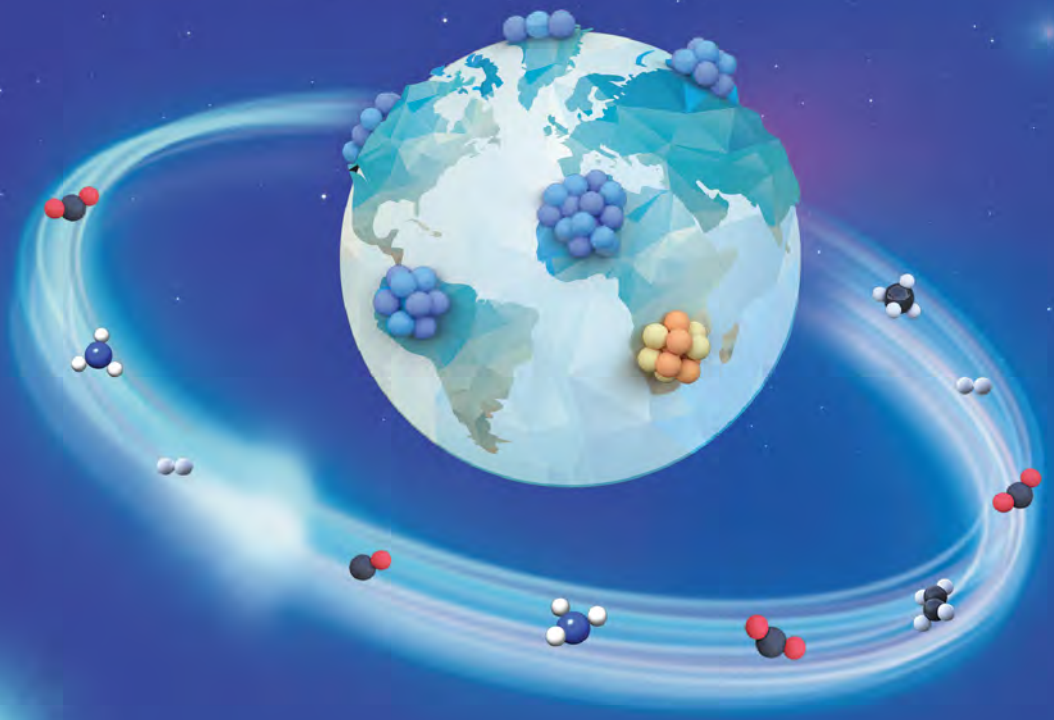
AI for Multidisciplinary Exploration and Discovery Workshop

Heterogeneous Catalysis



Oct. 10–11, 2024
(hybrid)

Big Ten Conference Center
Rosemont, IL

AIMED
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Acknowledgements

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Journal of Catalysis

Catalysis Science & Technology

APL Machine Learning

Chem Catalysis

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Workshop Vision and Objectives

The **Artificial Intelligence for Multidisciplinary Exploration and Discovery (AIMED) on Heterogeneous Catalysis** workshop brings together pioneering minds to explore how AI can accelerate breakthroughs in catalysis research. Focusing on the intersection of AI and heterogeneous catalysis, this event addresses complex challenges in catalysis by integrating AI's predictive power with human expertise.

Designed to foster cross-disciplinary collaborations, the workshop highlights AI's transformative potential in data analysis, experimental automation, and multiscale modeling, from the lab to industrial applications. By examining AI's role in augmenting scientific discovery and practical implementation, participants will engage in dynamic discussions on how AI can enhance catalytic processes, shape future innovations, and build a roadmap for sustainable development.

Through insightful keynote lectures, panel discussions, and poster presentations, AIMED aspires to define the future of catalysis research in the age of AI, empowering scientists to harness AI tools for more efficient, scalable, and innovative solutions.

The workshop is convened by the **National Science Foundation (NSF) CBET Catalysis** and **CHE Chemical Catalysis** Programs.

Key Information

Dates: October 10–11, 2024

Time: Central Daylight Time (CDT), 7:00 AM Day 1 – Noon Day 2

Location: Big Ten Conference Center, Rosemont, IL

Room: 202+203+205

Zoom Webinar:

Meeting ID: 837 9513 0756

Passcode: 867498

Schedule

Day 1 - October 10, 2024

7:00 - 8:00 AM: Badge Pickup & Breakfast (provided)

8:00 - 8:10 AM: **Hongliang Xin**, Virginia Tech

Opening Remarks

Robert McCabe & Kenneth Moloy, NSF

Program Remarks

Neil Schweitzer, Northwestern University

Local Logistics

AM 1 Session: **Foundational Models**

Chair: **John Kitchin**, Carnegie Mellon University

8:10 - 8:30 AM: **Boris Kozinsky**, Harvard University

Foundational Models for Predicting Quantum-Level Phenomena in Materials Design

8:30 - 8:50 AM: **Andy Peterson**, Brown University

Towards electronically grand-canonical machine-learned simulations, for electrochemical systems

8:50 - 9:10 AM: **Shyue Ping Ong**, University of California, San Diego

Foundational Software and Data for Materials Foundational Models

9:10 - 9:30 AM: **Marc Porosoff**, University of Rochester

Accelerating decarbonization with natural language processing

9:30 - 9:50 AM: **Amir Barati Farimani**, Carnegie Mellon University

Multimodal Language and Graph Learning in Catalysis

9:50 - 10:20 AM: Coffee Break

Day 1 - October 10, 2024

AM 2 Session: **Materials & Knowledge Discovery**

Chair: **Hongliang Xin**, Virginia Tech

10:20 - 10:40 AM: **Anatoly Frenkel**, BNL/Stony Brook University

Decoding the Structure of Active Species in Catalysts by Machine Learning Analysis of Spectra

10:40 - 11:00 AM: **Bryan Goldsmith**, University of Michigan

Interpretable machine learning to understand heterogeneous catalysts

11:00 - 11:20 AM: **Randall Meyer**, ExxonMobil

Descriptors for Metal Oxide Reactivity and Transport

11:20 - 11:40 AM: **Kirsten Winther**, SLAC/Stanford University

Improving the accuracy of ML-models for metal oxide catalysis with electronic structure descriptors

11:40 AM - noon: **Hao Li**, Tohoku University

"Turing Scheme for Catalysis" and DigCat 3.0 - An Intelligent Digital Platform Powered by Ultra-Large-Scale Exp + Comput Data

12:00 - 1:30 PM: Lunch (provided)

Day 1 - October 10, 2024

PM 1 Session:	**Data & Software Infrastructures**
	Chair: **Núria López**, Institute of Chemical Research of Catalonia
1:30 - 1:50 PM:	**Johannes Voss**, SLAC/Stanford University
	From Data to Models for Heterogeneous Catalysts: The Power of Combined Experiments and Simulations
1:50 - 2:10 PM:	**Andrew Rosen**, Princeton University
	Accessible and Interoperable Computational Workflows to Satisfy the Data-Hungry Machines
2:10 - 2:30 PM:	**Kamal Choudhary**, National Institute of Standards and Technology
	Examining Generalizability of AI Models for Catalysis
2:30 - 2:50 PM:	**Joseph Montoya**, Toyota Research Institute
	Materials science on the client-side
2:50 - 3:10 PM:	**Núria López**, Institute of Chemical Research of Catalonia (ICIQ)
	Data in computational heterogeneous catalysis
3:10 - 3:40 PM:	Coffee Break

Day 1 - October 10, 2024

PM 2 Session: **Future Labs**

Chair: **Neil Schweitzer**, Northwestern University

3:40 - 4:00 PM: **Milad Abolhasani**, North Carolina State University

Human-AI-Robot Collaboration to Accelerate Materials and Molecular Discovery with Autonomous Labs

4:00 - 4:20 PM: **Shijing Sun**, University of Washington

Building a self-driving lab from scratch

4:20 - 4:40 PM: **Paulami Majumdar**, Dow

Applying AI in Industrial Heterogeneous Catalysis

4:40 - 5:00 PM: **Chong Liu**, University of California, Los Angeles

Machine-learning for automated if not autonomous electrochemistry

6:00 - 9:00 PM: Buffet Dinner at Bub City (badge required)

Address: Parkway Bank Park, 5441 Park Pl, Rosemont, IL 60018

Day 2 - October 11, 2024

7:00 - 8:00 AM: Breakfast (provided)

AM 1 Session: **Theme Panel 1: Current Barriers**

What are the technological gaps and barriers in AI that hinder achieving scientific breakthroughs, particularly in catalysis for a sustainable future?

Moderator: **Hongliang Xin**, Virginia Tech

8:00 - 8:10 AM: **Long Qi**, Ames Lab

Accelerating Manufacturing through Automation and Artificial Intelligence

8:10 - 8:20 AM: **Teodoro Laino**, IBM Research Europe – Zurich (Virtual)

Multimodal Foundation Models for Molecular Structure Elucidation

8:20 - 8:30 AM: **Zack Ulissi**, Meta/Carnegie Mellon University

Beyond Relaxations: Extrapolation of Open Catalyst Models to Transition States, Vibrational Frequencies, Free Energies, and High Entropy Alloys

8:30 - 8:40 AM: **Xiaonan Wang**, Tsinghua University (Virtual)

AI-Driven Materials Discovery and Catalyst Development for a Sustainable Future

8:40 - 9:40 AM: Panel Discussion

9:40 - 10:10 AM: Coffee Break

Day 2 - October 11, 2024

AM 2 Session: **Theme Panel 2: Future Opportunities**

What is the future of AI for driving scientific discovery, and how different stakeholders can help shape the vision in catalysis?

Moderator: **John Kitchin**, Carnegie Mellon University

10:10 - 10:20 AM: **Suljo Linic**, University of Michigan

Shedding Light on the Physics of Chemisorption Using Machine Learning

10:20 - 10:30 AM: **Wendy Shaw**, Pacific Northwest National Laboratory

Accelerating Catalyst Discovery with AI/ML

10:30 - 10:40 AM: **AJ Medford**, Georgia Tech

Opportunities for AI in Catalysis Beyond Atomistic Models

10:40 - 10:50 AM: **Tian Xie**, Microsoft Research

Accelerating Materials Design with AI Emulators and Generators

10:50 - 11:50 AM: Panel Discussion

11:50 AM - noon: Concluding Remarks by **John Kitchin**

Early Career Investigators' Poster Showcase

(There is no specific time slot for poster presentations, encouraging interactions and discussions during coffee breaks and lunch.)

Brandon Bukowski, Johns Hopkins University
Accelerating Models for Catalyst Structure and Dynamics

Fanglin Che, University of Massachusetts Lowell
Multi-Scale Guided Machine Learning for Heterogeneous Catalysis for Hydrogen Economy

Rui Ding, The University of Chicago
Leveraging Data Mining, Active Learning, and Domain Adaptation in a Multi-Stage, Machine Learning-Driven Approach for the Efficient Discovery of Advanced Acidic Oxygen Evolution Electrocatalysts

Kasun Gunasooriya, The University of Oklahoma
Accelerated Discovery of Stable and Active Materials for Sustainable Electrochemical Processes

Emma Hu, Georgia Institute of Technology
Machine Learning Assisted Design of Multi-Metal Catalysts for Oxygen Reduction and Evolution Reactions

Tyler Josephson, University of Maryland, Baltimore County
Automated Reasoning to Advance Chemical Theory

Ritesh Kumar, The University of Chicago
In Silico Materials Design and Discovery for Electrocatalysis and Energy Storage

Mingjie Liu, University of Florida
Data-Driven Discovery in Chemistry and Materials Science

Pengfei Ou, National University of Singapore
High-Entropy Alloy Electrocatalysts Screened Using Machine Learning Informed by Quantum-Inspired Similarity Analysis

Daniel Schwalbe-Koda, University of California, Los Angeles
Digital Synthesis Lab: Towards Predictive Synthesis of Inorganic Materials

Evan Spotte-Smith, Carnegie Mellon University
Chemical Reaction Network Machine Learning (CRN-ML): A Frontier for Reactivity Studies

Tibor Szilvasi, The University of Alabama
Effect of Metal-Support Interactions on Nanoparticle Catalyst Structure

Siwen Wang, Toyota Research Institute of North America
Artificial Intelligence for Materials Research in Toyota

Zisheng Zhang, SLAC/Stanford University
Grand Canonical Ensemble Representation of Dynamic Electrocatalysts: From Clusters to Surfaces

Jiayu Peng, Massachusetts Institute of Technology
Learning Ordering in Crystalline Materials with Symmetry-Aware Graph Neural Networks

Joseph Gauthier, Texas Tech University
Understanding the Active Surface Phase for Improved Catalyst Design

Muhammed Shuaibi, Meta
Towards AI Accelerated Catalyst Discovery: Bridging the Gap Between Theory and Experiments

Biographies

Organizing Committee

Hongliang Xin
Virginia Tech

Hongliang Xin is an Associate Professor in the Department of Chemical Engineering at Virginia Tech, where he leads research on developing interpretable AI frameworks to advance the theory of heterogeneous catalysis and accelerate catalytic materials discovery.

John Kitchin
Carnegie Mellon University

John Kitchin is a Professor of Chemical Engineering at Carnegie Mellon University, with a courtesy appointment in Materials Science and Engineering. His research focuses on catalysis on metals and metal oxides using density functional theory, software development for materials modeling, and CO_2 capture materials.

Núria López
Institute of Chemical Research of Catalonia (ICIQ)

Núria López is a Professor at the Institute of Chemical Research of Catalonia (ICIQ). Her research focuses on heterogeneous photo-electro-catalysis using atomistic modeling. She has co-authored over 300 publications and contributed to software development such as Solvent contributions for VASP and ioChem-BD.

Neil Schweitzer
Northwestern University

Neil Schweitzer is the REACT Operations Director and a Research Associate Professor at Northwestern University. His expertise includes heterogeneous catalyst characterization and reaction kinetics.

Keynote Session: Foundational Models

Boris Kozinsky
Harvard University

Boris Kozinsky is the Thomas D. Cabot Associate Professor of Computational Materials Science at Harvard University and Principal Scientist at Bosch Research. He leads the Materials Intelligence Research group, focusing on materials discovery through computational methods and machine learning to design materials for energy storage and conversion systems.

Shyue Ping Ong
University of California, San Diego

Shyue Ping Ong is a Professor of NanoEngineering at the University of California, San Diego. He leads the Materials Virtual Lab, focusing on materials design using data science and machine learning.

Andy Peterson
Brown University

Andrew Peterson is an Associate Professor in the School of Engineering at Brown University. His research focuses on sustainable energy, particularly in the theory of reactions at electrified interfaces, and in developing computational tools for better optimization of electrochemical systems.

Marc Porosoff
University of Rochester

Marc Porosoff is an Associate Professor of Chemical Engineering at the University of Rochester. His research focuses on developing low-cost, alternative catalysts for CO_2 hydrogenation into value-added chemicals and fuels. Porosoff combines experimental techniques and computational methods to accelerate the deployment of decarbonization technologies.

Amir Barati Farimani
Carnegie Mellon University

Barati Farimani is the Russel V. Trader Associate Professor of Mechanical Engineering at Carnegie Mellon University. His lab focuses on the intersection of mechanical engineering, data science, and machine learning, using advanced algorithms to learn, infer, and predict physical phenomena

Keynote Session: Materials & Knowledge Discovery

Anatoly Frenkel
BNL/Stony Brook University

Anatoly Frenkel is a Professor in the Department of Materials Science and Chemical Engineering at Stony Brook University and a Senior Chemist at Brookhaven National Laboratory. His research focuses on developing and applying in situ and operando synchrotron methods to address materials challenges, with an emphasis on catalysis, electromechanical materials, quantum dots, and filtration materials. Frenkel is also recognized for advancing machine learning methods for the structural analysis and design of nanomaterials.

Bryan Goldsmith
University of Michigan

Bryan Goldsmith is an Associate Professor of Chemical Engineering at the University of Michigan, Ann Arbor. His research focuses on using first-principles computational modeling and data science to design catalysts and materials for sustainable chemical conversion, pollution reduction, and energy generation/storage.

Randall Meyer
ExxonMobil

Randall Meyer is a scientist at ExxonMobil Technology and Engineering, where he has worked since 2014. Prior to that, he was a faculty member in the Chemical Engineering department at the University of Illinois Chicago for nine years. Meyer's expertise is in heterogeneous catalysis, and more recently, he has become involved in data-driven approaches for catalyst development.

Kirsten Winther
SLAC/Stanford University

Kirsten Winther is an Associate Scientist at the SUNCAT Center for Interface Science and Catalysis at SLAC/Stanford, where she has worked since 2017. Her research focuses on combining density functional theory simulations with data science to accelerate the discovery of novel catalytic materials. Her interests include developing machine learning models for predicting catalyst stability and adsorption energetics, active learning frameworks for catalyst discovery, and contributing to scientific software and the open database catalysis-hub.org.

Hao Li
Tohoku University

Hao Li is an Associate Professor and Principal Investigator at the Advanced Institute for Materials Research (WPI-AIMR), Tohoku University, Japan, and an Adjunct Investigator at the ARC Centre of Excellence for Green Electrochemical Transformation of Carbon Dioxide (GETCO2) at the University of Queensland, Australia.

Keynote Session: Data & Software Infrastructures

Johannes Voss
SLAC/Stanford University

Johannes Voss is a staff scientist at SLAC National Accelerator Laboratory, where he leads the data science efforts at the SUNCAT Center for Interface Science and Catalysis. His team develops machine learning models for the prediction of catalytic reaction energies and materials properties, including empirical models for practical performance predictions and exchange-correlation functionals for surface science.

Andrew Rosen
Princeton University

Andrew Rosen is an Assistant Professor of Chemical and Biological Engineering at Princeton University. His research group utilizes high-throughput computing, machine learning, and quantum-chemical calculations to design new materials for a sustainable future.

Kamal Choudhary
National Institute of Standards and Technology

Kamal Choudhary is a Staff Scientist in the Material Measurement Laboratory at the National Institute of Standards and Technology (NIST) in Maryland, USA. His research focuses on atomistic materials design using classical, quantum, and machine learning methods. He developed the widely used JARVIS database and tools.

Joseph Montoya
Toyota Research Institute

Joseph Montoya leads the Accelerated Materials Design and Discovery (AMDD) team at the Toyota Research Institute (TRI). His work focuses on developing AI-accelerated, end-to-end materials discovery methods, drawing on his expertise in computational catalysis, materials informatics, and AI for materials.

Núria López
Institute of Chemical Research of Catalonia (ICIQ)

Núria López is a Professor at the Institute of Chemical Research of Catalonia (ICIQ). Her research focuses on heterogeneous photo-electro-catalysis using atomistic modeling. She has co-authored over 300 publications and contributed to software development such as Solvent contributions for VASP and ioChem-BD.

Keynote Session: Future Labs

Milad Abolhasani
North Carolina State University

Milad Abolhasani is the ALCOA Professor and a University Faculty Scholar in the Department of Chemical and Biomolecular Engineering at North Carolina State University. His research focuses on self-driving labs for the accelerated discovery, development, and manufacturing of advanced functional materials and molecules using fluidic micro-processors.

Shijing Sun
University of Washington

Shijing Sun is an assistant professor at the University of Washington, where she leads research in collaborative intelligence, robotics, and AI for clean energy innovation. Before joining UW, she worked at the Toyota Research Institute and MIT, focusing on AI-driven materials discovery and high-throughput experimentation.

Paulami Majumdar
Dow

Paulami Majumdar is an Associate Research Scientist in Core R&D at Dow in Midland, Michigan. Her research focuses on computational catalysis for materials design and optimization.

Chong Liu
University of California, Los Angeles

Chong Liu is an Associate Professor at UCLA. His research combines electrochemistry, nanomaterials, and machine learning to develop AI-augmented environments for advanced catalysis and electrochemistry.

Theme Panel 1: Current Barriers

Long Qi
Ames Laboratory

Long Qi is a Scientist at Ames National Laboratory. His research focuses on heterogeneous catalysis and automation of reactor design to accelerate sustainable chemical conversions. He specializes in developing interfacial spectroscopy to decipher catalytic processes.

Teodoro Laino
IBM Research Europe – Zurich

Teodoro Laino is a Distinguished Research Scientist and Manager at IBM Research Europe – Zurich. He leads the team behind IBM RXN for Chemistry, focusing on multimodal foundation models for molecular structure elucidation and the digitalization of chemical processes using AI.

Zack Ulissi
Meta/Carnegie Mellon University

Zack Ulissi is a Senior Research Manager on the FAIR Chemistry team at Meta's Fundamental AI Research lab and an Adjunct Professor of Chemical Engineering at Carnegie Mellon University. He works on applying machine learning to catalyst discovery and design, bridging the gap between theory and experiments for materials research. He has led several open science initiatives and community efforts.

Xiaonan Wang
Tsinghua University

Xiaonan Wang is a tenured Associate Professor and team lead in the Department of Chemical Engineering at Tsinghua University. Wang leads the Smart Systems Engineering research group and AI Accelerated Materials Development programs at NUS and Tsinghua for sustainable technologies.

Theme Panel 2: Future Opportunities

Suljo Linic
University of Michigan

Suljo Linic is the Martin Lewis Perl Collegiate Professor of Chemical Engineering at the University of Michigan. His research focuses on developing predictive theories of surface chemistry related to heterogeneous catalysis, electrocatalysis, and photocatalysis. His group combines experimental techniques, such as kinetic analysis and in operando spectroscopy, with first-principles theoretical tools, including density functional theory (DFT) and ab initio kinetics, to advance sustainable energy generation, functional nanomaterials, and catalyst design.

Wendy Shaw
Pacific Northwest National Laboratory

Wendy Shaw is the Chief Science and Technology Officer for the Physical and Computational Sciences Directorate at Pacific Northwest National Laboratory, where she leads strategy and internal investments with a focus on leveraging AI and machine learning to accelerate scientific discovery. Her research centers on developing bioinspired catalysts for renewable energy and investigating protein structures to understand biomineralization processes.

AJ Medford
Georgia Tech

AJ Medford is an Associate Professor in the School of Chemical & Biomolecular Engineering at Georgia Tech. His research lies at the intersection of data science, electronic structure theory, and catalysis, with key contributions including the development of machine-learned exchange-correlation functionals for density functional theory, neural network models for transient kinetic datasets, and mechanistic insights into nitrogen conversion reactions.

Tian Xie
Microsoft Research

Tian Xie is a principal research manager and project lead at Microsoft Research AI4Science. He leads a team of researchers, engineers, and program manager to develop the next generation machine learning models for materials discovery.

Early Career Investigators

Brandon Bukowski
Johns Hopkins University

Brandon C. Bukowski is an Assistant Professor in Chemical and Biomolecular Engineering at Johns Hopkins University. His research focuses on using computational chemistry and data science to design nanoporous catalysts and supported nanoparticles for sustainable energy and environmental applications.

Fanglin Che
University of Massachusetts Lowell

Fanglin Che is an Assistant Professor of Chemical Engineering at UMass Lowell, where she leads research focused on advancing electrified interfacial phenomena using AI-driven multi-scale and multi-physics computational models.

Rui Ding
The University of Chicago

Rui Ding is a postdoctoral researcher at the University of Chicago, where his work focuses on integrating machine learning with material science to design advanced materials for sustainable energy applications. His research interests include catalysts, batteries, and sensors, with an emphasis on accelerating material discovery through computational approaches

Joseph Gauthier
Texas Tech University

Joe Gauthier is an Assistant Professor of Chemical Engineering at Texas Tech University. His research focuses on heterogeneous (electro)catalysis, with the goal of addressing challenges in renewable energy conversion, storage, and the decarbonization of the chemical industry.

Kasun Gunasooriya
The University of Oklahoma

Kasun Gunasooriya is an Assistant Professor of Sustainable Chemical, Biological, and Materials Engineering at the University of Oklahoma, where he is also a faculty affiliate in the Data Science and Analytics Institute. His research focuses on developing materials and processes for renewable energy, fuels, and chemicals by integrating computational catalysis, kinetic modeling, machine learning, and techno-economic analysis to enhance efficiency, durability, and sustainability while minimizing environmental impacts.

Emma Hu
Georgia Institute of Technology

Emma Hu is an Assistant Professor in the School of Materials Science and Engineering at the Georgia Institute of Technology. Her research focuses on atomistic modeling and machine learning to study functional materials for energy applications, including electrochemical catalysis and light harvesting, with an emphasis on understanding electron transfer and chemical reactions at electrochemical interfaces.

Tyler Josephson
University of Maryland, Baltimore County

Tyler R. Josephson is an Assistant Professor of Chemical, Biochemical, and Environmental Engineering at the University of Maryland, Baltimore County, where he leads the AI & Theory-Oriented Molecular Science (ATOMS) Lab. His research focuses on developing computational methods for molecular simulation and the automated discovery of scientific theories, using techniques such as quantum chemistry, Monte Carlo, symbolic regression, and formal theorem proving.

Ritesh Kumar
The University of Chicago

Ritesh Kumar is an Eric and Wendy Schmidt AI in Science Postdoctoral Fellow at the Pritzker School of Molecular Engineering, University of Chicago, where he leads initiatives combining modeling and data science with experimental collaboration to address challenges in electrocatalysis and next-generation batteries.

Mingjie Liu
University of Florida

Mingjie Liu is an Assistant Professor in the Department of Chemistry at the University of Florida, where her research focuses on developing AI-driven computational platforms for designing and discovering carbon-based materials for energy applications.

Pengfei Ou
National University of Singapore

Pengfei Ou is an Assistant Professor in the Department of Chemistry at the National University of Singapore. His research focuses on catalyst design for electrochemical reactions, dynamic simulations of chemical processes, and methods for accelerating catalyst discovery.

Jiayu Peng
Massachusetts Institute of Technology

Jiayu Peng is an incoming Assistant Professor in the Department of Materials Design and Innovation at the University at Buffalo, starting in January 2025. His research integrates materials physics and surface science with data science and machine learning to accelerate materials discovery for sustainable applications.

Daniel Schwalbe-Koda
University of California, Los Angeles

Daniel Schwalbe-Koda is an Assistant Professor of Materials Science and Engineering at UCLA. His research focuses on computational materials design, digital synthesis models, high-throughput simulations, and scientific machine learning.

Muhammed Shuaibi
Meta

Muhammed Shuaibi is a Research Engineer at Meta's Fundamental AI Research (FAIR) lab, where he works on AI applications for chemistry and materials science as part of the Open Catalyst Project.

Evan Spotte-Smith
Carnegie Mellon University

Evan Spotte-Smith (they/them) is a Carnegie Bosch Institute Postdoctoral Fellow and incoming Assistant Professor of Chemical Engineering at Carnegie Mellon University, starting in Fall 2025. Their research focuses on using computational chemistry, data science, and high-throughput experimentation to optimize reactivity for sustainable technologies.

Tibor Szilvasi
The University of Alabama

Tibor Szilvási is an Assistant Professor in the Department of Chemical and Biological Engineering at The University of Alabama. His research focuses on understanding nanoparticle-catalyzed thermal reactions and the influence of the electric double layer on electrocatalytic reactions.

Siwen Wang
Toyota Motor North America

Siwen Wang is a Senior Research Scientist in the Materials Research Department at the Toyota Research Institute of North America (TRINA) in Ann Arbor, Michigan. She leads a team focused on material informatics for applications in carbon neutrality and electrification.

Zisheng Zhang
SLAC/Stanford University

Zisheng Zhang is a Stanford Energy Fellow at the SUNCAT Center for Interface Science and Catalysis. His research focuses on realistic modeling of complex interfaces, inverse design of functional molecules and materials, and physics-informed machine learning.

Attendees

Bin Liu
Kansas State University

Chris Paolucci
University of Virginia

Cong Liu
Argonne National Laboratory

Cory Phillips
U.S. Department of Energy

De-en Jiang
Vanderbilt University

Eric Sacia
AbbVie

Jacob Saldinger
BP

Jae Young Kim
University of Delaware

Jiayi Xu
Argonne National Laboratory

Jose Rebolledo
University of Notre Dame

Kat Stephan
Chem Catalysis

Lars Grabow
University of Houston

Líney Árnadóttir
Oregon State University

Michael Bradford
GTI Energy

Moses Abraham Bokinala
Drexel University

Pranav Ramachandra
University of California, Berkeley

Qin Wu
Brookhaven National Laboratory

Randy Snurr
Northwestern University

Roushan Singh
University of Illinois Chicago

Siobhan Brown
Northwestern University

Srikar Bhattar
AVN Corporation

Tracee Whitfield
U.S. Army

Yezhi Jin
University of Chicago

Yinan Xu
University of Chicago

Zuhal Cakir
Purdue University

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