

## Sponsors



# 9th Annual CBE Graduate Research Symposium

## Hosted By:

University of Notre Dame  
Department of Chemical & Biomolecular  
Engineering  
Graduate Student Organization

Oct 5<sup>th</sup> & 6<sup>th</sup> 2023  
Dahnke Ballroom,  
Duncan Student Center

## Organizing Committee

### Welcome

Welcome to the 9th Annual CBE Graduate Research Symposium!

The goal of the CBE Symposium is to provide a forum for CBE graduate students to present their research, network with professionals from both industry and academia, and develop their professional identity.

Over the course of the symposium, students will showcase research from a wide range of disciplines, including catalysis, energy and sustainability, nano-fluidics, micro-fluidics, simulation and theory, materials science, nanotechnology, and bioengineering.

The Symposium also features invited talks by experienced and renowned personalities in chemical engineering to provide a variety of perspectives on career development for PhD Chemical Engineers.

As this event has continued to grow, so too has the impact on CBE graduate student professional development and sense of community.

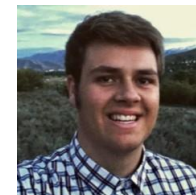
Thank you for attending the CBE Graduate Research Symposium.



Amish Chovatiya



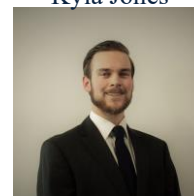
Kyla Jones



Denver Haycock



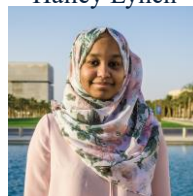
Hailey Lynch



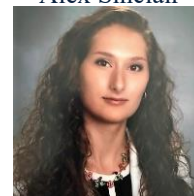
Alex Sinclair



Jose Rebolledo Oyarce



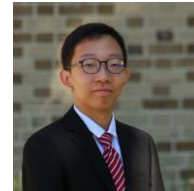
Fathya Salih



Montana Carlozo



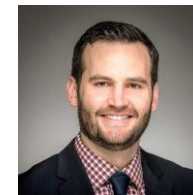
Lingyu Yang



Xuyao Gao



William Schnieder



William Phillip

## Event Schedule

### DAY 1 PROGRAM

Arrivals/Sign-in	1:00 pm
Opening Remarks and Seating	1:50 pm
Student Presentations (1 - 3)	2:00 pm
Industry Panel and Refreshments	3:00 pm
Break and Refreshments	4:15 pm
Student Presentations (4 - 6)	4:30 pm
Dinner and Networking	5:30 pm
Conclusion to Day 1 Events	7:00 pm

### DAY 2 PROGRAM

Poster Setup/Check-in and Breakfast	8:30 am
Poster Session 1	9:30 am
Invited Speaker: Dr. Rebecca Lindsey	11:15 am
Lunch	12:00 pm
Poster Session 2	1:15 pm
Invited Speaker: Dr. Kevin Dahm	3:00 pm
Poster Awards and Closing Remarks	3:45 pm
Conclusion to Day 2 Events	4:00 pm

## Guest Speakers

### Dr. Rebecca K. Lindsey

Assistant Professor  
Department of Chemical  
Engineering  
University of Michigan



#### About the Speaker

Dr. Lindsey is an Assistant Professor of Chemical Engineering and by courtesy, of Applied Physics, Materials Science & Engineering, and Nuclear Engineering & Radiological Sciences at the University of Michigan. She is a member of the KIM Review Editorial Board and the Institute of Computational Science & Engineering Advisory Board, and is an Executive Committee Member of the APS Topical Group on Shock Compression of Condensed Matter. Dr. Lindsey received her B.S. in Chemical Engineering from Wayne State University and her M.S. and Ph.D. in Chemical Physics from the University of Minnesota, Twin Cities. She went on to become a Postdoctoral Research Fellow at LLNL, where she worked as a Staff Research Scientist leading research teams within the Energetic Materials Center. Throughout, Dr. Lindsey's work has been underpinned by a strong interest in developing tools enabling exploring inaccessible problem spaces. Her group also leverages data science, machine learning, and computer vision to aid in interpretation of large experimental datasets and develop material and device performance models from them. Her efforts were recently recognized through the LLNL Physical and Life Sciences Directorate Research Award and the Young Investigator Award from the AIChE's Computational Molecular Science and Engineering Forum.

### Dr. Kevin Dahm

Professor & Undergraduate  
Program Chair  
Department of Chemical  
Engineering  
Rowan University



#### About the Speaker

Dr. Kevin Dahm is Professor and Undergraduate Program Chair of Chemical Engineering at Rowan University. He earned his B.S. from Worcester Polytechnic Institute in 1992 and his Ph.D. from Massachusetts Institute of Technology in 1998. Prior to joining Rowan University he was a Postdoctoral Researcher at University of California at Berkeley and an Adjunct Professor at North Carolina A&T State University. He has published articles on several aspects of engineering pedagogy, including assessment of student learning, teaching technical communication and engineering design, and game-based learning. He has co-authored two books: Fundamentals of Chemical Engineering Thermodynamics, with Donald Visco Jr., and Interpreting Diffuse Reflectance and Transmittance, with his father Donald Dahm. He received the Lindback Distinguished Teaching Award in 2019, and is the recipient of several national awards from ASEE including the Joseph J. Martin Award, the Raymond W. Fahien Award, the Corcoran Award, and the mid-Atlantic section Outstanding Teaching Award.

## Student Oral Presentations

P.N.	Student Name	Presentation Title	Time
1	<a href="#">Rachel Ollier</a>	Biomimetic Strain-Stiffening in Fully Synthetic Dynamic-Covalent Hydrogel Networks	2:00 pm
2	<a href="#">Ning Wang</a>	Machine Learning Enabled Development of Accurate Force Fields for Refrigerants	2:20 pm
3	<a href="#">Runyao Zhu</a>	Blocking Tau Transmission by Biomimetic Graphene Nanoparticles	2:40 pm
4	<a href="#">Mayesha Sahir Mim</a>	Shining Light on Calcium-Mediated Morphogenesis: Forward Engineering Organ Development with Optogenetics and Mechanosensation	4:30 pm
5	<a href="#">Bo Su</a>	Dissipative Non-Equilibrium Host-Guest Hydrogels Regulated by Consumable Fuels	4:50 pm
6	<a href="#">Mengdi Liu</a>	Polybenzimidazole-based Membranes with Semi-Interpenetrating Network (s-IPN) Structures for High-Temperature Precombustion Carbon Capture	5:10 pm

# Poster Presentations

## SESSION 1

<b>P.N.</b>	<b>Presenter</b>	<b>Advisor/s</b>	<b>Poster Title</b>
<b>P1</b>	Piyush Deshpande	Jennifer Schaefer	Characterization of Solid-State Lithium-Sulfur Battery Reaction Intermediates
<b>P3</b>	Jialing Xu	William Phillip	Using Green Solvents for the Fabrication of Adsorptive Membranes via Surface Segregation and Vapor Induced Phase Separation Method
<b>P5</b>	Kyle McCarthy	Hsueh-Chia Chang	A microfluidic platform for the detection of Alzheimer's Disease from colocalized surface proteins on exosomes
<b>P7</b>	Lingyu Yang	Jennifer Schaefer	Water-Assisted Ion Conduction in Solid-State Charge-Transfer Complex Electrolytes for Lithium Batteries
<b>P9</b>	Bernice Webber	Matthew Webber	Supramolecular hydrogels utilizing polymer-nanoparticle interactions for ultra-long acting basal insulin delivery
<b>P11</b>	Connor Schmidt	Matthew Webber	A Non-Equilibrium Steady State Host-Guest Cross-linked Hydrogel
<b>P13</b>	Anna O'Keefe	Casey O'Brien	Development of Composite Membrane Preparation Approaches to Enable Operando Transmission FTIR Characterization
<b>P15</b>	Alejandro Chaperro-Planell	Casey O'Brien	Tuning CO <sub>2</sub> Conversion of Amine-based Polymer Catalyst through Structural Modification via Quaternization
<b>P17</b>	Audrey Hansrisuk	Matthew Webber	Development of a supramolecular hydrogel for prime-boost vaccine delivery
<b>P19</b>	Maria Unger	Jeremiah Zartman	G $\alpha$ q homeostasis is required in organ size regulation, initiation of larval to pupal metamorphosis and larval survival in <i>Drosophila melanogaster</i> .

<b>P21</b>	Stephen Cini	Başar Bilgiçer	Utilizing a Nucleotide Binding Site Ligand for Antibody Purification
<b>P23</b>	Annabelle Li	William Phillip	Development of Composite Block Copolymer Adsorptive Membranes on a Nonwoven Support
<b>P25</b>	Deanna Poirier	Jason Hicks	Plasma-Assisted Approaches for the Direct Conversion of Natural Gas to Value-Added Products
<b>P27</b>	David Gazzo	Jeremiah Zartman	A Dynamic Interaction Between Ion Channels: Piezo and SERCA
<b>P29</b>	Bo Wei Cynthia Chen	Casey O'Brien	Olefin/Paraffin Separation Performance of Amine-modified PIM-1 Membrane
<b>P31</b>	Daniel Montes Pinzon	Hsueh-Chia Chang / Donny Hanjaya-Putra	Development of a High-Throughput Drug Screening Platform Via Pipetting Gel Droplet Micro-Organoids Models
<b>P33</b>	Shuman Liu	Jeremiah Zartman	Deciphering the interplay of morphogen and bioelectric signaling during growth and morphogenesis
<b>P35</b>	Christopher Addonizio	Matthew Webber	Material Consequences of Guest Orientation in Host-Guest Supramolecular Complex Crosslinking
<b>P37</b>	Sandra Weber	Ruilan Guo	Organosoluble Pentiptycene-Containing Polybenzoxazole Membranes for High Temperature Gas Separations
<b>P39</b>	Emily DeWolf	Matthew Webber	Leveraging Dynamic-Covalent Bonds for Glucose-Responsive Peptide Structures
<b>P41</b>	Russell Clarke	Jason Hicks	Coke Suppression and Pattern Formation in Light Alkane Plasma
<b>P43</b>	Weike Chen	Matt Webber	Sustained Release of Glucagon Like Peptide-1 (GLP-1) From An Injectable Hydrogel Protects Mice From Hyperglycemia
<b>P45</b>	Alba Scotto d'Apollonia	Jason Hicks	Polyoxometalates as Platforms for the Design of Single Site Catalysts for Light Olefin Oligomerization

# Poster Presentations

## SESSION 2

<b>P.N.</b>	<b>Presenter</b>	<b>Advisor/s</b>	<b>Poster Title</b>
<b>P2</b>	Ramón González-Pérez	Jonathan Whitmer	Characterization of Ion Binding Guided by Free Energy Calculations
<b>P4</b>	Krishnendu Mukherjee	Yamil Colón	Active learning for efficient navigation of multi-component gas adsorption landscapes in a MOF
<b>P6</b>	James Carpenter	Yamil Colón	Modeling Adsorption in Soft Porous Coordination Polymers
<b>P8</b>	Orlando A. Mendible Barreto	Yamil Colón	Considerations in the use of ML interaction potentials for free energy calculations
<b>P10</b>	Fathya Salih	Yamil Colón	Developing an Open-Source Sigma Profile Generator for Accelerated Active-Learning Driven Molecular Discovery
<b>P12</b>	Wilson Raney	Yamil Colón	Entangled Photon Properties of Functionalized Metal-Organic Frameworks
<b>P14</b>	Kyla Jones	Alexander Dowling	Optimization Under Uncertainty with Bayesian Hybrid Models
<b>P16</b>	Damian Agi	Alexander Dowling	Modeling & Optimization of Pd-based Water-Gas Shift Membrane Reactors for Low-Cost Blue Hydrogen Production
<b>P18</b>	Madelynn Watson	Alexander Dowling	A Risk-conscious Optimization Model for Sustainable Aviation Fuel Production in the Brazilian Sugarcane Industry
<b>P20</b>	Dinis Abranches	Edward Maginn / Yamil Colón	Novel Sustainable Materials Design with Thermodynamics-Informed Machine Learning
<b>P22</b>	Etinosa Osaro	Yamil Colón	Active Learning of alchemical adsorption simulations, towards a universal adsorption model



<b>P24</b>	Raghav Saxena	William Schneider	First-principles Investigation of N <sub>2</sub> O formation over H-SSZ-13 zeolite catalyst
<b>P26</b>	Xinhe Chen	Alexander Dowling	Multiscale Optimization of Integrated Energy Systems that Co-Produce Electricity and Hydrogen Using Market Surrogate Models
<b>P28</b>	Hailey Lynch	Alexander Dowling	Science-Based Design of Experiments and Pyomo.DoE
<b>P30</b>	Logan Hennes	Jonathan Whitmer	Coarse-Grained Modeling of Ionic Liquid Crystals
<b>P32</b>	Barnabas Agbodekhe	Edward Maginn	From elements to screened molecules: Towards the molecular design and discovery of green refrigerants
<b>P34</b>	Molly Dougher	Alexander Dowling	Opportunities for Membranes to Enhance Critical Mineral Processes
<b>P36</b>	Jonathan Aubuchon Ouimet	William Phillip	Guiding Material Design to Harness Unsteady State Transport Phenomena for Selective Solute Recovery
<b>P38</b>	Hyunsu Jeon	Yichun Wang	Chiral Nanocarriers: Enhancing Drug Transport and Delivery in Tumor-like Spheroids
<b>P40</b>	Gaeun Kim	Yichun Wang	Unraveling Origin-Dependent Exosome Uptake and Cargo Release using Chiral Nanoparticles
<b>P42</b>	James Johnston	Yichun Wang	Stimulated Biomaterials for understanding the biogenesis of Extracellular Vesicles (EVs)
<b>P44</b>	Jordan Smith	Jennifer Schaefer	Understanding and Quantifying the Benefits of Gel Polymer Electrolytes in Rechargeable Batteries to Improve Safety
<b>P46</b>	Garam Lee	Casey O'Brien / David Go	Investigation of Intermediate Species on a Catalytic Surface in Non-Thermal Plasma-Activated Carbon-Nitrogen Coupling from Methane and Nitrogen
<b>P48</b>	Xuyao Gao	William Schneider	Influence of N,N,N-trimethyl-1-adamantyl Ammonium on Defects/Al Siting Energetics and Accessible Si/Al /Defect Ratio in CHA