systems for thermal management of power and microelectronic systems, as well as for thermochemical and electrochemical energy storage applications. His goal is to achieve transformational changes in technologies by tuning and controlling solid-liquid-vapor interactions at micro-/nano length scales. Specific areas of focus include the development of novel materials and micro-/nanostructures for phase change heat transfer, thermochemical energy storage, and interfacial transport phenomena. Applications of his work include cooling high-powered electronics, battery thermal management, and data center cooling, and improving the efficiency of HVAC systems.

## YAMIL COLÓN



#### Assistant Professor of Chemical and Biomolecular Engineering University of Notre Dame; ycolon@nd.edu

Professor Yamil Colón's group leverages molecular modeling, statistical mechanics, thermodynamics, material science, and machine learning. Within EARTH, he works on studying separations of refrigerants in ionic liquids, deep eutectic solvents, and porous materials using molecular modeling tools. He also is leveraging machine learning and molecular design to discover new refrigerant blends. Lastly, he is modeling water vapor separations in porous materials for dehumidification. The computational skill set from his group lends itself to anyone who wants molecular insights into observed phenomena, predictions of thermophysical properties, discover new materials for a given task, or use machine learning to process data or guide material and molecular design.



### ALEX DOWLING

#### Associate Professor of Chemical and Biomolecular Engineering and Applied and Computational Mathematics and Statistics University of Notre Dame; adowling@nd.edu

Professor Alex Dowling's research combines chemical engineering, computational optimization, machine learning, and data science organized in three research themes: (1) molecular-to-systems (multiscale) modeling and optimization, (2) optimal design of experiments and statistical inference, and (3) machine learning for bridging timescales. Applications domains include energy markets and infrastructure, integrated energy systems, carbon sequestration, sustainable hydrogen, critical mineral recycling, and advanced separations (membranes, ionic liquids).



### CHRISTOPHER DEPCIK

Associate Professor Mechanical Engineering, Courtesy Professor Aerospace Engineering American Society of Mechanical Engineering Fellow University of Kansas; depcik@ku.edu



Professor Christopher Depcik specializes in developing numerical models that bridge fundamental reaction kinetics and thermodynamics with real-world engineering applications, particularly in HVACR technologies. With expertise in homogeneous and heterogeneous reaction modeling, he simulates complex phenomena such as refrigerant combustion and surface reactions in catalytic converters, biomass gasifiers, and particulate filters. His background in zero- and one-dimensional modeling, from adiabatic flame temperatures to internal combustion engines and flow-through reactors, enables him to translate fundamental chemistry into predictive tools for macroscopic systems. He brings extensive programming experience (FORTRAN, C/C++, MATLAB, and GUI development) and a strong foundation in advanced thermodynamics, which he teaches at the graduate level. Currently, his research focuses on refrigerant combustion and the development of HVACR innovations, such as ultrahigh-speed centrifugal compression. He is eager to collaborate on projects that leverage his modeling and simulation expertise to advance next-generation refrigerant technologies and improve system performance.



## LISA FREDIN

#### Assistant Professor of Chemistry Lehigh University; lafredin@lehigh.edu



Focusing on the development of models at the interface of experiment and theory, Professor Lisa Fredin uses quantum chemistry to interrogate the chemical physics of catalytic materials and improve fundamental understanding of structure-activity relationships in catalytic processes. Working with experimental collaborators, her group will discover new photocatalysts to harness waste fluorene sources for biomedical and commodity chemical formation. In addition, using quantum understanding of the mechanisms of these systems we will be able to improve reaction yields and selectivities, as well as modify catalysts to use more difficult substrates and conditions.



### XU HAN

Assistant Professor of Civil, Environmental, and Architectural Engineering University of Kansas; xuhan@ku.edu

Dr. Xu Han's research focuses on smart, sustainable, and resilient building and cities. His expertise lies in design, modeling, and controls of building thermal and HVAC systems. He develops multi-domain thermal and energy simulation models from the refrigeration cycle scale, building scale, to community/urban scale. He also develops advanced optimal control strategies for building HVAC systems by integrating data science, machine learning, IoT, and optimization.



### YUNHO HWANG





#### Research Professor of Mechanical Engineering University of Maryland; yhhwang@umd.edu

Professor Yunho Hwang is a research professor and co-director of the Center for Environmental Energy Engineering (CEEE). He is an expert in "Energy Efficiency and New Innovative Energy Systems Research" in the field of refrigeration, air-conditioning, and heat-pumping (RAH) technologies. His expertise includes the development of efficient polymer & zeolite dehumidification, sorption cooling, sorption energy storage, electrochemical dehumidification, and hybrid separate sensible and latent cooling technology.

### CHRISTINA KARAMPERIDOU



Professor of Atmospheric Sciences University of Hawai'i, Mānoa; ckaramp@hawaii.edu



Professor Christina Karamperidou's research focuses on ENSO dynamics and predictability, extreme events in response to large-scale climate variability and change, paleoclimate, and machine learning applications in environmental science and climate model optimization. She uses a hierarchy of climate models (from simple theoretical models to comprehensive Earth System Models) and leverages advanced statistics and machine learning techniques to model and understand the dynamics of climate and its impact on weather risk.



#### HUIJEONG KIM

Assistant Professor of Civil, Environmental, and Architectural Engineering University of Kansas; hjkim@ku.edu

Professor Huijeong Kim's research areas include architectural engineering, building technology, and decision science. She focuses on human-building interactions, data-driven decision support systems, smart and connected communities, equitable clean energy transitions, and integrative intervention design using technological innovations and community engagement.



### **BING PU**



#### Assistant Professor of Geography and Atmospheric Science University of Kansas; bpu@ku.edu

Professor Bing Pu's research focuses on the variability of dust aerosols, dust-climate interactions, and regional climate change. Within EARTH, Bing primarily works on understanding the atmospheric and climate impacts of HFC-based processes using observations and climate models.



#### **RUI SUN**

#### Associate Professor of Chemistry University of Hawai'i at Mānoa; ruisun@hawaii.edu

Professor Rui Sun's research expertise is to develop and apply computational chemistry modeling and simulation methodologies to tackle outstanding chemical and biophysical problems. Through simulations of both gas and condensed phase, Rui Sun will lead EARTH's efforts on understanding the fate of refrigerant molecules in the atmosphere and assess their environmental impact.

#### BESS VLAISAVLJEVICH



Associate Professor of Chemistry University of Iowa; bess-vlaisavljevich@uiowa.edu

Professor Bess Vlaisavljevich's research focuses on using quantum chemistry methods to solve problems in energy, sustainability, and catalysis. In EARTH, her group will model how small molecules adsorb in porous materials, the impact of guest-guest interactions, and assess water stability at metal-nodes. Additionally, her group will provide computational support for deconvoluting reaction mechanisms in the design of new refrigerants and provide high-level quantum chemical data to assess and improve machine learning potentials developed by others in the center. Her team is currently working in Project 1.1 and 3.2.





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### ED MAGINN



#### Associate Vice President for Research Keough-Hesburgh Professor of Engineering University of Notre Dame; ed@nd.edu



Professor Ed Maginn's research group develops and applies atomistic simulations along with machine learning tools to compute the thermophysical properties of fluids. For EARTH, we focus on calculating the properties of existing and new refrigerants, including phase equilibria and transport properties. We also use simulations to examine solvation of refrigerants in fluids such as deep eutectic liquids, in support of efforts to develop efficient methods for separating refrigerant mixtures. Our simulation tools are quite versatile, however, and can me applied to many systems. Talk to me about your system and maybe we can help out with simulations.

## JOHN ONYANGO

#### Associate Professor of Architecture University of Notre Dame; jonyang1@nd.edu



Professor John Onyango's research primarily focuses on Sustainability in the broad sense that takes holistic approaches to the creative practices at the building and urban design levels that is both interdisciplinary as well as multidisciplinary in collaboration with other colleagues in the allied fields such as engineering, sociology, healthcare, and IT communications. John is interested in understanding energy use in traditional buildings using simulation and biomimetic epidemiology, built environment and aging & wellbeing.

## Safety Tips: Ergonomics

Situate computer monitor an arm's length away.

When typing, keep wrists straight and hands at or below elbow level.

Adjust chair height so knees are level with hips.

When seated, occasionally stretch hands, fingers, and arms.

Get up and walk around as often as possible!

View more tips from the Mayo Clinic here.









## Announcements and Reminders



FROST: Fostering Research Opportunities in Sustainable Technologies

Applications due on March 31st!

HEART: Harnessing Educators for Advancing Refrigerant Technologies



Our first webinar speaker will be **Professor John Bischof** from the University of Minnesota on May 6th from 2-3 pm CST! John is the Center Director of the NSF ERC for Advanced Technologies for the Preservation of Biological Systems (<u>NSF ATP-Bio</u>). *Please join us virtually on Zoom! More details to come.* 



If you attended our Biannual Team Meeting, please take our <u>exit survey</u>!

Your input will help us make our following meetings even better.





Please use the following statement in your publication acknowledgements if your research was funded by EARTH.

"This research is based upon work supported by the National Science Foundation under award number **ERC-2330175** for the Engineering Research Center EARTH."









