

Automating Chemical Laboratories

The Third Annual Scialog Conference
April 16 – 19, 2026

scialog2026[®]



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Scialog: Automating Chemical Laboratories

Objectives

1. Engage in dialogue with the goal of accelerating high-risk, high-reward research.
2. Analyze bottlenecks related to when, what and how to automate the chemical discovery workflow and develop approaches to surmount those barriers.
3. Build a creative better-networked community of scientists that crosses disciplinary silos.
4. Form new teams to write proposals to seed novel projects based on innovative ideas that emerge from the dialogue.
5. Most importantly, enjoy the discussions about where this field should go and how we can work together to get there.

Process

Brainstorming is welcome; don't be afraid to say what comes to mind.

Consider the possibility of unorthodox or unusual ideas without immediately dismissing them.

Discuss, build upon and constructively criticize each other's ideas in a spirit of cooperative give and take.

Make comments concise to avoid monopolizing the dialogue.

Conduct at RCSA Meetings

Research Corporation for Science Advancement fosters a welcoming and respectful environment for listening in which the different identities, backgrounds, and perspectives of all participants are valued, and in which everyone is empowered to share ideas as fellow scientists.

RCSA does not tolerate any form of harassment, which could include verbal or physical conduct that has the purpose or effect of substantially interfering with anyone else's participation or performance at this conference, or of creating an intimidating, hostile, or offensive environment; any such harassment may result in dismissal from the conference.

[Read RCSA's Code of Conduct](#)



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Scialog: Automating Chemical Laboratories

From the President

Welcome to the 2026 **Scialog: Automating Chemical Laboratories**. This meeting, co-sponsored by **Research Corporation**, the **Arnold and Mabel Beckman Foundation** and the **Frederick Gardner Cottrell Foundation**, marks the third and final convening on this important and rapidly advancing theme.



We are at a pivotal moment in the chemical sciences. The convergence of artificial intelligence and laboratory automation, including robotics, is not only accelerating research, it is redefining how it is done. From autonomous experimentation to AI-driven hypothesis generation and analysis, we are seeing the emergence of laboratories that can operate with unprecedented speed, adaptability, and intelligence.

Scialog is built on the idea that breakthrough science happens at the intersection of disciplines and perspectives. By bringing together early-career scientists from diverse fields, we create an environment designed to foster creativity, challenge assumptions, and spark new directions. Many of you are meeting for the first time; that is by design, and it is where innovation begins.

With that in mind, I want to recognize the leadership of our Program Directors—**Andrew Feig, Richard Wiener, Eileen Spain, and Silvia Ronco**—and the support of our partners **Anne Hultgren and Catrina Bryant** from the Arnold and Mabel Beckman Foundation, and **Shaun Kirkpatrick** from the Frederick Gardner Cottrell Foundation.

What we've built here is a process designed to get you talking—really talking—with one another. The goal is to spark ideas that might not emerge in your own lab or within your usual collaborations but become possible when you start working across disciplines and perspectives. If it works the way it's meant to, this won't feel like a typical meeting, it should feel more dynamic, more open, and ultimately more productive.

Over the next two days, we encourage you to share ambitious ideas, test unproven hypotheses, and engage openly with potential collaborators. This is the time to take intellectual risks and explore possibilities that may not yet have a clear path forward.

We look forward to the ideas and partnerships that will emerge from this meeting—and to the lasting impact they may have on the future of science.

Welcome, and thank you for being part of this effort.

Eric Isaacs

President

Research Corporation for Science Advancement

Scialog: Automating Chemical Laboratories

From the Program Director

Research Corporation's highly interactive Scialog meetings have the goal of catalyzing new collaborations based on blue-sky ideas among Scialog Fellows who constitute a highly select group of exemplary early-career scientists from the U.S. and Canada. The emphasis is on dialogue, networking, and building new collaborations to pursue novel, high-risk discovery research.



Research Corporation, the Arnold and Mabel Beckman Foundation, and the Frederick Gardner Cottrell Foundation chose to focus on Automating Chemical Laboratories because we believe we are on the cusp of a revolution in how science gets done. This will change every aspect of the chemical experimental workflow if successful, from what molecules are made to how they are synthesized, purified, and analyzed. These technologies also have the ability to democratize science by making discovery open to those with interesting ideas and not just the laboratories with the most expensive cutting-edge instrumentation. We believe these breakthroughs can be accelerated by bringing together chemists, physicists, engineers, computer scientists, and roboticists to work together collaboratively on novel, high-risk projects.

We have an outstanding keynote speaker, **Christopher Welch** (Indiana Consortium for Analytical Sciences and Engineering), to set the stage for breakout discussions. We also have a terrific group of senior scientists to round out the team of Facilitators:

Rajeev Surendran Assary (Argonne National Laboratory)

Lane Baker (Texas A&M University)

Malika Jeffries-EL (Boston University)

Anne LaPointe (Cornell University)

Philip LeDuc (Carnegie Mellon University)

Karl Mueller (Ames National Laboratory)

Nikki Pohl (Indiana University, Bloomington)

Sarah Reisman (California Institute of Technology)

Scialog meetings focus on dialogue and team building with the goal of creating novel strategies and collaborative approaches. An important feature is the opportunity for Scialog Fellows to form teams and write proposals to pursue particularly creative ideas that emerge through the discussions. We hope this competition is exciting, but regardless of which proposals are funded, the primary purpose is to catalyze a deeper and more meaningful exchange of ideas than ordinarily occurs at scientific conferences. Our intent is for this process to help participants gain new insights and connections that significantly advance fundamental science to enable major advances in automated laboratory technologies.

We hope each participant finds the Scialog experience of great value. Please do not hesitate to provide feedback on how to make the conference better. My fellow Program Directors, **Richard Wiener**, **Silvia Ronco**, and **Eileen Spain**, the RCSA staff, and I are here to help make the meeting a great experience!

Andrew Feig

Senior Program Director

Research Corporation for Science Advancement

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Conference Agenda

April 16 – 19, 2026

Thursday, April 16

2:00 pm	Registration Opens	Sonoran Foyer
2:00 – 5:00 pm	Snacks & Informal Discussions	Sonoran Foyer
5:00 – 6:30 pm	Poster Session and Reception	Javelina/Sonoran Terrace
6:00 – 6:30 pm	Meeting for Discussion Facilitators	Sonoran Ballroom
6:30 – 7:30 pm	Dinner	Sonoran Rooftop Patio
7:30 – 8:30 pm	Welcoming Remarks Eric Isaacs, President, RCSA Anne Hultgren, Director, Arnold & Mabel Beckman Foundation Conference Overview Andrew Feig, Senior Program Director, RCSA Introductions	Sonoran Ballroom
8:30 – 11:00 pm	Starlight Cafe	Sonoran Rooftop Patio

Friday, April 17

7:00 – 8:00 am	Breakfast	Sonoran Rooftop Patio
8:00 – 8:45 am	Keynote Presentation <i>Advancing the Automation of Chemical Laboratories through Industry-Academia Research Collaborations</i> Christopher Welch, Indiana Consortium for Science and Engineering (ICASE)	Sonoran Ballroom
8:45 – 9:00 am	Orientation to New PRISM System	Sonoran Ballroom
9:00 – 10:15 am	Breakout Session Overview and Instructions Breakout Session I	Wayne or Vigas Patio, Mesa, Canyon, Desert, Sonoran Ballroom
10:15 – 10:35 am	Report Out	Sonoran Ballroom
10:35 – 11:15 am	Conference Photo and Morning Break	Stairs Near the Main Pool
11:15 – 11:45 am	Mini Breakout Session I (Fellows)	All Spaces
	Facilitator Meeting	Sonoran Ballroom
11:45 – 1:00 pm	Lunch	Sonoran Rooftop Patio
1:00 – 2:15 pm	Breakout Session II	Wayne or Vigas Patio, Mesa, Canyon, Desert, Sonoran Ballroom
2:15 – 2:35 pm	Report Out	Sonoran Ballroom
2:35 – 3:05 pm	Mini Breakout Session II (Fellows)	All spaces
3:05 – 5:15 pm	Afternoon Break, Informal Discussions and Leisure Time	Sonoran Foyer
5:15 – 6:30 pm	Poster Session and Reception	Javelina/Sonoran Terrace
6:30 – 7:30 pm	Dinner	Sonoran Rooftop Patio
7:30 – 8:30 pm	2025 Team Award Presentations	Sonoran Ballroom
8:30 – 11:00 pm	Starlight Café	Sonoran Rooftop Patio

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Conference Agenda

April 16 – 19, 2026

Saturday, April 18

7:00 – 8:00 am	Breakfast	Sonoran Rooftop Patio
8:00 – 8:45 am	2025 Team Award Presentations	Sonoran Ballroom
8:45 – 9:15 am	Project Gemini Opportunities Karl Mueller, Rajeev Ansary and Eric Isaacs	Sonoran Ballroom
9:15 – 9:45 am	Mini Breakout Session III (Fellows)	All Spaces
9:45 – 10:00 am	Morning Break	Sonoran Foyer
10:00 – 11:15 am	Breakout Session III	Wayne or Vigas Patio, Mesa, Canyon, Desert, Sonoran Ballroom
11:15 – 11:35 am	Report Out	Sonoran Ballroom
11:35 – 12:05 am	Mini Breakout Session IV (Fellows)	All Spaces
	Facilitator and Funding Partners Discussion	Sonoran Ballroom
12:05 – 1:15 pm	Lunch	Sonoran Rooftop Patio
1:15 – 5:45 pm	Team Formation, Informal Discussions and Proposal Writing	Santa Catalina Ballroom & Terrace
5:45 – 6:30 pm	Reception	Santa Catalina Ballroom & Terrace
6:30 – 7:30 pm	Dinner	Gold Room & Gold Terrace
7:30 – 11:00 pm	Starlight Cafe	Santa Catalina Ballroom & Terrace

Sunday, April 19

6:30 – 7:30 am	Breakfast	Sonoran Rooftop Patio
7:30 – 11:00 am	Presentation of Proposals	Sonoran Ballroom
	Assessment Survey and Wrap-up	
10:00 – 12:00 pm	Lunch (available to go)	Sonoran Foyer

Scialog: Automating Chemical Laboratories

Keynote Presentation

Advancing the Automation of Chemical Laboratories through Industry-Academia Research Collaborations

Christopher J. Welch

Indiana Consortium for Science and Engineering (ICASE)



Abstract:

In this presentation we will highlight the importance of industry-academia research collaborations in developing new research technologies for automating chemical laboratories. Case studies from projects carried out over two decades at Merck Research Laboratories will be complemented with lessons learned from recent projects carried out at the NSF Center for Bioanalytic Metrology, an industry-university cooperative research center involving Notre Dame, Purdue, Indiana University and Abbvie, Agilent, Bristol Myers Squibb, Corteva Agriscience, Evonik, Exxon Mobil, Genentech, Eli Lilly, Merck, Pfizer, Procter & Gamble, SciEx and Takeda.

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2024 Team Awards

James Grinias, Chemistry & Biochemistry, Rowan University

Connor Coley, Chemical Engineering & Electrical Engineering and Computer Science, Massachusetts Institute of Technology

Jessica Sampson, Chemistry and Biochemistry, University of Delaware

Calibration-Free Quantitation of Reaction Yields in High-Throughput Reaction Screening through Absolute Carbon Quantification by LC-FID

Michael McGuirk, Chemistry, Colorado School of Mines

Andrea Pickel, Mechanical Engineering, University of Rochester

Getting on the Grid: Parallel Nano-Crystallography for Large-Scale Data Generation

Grant Rotskoff, Chemistry, Stanford University

Aditi Krishnapriyan, Chemical Engineering / Computer Science, University of California, Berkeley

Andrew Zahrt, Chemistry, University of Pennsylvania

Automated Workflows to Assess Physical Constraints in Neural Networks for Molecular Property Prediction

Martin Seifrid, Materials Science and Engineering, North Carolina State University

Cory Simon, Chemical Engineering, Oregon State University

Connor Bischak, Chemistry, University of Utah

Reducing the Cost of Device Development with Closed-Loop Proxy Measurements and Supplemental Characterization

Jolene Reid, Chemistry, University of British Columbia

Yu Gan, Biomedical Engineering, Stevens Institute of Technology

Closed-Loop Hypothesis Generation for Automated Chemical Synthesis

Daniel Schwalbe-Koda, Materials Science and Engineering, University of California, Los Angeles

Gabe Gomes, Chemistry / Chemical Engineering, Carnegie Mellon University

Jeffrey Lopez, Chemical and Biological Engineering, Northwestern University

Structure Identification in Complex Chemical Mixtures Using Boltzmann Spectroscopy

Laura Ackerman-Biegasiewicz, Chemistry, Emory University

Gabe Gomes, Chemistry / Chemical Engineering, Carnegie Mellon University

A Data-Driven Approach for Derisking Chemical Synthesis

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2025 Team Awards

Daniel Schwalbe-Koda, Materials Science and Engineering, University of California, Los Angeles

Shijing Sun, Mechanical Engineering, University of Washington

Achieving the Theoretical Limits of Information Gains in Automated Experimentation under Hardware Restrictions

Zakaria Al Balushi, Materials Science and Engineering, University of California, Berkeley

Pieremanuele Canepa, Electrical and Computer Engineering, University of Houston

Shijing Sun, Mechanical Engineering, University of Washington

Autonomous Discovery of Single-phase High-Entropy Transition Metal Chalcogenides

Michael McGuirk, Chemistry, Colorado School of Mines

Andrew Zahrt, Chemistry, University of Pennsylvania

CrySolv: A Predictive Program for Solvent-Mediated Molecular Crystallization

Cailin Buchanan, Materials Science Division, Argonne National Laboratory

Daniel Tabor, Chemistry, Texas A&M University

Temporally Adaptive Design of Organic Flow Battery Systems

James Grinias, Chemistry & Biochemistry, Rowan University

Long Luo, Chemistry, University of Utah

Glen O'Neil, Chemistry & Biochemistry, Montclair State University

An Open-Source Modular Automated Laboratory System for Real-Time Monitoring of Continuous Electrosynthesis

Cailin Buchanan, Materials Science Division, Argonne National Laboratory

Badri Narayanan, Mechanical Engineering, University of Louisville

Johanna Schwartz, Materials Science Division/Physical Life Sciences, Lawrence Livermore National Laboratory

Automated Design of Next-Generation Anion Exchange Membranes for Fuel Cells and Beyond

Mark Hendricks, Chemistry, Whitman College

Jessica Sampson, Chemistry and Biochemistry, University of Delaware

Martin Seifrid, Materials Science and Engineering, North Carolina State University

CRISIS: Comprehensive Reproducibility Initiative for Scientific Integrity and Standardization

Scialog: Automating Chemical Laboratories

2026 Proposal Guidelines

1. Awards are intended to provide seed funding for teams of two to three Scialog Fellows formed at this conference for high-risk, high-impact projects.
2. The application package should be submitted as a single PDF file. Pages one and two should describe the project and role of each team member. A third page may be used for references. No budget is necessary.
3. Awards will be in the amount of \$66K direct funding per team member, plus a small percentage for overhead. Grant duration will be one year.
4. No Scialog Fellow can be a member of more than two teams. If a Scialog Fellow is a member of two teams, other members of the teams must be different. No team can submit more than one proposal.
5. No Scialog Fellow who previously has won a Scialog: AUT Collaborative Award can be a member of more than one team. The other team members must be different from the members of the previously awarded team.
6. Scialog Fellows who have previously won two Scialog: AUT Collaborative Awards are not eligible to be funded members of a team, but they can participate as a non-funded team member.
7. Teams cannot include members who have previously collaborated with one another. If you are unsure of your status (e.g., prospective team members were part of a large collaboration but did not significantly interact), please check for clarification with an RCSA Program Director.
8. Teams are encouraged (but not required) to:
 - a. Include members with different research approaches and methods.
 - b. Include members from different disciplines.
9. Proposals must be submitted electronically by **6:00 a.m. PST Sunday, April 19, 2026**. Instructions for submission will be provided at the meeting.
10. Awards are anticipated to start **July 1, 2026**.

Scialog: Automating Chemical Laboratories

Scialog Fellows

Laura Ackerman-Biegasiewicz laura.ackerman@emory.edu

Chemistry, Emory University

Our lab is interested in the design and development of sustainable catalysts using informed high-throughput screening. We collect data on catalysts that are generalizable to many methods such as ligation, coordination, and stability trends via spectral databases.

Jason Adams Ja116@rice.edu

Chemical and Biomolecular Engineering, Rice University

Interested in high-throughput methods to determine fundamental and mechanistic descriptors for thermal and electrochemical catalysis.

Amirali Aghazadeh amiralia@gatech.edu

Electrical and Computer Engineering, Georgia Institute of Technology

My research transforms chemical discovery from trial-and-error into autonomous, AI-driven science. We build agentic AI to interpret data, generate hypotheses, and design combinatorial libraries, enabling cloud-robotic tele-experimentation that accelerates discovery.

Mahshid Ahmadi mahmadi3@utk.edu

Materials Science and Engineering; Chemistry, University of Tennessee, Knoxville

My research focuses on ML guided automated synthesis and characterization of halide perovskites and related materials, recently expanded with large language models (LLMs) for hypothesis generation and experimental planning toward fully autonomous materials discovery and design.

Halleh Balch balch@stanford.edu

Oceans and Electrical Engineering, Stanford University

We develop optical methods for next-generation spectroscopic and imaging sensors with a focus on applications in oceanography and water sustainability. Towards this, we work to integrate these platforms in situ with robotic chemical processing on autonomous underwater vehicles.

Oceane Bel obel@pnnl.gov

Physical and Computational Sciences Directorate, Pacific Northwest National Laboratory

I worked on performance enhancement projects focusing on data movement and placement on scientific networks and systems. My research interests include network simulation, performance enhancement of networks and systems, and Artificial Intelligence (AI).

Connor Bischak connor.bischak@utah.edu

Chemistry, University of Utah

I develop robotic platforms to accelerate discovery in organic and hybrid semiconductors, enabling high-throughput synthesis, characterization, and data-driven insights that reveal structure–property relationships and guide the design of functional materials.

Cailin Buchanan cbuchanan@anl.gov

Materials Science Division, Argonne National Laboratory

Interested in developing autonomous electrochemistry platforms to accelerate discovery of cost-effective, low-environmental impact materials for a range of electrochemistry applications, including energy storage, e.g., aqueous batteries, and critical materials extraction.

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Scialog Fellows Continued

Justin Bui justinbui@nyu.edu

NYU Tandon - Department of Chemical and Biomolecular Engineering, New York University

My group develops electrochemical reactors to decarbonize chemical synthesis, coupling reaction engineering with multi-physics modeling, machine learning, and electroanalytical methods to discover and optimize new, industrially relevant electrochemical reactions.

Stacy Copp stacy.copp@uci.edu

Materials Science and Engineering, University of California, Irvine

High-throughput experimental screening and machine learning-guided design of DNA nanomaterials e.g. fluorescent silver nanoclusters; interpretable machine learning models; near-infrared emitters for deep tissue imaging; molecular nanomaterials.

Emily Davidson edavidson@princeton.edu

Chemical Engineering, Princeton University

I am interested in controlling material structure from the molecular scale (for example, through sequence-defined polymers) through macroscopic scales (by controlling material microstructure through 3D printing). Both efforts are aided by automation!

Luis De Jesús Báez ldjesus@buffalo.edu

Chemistry, University at Buffalo SUNY

Our research focuses on evaluating different synthetic methods for materials discovery with a focus on catalysis and energy storage.

Sijia Dong s.dong@northeastern.edu

Chemistry and Chemical Biology, Northeastern University

We combine first principles simulations and data-driven methods to study and design proteins and synthetic polymers to control chemistry, especially under external stimuli. We develop computational methods for both classical and quantum computers to accelerate chemical discovery.

Victor García-López vglopez@lsu.edu

Chemistry, Louisiana State University

We design and synthesize stimuli-responsive organic molecules that modulate cell membrane structure and function. Our work targets the development of new antimicrobials and molecular components for biomimetic memristors and memcapacitors aimed at mimicking neuron synapses.

Mengyang Gu mengyang@pstat.ucsb.edu

Statistics and Applied Probability, University of California, Santa Barbara

Develop efficient surrogate models to predict expensive experiments with quantified uncertainty, and build generally applicable AI agents for design optimization to reduce experimental costs and time in physics, chemistry, materials science, and engineering.

Mark Hendricks hendrimp@whitman.edu

Chemistry, Whitman College

I am a synthetic chemist focused on the pathways through which nanocrystals form; we're interested in both semiconducting and metallic nanocrystals. My lab uses automated liquid-handling robots to synthesize nanocrystals, and have developed an autonomous system as well.

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Scialog Fellows Continued

Olexandr Isayev olexandr@olexandrisayev.com

Chemistry, Carnegie Mellon University

My research has been focused on ML and QM, paving the way for developing atomistic molecular ML potentials that approximate the solution of the Schrodinger equation. We also develop generative AI methods and autonomous experiments that solve a so-called inverse design problem.

Vida Jamali vjamali3@gatech.edu

Chemical and Biomolecular Engineering, Georgia Institute of Technology

My research lies at the intersection of nanoscience, in situ microscopy, and AI. We build feedback-controlled, cloud-connected experimentation platforms that transform characterization tools into autonomous engines for chemical and materials discovery.

Metin Karayilan metin.karayilan@case.edu

Chemistry, Case Western Reserve University

My research lab designs responsive, degradable, and multifunctional polymers using automated synthesis and controlled radical polymerization. My work targets biomaterials, sustainability, and structure–property discovery, leveraging robotics and AI to accelerate innovation.

Haegyum Kim haegyumkim@lbl.gov

Materials Sciences Division, Lawrence Berkeley National Laboratory

Materials design for energy storage and conversion materials; In situ and operando multi-modal structure characterization; Materials synthesis of diverse compounds; AI-driven autonomous laboratory for accelerated materials discovery.

Sten Lambeets sten.lambeets@pnnl.gov

Physics and Computers Sciences Directorate, Pacific Northwest National Laboratory

I am a domain scientist interest in material sciences, nuclear energy and catalysis. I am interested how to build AI agent networks to conduct scientific research autonomously using variety of specialized AI agents.

Zhou Lin zhoulin@umass.edu

Chemistry, University of Massachusetts Amherst

Computational modeling of chemical reactions and material properties in complex systems with significance in energy and environment, using a combination of quantum mechanics, statistical mechanics, and artificial intelligence.

Chong Liu chongliu@chem.ucla.edu

Chemistry and Biochemistry, University of California, Los Angeles

One research interest of the Liu group at UCLA Chemistry & Biochemistry is developing machine-learning models for electrochemistry and establishing autonomous experimentation platforms for electrochemistry.

Mingjie Liu mingjieliu@ufl.edu

Chemistry, University of Florida

AI tools development for AUT. Generative AI for molecules and materials design. Bayesian Optimization for reaction design. Deep learning models for structure-property relationships prediction.

Scialog: Automating Chemical Laboratories

Scialog Fellows Continued

Jeffrey Lopez jlopez@northwestern.edu

Chemical and Biological Engineering, Northwestern University

In the Lopez Research Group, we work to identify and understand molecular phenomena that can be utilized to design and develop materials to meet these demands and enable the global transition to clean energy.

Long Luo long.luo@utah.edu

Chemistry, University of Utah

Controlling chemical reactions by space and time.

Marilyn Mackiewicz marilyn.mackiewicz@oregonstate.edu

Chemistry, Oregon State University

Automating chemistry using continuous flow chemistry.

Mike McGuirk cmmcguirk@mines.edu

Chemistry, Colorado School of Mines

My work addresses fundamental scientific challenges related to organic and hybrid materials, supramolecular assembly, and environmental sustainability, leveraging expertise in noncovalent interactions, structural order, and chemical reactivity.

Arun Moorthy arunmoorthy@trentu.ca

Forensic Science, Trent University

I am interested in developing novel algorithms and models to support the interpretation of analytical measurements. My primary application area is mass spectral analysis of seized drugs and other forensically relevant materials.

Melody Morris melodymorris@umass.edu

Polymer Science & Engineering, University of Massachusetts Amherst

The Morris group uses automation on both synthetic and biobased polymer systems, specializing in harnessing chemical methods to enable proxy screening techniques. We aim to connect these accessible low fidelity measurements to costly high fidelity findings to accelerate science.

Jin Qian jqian2@lbl.gov

Chemical Sciences Division, Lawrence Berkeley National Laboratory

My research develops digital twins for chemical systems by combining real-space DFT with automation. This enables large-scale, data-driven simulations to interface with robotic labs, accelerating discovery through predictive modeling and experiment–theory integration.

Trevor David Rhone rhonet@rpi.edu

Physics, Rensselaer Polytechnic Institute

AI guided materials discovery with a focus on two-dimensional materials and their magnetic and topological properties.

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Scialog Fellows Continued

Nicholas Riley nmriley@uw.edu

Chemistry, University of Washington

My research group uses mass spectrometry and chemical biology to study protein glycosylation and its role in numerous aspects of cell surface biology. We seek to automate sample preparation (e.g., enzymatic treatments, enrichments) and glycoengineering efforts in our lab.

Jessica Sampson jrsampso@udel.edu

Chemistry and Biochemistry, University of Delaware

I am interested in the applications and improvement of high throughput experimentation for small molecule synthesis.

Carly Schissel ckschissel@psu.edu

Chemistry, Pennsylvania State University

The Schissel Lab focuses on the discovery, design, and synthesis of bioactive peptides with unusual amino acids and structures. We aim to create novel molecules with therapeutic potential, leveraging chemical synthesis, molecular biology, and computational tools.

Daniel Schwalbe-Koda dskoda@ucla.edu

Materials Science and Engineering, University of California, Los Angeles

We seeks to accelerate materials theory by integrating high-performance computing, machine learning (ML), literature data, and atomistic simulations, with a specific focus on understanding the synthesis of energy materials from a computational setting.

Johanna Schwartz schwartz28@llnl.gov

Materials Science Division/Physical Life Sciences, Lawrence Livermore National Laboratory

Expanding the chemistries accessible to additive manufacturing methods. Inventing new AM methods to access novel materials. Using AM as a tool for autonomous, automated materials discovery, characterization, and accelerated optimization.

Cory Simon cory.simon@oregonstate.edu

Chemical Engineering, Oregon State University

Bayesian optimization for the adaptive design of experiments to efficiently discover and synthesize molecules and materials.

Nathan Szymanski nszymanski@seas.ucla.edu

Materials Science and Engineering, University of California, Los Angeles

Modeling solid-state phase transformations and synthesis kinetics, coupled with automated in-situ X-ray diffraction, to accelerate the development of inorganic materials for energy technologies.

Daniel Tabor daniel_tabor@tamu.edu

Chemistry, Texas A&M University

My group works on machine learning methods development and applications for organic materials design, spectroscopy, and new reaction discovery.

Scialog: Automating Chemical Laboratories

Scialog Fellows Continued

Allison Walker allison.s.walker@vanderbilt.edu

Chemistry, Vanderbilt University

My research focuses on the development of AI and other computational methods for natural product discovery and biosynthesis. We are interested in automating data collection and model validation using chemical lab automation techniques.

Yinan Wang wangy88@rpi.edu

Industrial and Systems Engineering, Rensselaer Polytechnic Institute

Engineering-driven machine learning and optimization for designing, monitoring, and controlling complex physical systems.

Jie Xu xuj@anl.gov

Nanoscience and Technology Division, Argonne National Laboratory

I develop advanced functional polymers using high-throughput experimentation, AI/ML-guided design, and robotic labs. I lead Polybot at DOE, advancing sustainable, high-performance materials for electronics, thermal management, and green polymers.

Yan Zeng yan.zeng.helen@gmail.com

Chemistry and Biochemistry, Florida State University

Discovering and exploring synthesis science of solid-state materials, developing self-driving autonomous laboratories integrating automation, AI/ML, and thermochemical theories, and designing chemical processes to convert minerals to advanced materials.

Zach Zheng z.z@wustl.edu

Chemistry, Washington University in St. Louis

I use large language model agents and high-throughput experiments to design and synthesize metal-organic frameworks and other porous crystals. We aim to create new materials for gas separations, pollutant removal, materials recovery, and nutrition delivery applications.

Qilei Zhu q.zhu@utah.edu

Chemistry, University of Utah

My research focuses on developing sustainable strategies for organic synthesis using electrochemistry and photocatalysis, combining mechanistic insight, catalysis design, and reactive intermediate control to enable greener chemical transformations.

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Discussion Facilitators

Rajeev Assary assary@anl.gov

Materials Science Division, Argonne National Laboratory

Energy Storage. Computational Materials Chemistry. Computational Catalysis and Electrochemistry. Artificial Intelligence for Materials Chemistry.

Lane Baker lane.baker@tamu.edu

Chemistry, Texas A&M University

High throughput electrochemistry, general analytical chemistry, data science, machine learning.

Malika Jeffries-EL malikaj@bu.edu

Chemistry, Boston University

Expediting the design and synthesis of organic semiconductors using automation and machine learning.

Anne LaPointe lapointe@cornell.edu

Chemistry and Chemical Biology, Cornell University

Catalysis, green chemistry, polymers, high throughput experimentation.

Philip LeDuc prl@andrew.cmu.edu

Mechanical Engineering, Biological Sciences, Computational Biology, Biomedical Engineering, Electrical and Computer Engineering, Carnegie Mellon University

Philip LeDuc is the William J. Brown Professor works at the intersection of mechanical engineering and biology by envisioning cells and molecules as systems that can be investigated with some of the same fundamental approaches used on machines such as planes and automobiles.

Karl Mueller drktmueller@gmail.com

Ames National Laboratory

I am currently interested in automation and autonomy in chemical and materials sciences; energy storage research; new spectroscopic and imaging modalities; and data sciences coupled with AI for scientific discovery.

Nikki Pohl npohl@indiana.edu

Chemistry, Indiana University Bloomington

My lab develops open-source methods for automated synthesis of oligosaccharides/glycopeptides and designs tools to study the roles of carbohydrates in plant, microbial, human biology. We have also created low-cost teaching lab experiments with Python and automated flow synthesis.

Sarah Reisman reisman@caltech.edu

Chemistry & Chemical Engineering, California Institute of Technology

My research is focused on natural product synthesis and the discovery of new reactions. We are interested in using emerging methods in data science and machine learning to change how we approach chemical synthesis.

Chris Welch chris.welch@icase.center

ICASE, Indiana Consortium for Analytical Science and Engineering

Stereochemistry, chromatography, high throughput experimentation, pharmaceuticals, analytical chemistry.

Scialog: Automating Chemical Laboratories

Guests

Danny Abrams dmabrams@northwestern.edu

Engineering Sciences & Applied Mathematics, Northwestern University

My interests relevant to this Scialog are focused on how new scientific collaborations are established, and in particular the role conferences may play in that process.

Anne Hultgren ahultgren@beckman-foundation.org

Arnold and Mabel Beckman Foundation

Support for chemistry and life sciences, especially the invention of new methods, materials, and instruments.

Devora Najjar najjar@sloan.org

Technology and NYC Programs, Alfred P. Sloan Foundation

I am interested in the metascientific implications of automation and AI and generally supporting tools and networks focused on open scientific software and hardware.

Scialog: Automating Chemical Laboratories

Arnold and Mabel Beckman Foundation

Anne Hultgren ahultgren@beckman-foundation.org
Executive Director and CEO

Catrina Bryant cbryant@beckman-foundation.org
Deputy Director

Frederick Gardner Cottrell Foundation of Research Corporation Technologies, Inc.

Shaun Kirkpatrick skirkpatrick@rctech.com
President

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