Automating Chemical Laboratories

The Second Annual Scialog Conference
April 3 – 6, 2025

scialog2025®

ARNOLD & MABEL BECKMAN FOUNDATION

RESEARCH CORPORATION *for* SCIENCE ADVANCEMENT

THE FREDERICK GARDNER COTTRELL FOUNDATION

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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

From the President

Welcome to the 2025 ***Scialog: Automating Chemical Laboratories*** meeting, cosponsored by Research Corporation, the Arnold and Mabel Beckman Foundation, and the Frederick Gardner Cottrell Foundation. This is the second of three Scialog meetings on this theme.

The goal of this Scialog is to catalyze multidisciplinary collaboration on fundamental science projects that use artificial intelligence, machine learning, laboratory robotics, high-throughput synthesis, and automated analytical workflows to drive discovery and – even more boldly – to transform the way chemical laboratories operate.

Scialog's overarching purpose is to advance cutting-edge science of great significance to humanity by catalyzing innovative, basic research. Our focus is on scientists in the early years of their independent careers. Through the unique Scialog process, we seek to lay the foundation for an ongoing, highly creative, cross-disciplinary community of scientists that will prove adept at identifying exciting areas for research advances for decades to come.

To that end, under the guidance of Program Directors **Andrew Feig, Richard Wiener, Eileen Spain** and **Silvia Ronco** (Research Corporation), and with assistance from our initiative partners **Anne Hultgren and Catrina Bryant** (Beckman Foundation) and **Shaun Kirkpatrick** (Frederick Gardner Cottrell Foundation), we hope you will be engaged in passionate discussions with colleagues, many of whom you will meet for the first time at Scialog. The process is designed to stimulate new ideas that you might not be able to pursue on your own but become possible to try out in collaborative teams. The result, we expect, will be a meeting unlike others that you attend. We are confident that you will find the next two days to be extremely worthwhile.

This is your opportunity to air that wild idea you have been reluctant to share with others, or to discuss a nagging hunch that does not yet have sufficient supporting data, or to take a leap on a high-impact/high-risk project instead of concentrating all your effort on incremental studies. This is the time to come up with, and be open to, completely new ideas that may truly change the world and to find new colleagues and collaborators with whom to pursue them.

We hope this second meeting on this topic yields a crop of outstanding team proposals, which will make our job of determining who receives funding very challenging. For all Fellows, whether or not you develop a funded project, we are sure that this Scialog network will provide long-term benefits. I wish you every success in exploring new and compelling ideas over the next two days.

Have a terrific meeting!

Daniel Linzer
President
Research Corporation for Science Advancement

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, **Nikki Pohl** (Indiana University, Bloomington), 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 (Pacific Northwest National Laboratory)
Nancy Washton (Pacific Northwest National Laboratory)
Christopher Welch (Indiana Consortium for Analytical Sciences and Engineering)

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

Conference Agenda
April 3 – 6, 2025

Thursday, April 3

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** Dan Linzer, 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 4

7:00 – 8:00 am	**Breakfast**	Sonoran Rooftop Patio
8:00 – 8:45 am	**Keynote Presentation** *Toward Human-Centered Lab Automation* Nikki Pohl, Indiana University, Bloomington	Sonoran Ballroom
8:45 – 9:00 am	**Breakout Session Overview and Instructions**	Sonoran Ballroom
9:00 – 10:15 am	**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) **Facilitator Meeting**	All Spaces 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	**2024 Team Award Presentations**	Sonoran Ballroom
8:30 – 11:00 pm	**Starlight Café**	Sonoran Rooftop Patio

Conference Agenda
April 3 – 6, 2025

Saturday, April 5

6:45 – 7:30 am	**Optional Guided Nature Walk**	Meet on Vigas Patio
7:00 – 8:00 am	**Breakfast**	Sonoran Rooftop Patio
8:00 – 8:45 am	**2024 Team Award Presentations**	Sonoran Ballroom
8:45 – 9:15 am	**Mini Breakout Session III** (Fellows)	All Spaces
9:15 – 9:45 am	**Morning Break**	Sonoran Foyer
9:45 – 11:00 am	**Breakout Session III**	Wayne or Vigas Patio, Mesa, Canyon, Desert, Sonoran Ballroom
11:00 – 11:20 am	**Report Out**	Sonoran Ballroom
11:20 – 11:50 am	**Mini Breakout Session IV** (Fellows) **Facilitator and Funding Partners Discussion**	All Spaces Sonoran Ballroom
11:50 – 1:00 pm	**Lunch**	Sonoran Rooftop Patio
1:00 – 5:45 pm	**Team Formation, Informal Discussions and Proposal Writing**	All Spaces
5:45 – 6:30 pm	**Reception**	Sonoran Terrace
6:30 – 7:30 pm	**Dinner**	Sonoran Rooftop Patio
7:30 – 11:00 pm	**Starlight Cafe**	Sonoran Rooftop Patio

Sunday, April 6

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

Keynote Presentation

Toward Human-Centered Lab Automation

Nikki Pohl
Indiana University, Bloomington

Abstract:
Lab automation, and now artificial intelligence-based methods, promise to improve the productivity of scientists. However, the adoption rate for these technologies is still very low. Based on two decades of training and research related to solving the automated glycan synthesis problem, this talk will argue that a greater focus on people is needed in developing these technologies for broad impact. A training framework for designing experiments called SMART (Society, Machines, Analysis, Reproducibility, Trust) will also be introduced.

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

2025 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 $60K 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 6, 2025**. Instructions for submission will be provided at the meeting.

10. Awards are anticipated to start **July 1, 2025**.

Scialog Fellows

Mahshid Ahmadi mahmadi3@utk.edu
Materials Science and Engineering, Chemistry, University of Tennessee, Knoxville
My lab focuses on integrating ML to automate synthesis and characterization of optoelectronic materials, while leveraging human expertise for hypothesis making and goal setting. This synergy accelerates materials discovery and optimization, streamlines the path from lab to fab.

Zak Al Balushi albalushi@berkeley.edu
Materials Science and Engineering, University of California, Berkeley
The Al Balushi Research Group synthesizes electronic materials like thin films, 2D materials, and nanostructures via solution and vapor phase techniques. We focus on scalable growth and integration for microelectronics, quantum tech, and novel in situ growth platforms.

Herdeline Ann Ardoña hardona@uci.edu
Chemical and Biomolecular Engineering, University of California, Irvine
Our research group's program is centered on engineering macromolecular biomaterials, molecularly designed to convert and transduce exogenous cues at the cell-material/synthetic matrix interface — offering new avenues for tuning and monitoring electroactive living systems.

Oceane Bel obel@pnnl.gov
Physical and Computational Sciences Directorate, Pacific Northwest National Laboratory
My research revolves around automation and systems. My current work is making tools that isolate communications network attackers reconfiguring the network's topology. I also am interested in using generative AI to automate instrument maintenance.

Connor Bischak connor.bischak@utah.edu
Chemistry, University of Utah
Our group is interested in the fundamental processes that govern the performance of organic electronics using both high throughput synthesis and characterization platforms as well as nanoscale imaging.

Cailin Buchanan cbuchanan@anl.gov
Materials Science Division, Argonne National Laboratory
I am interested in using automated fundamental electrochemistry to accelerate solutions to clean energy challenges such as achieving economical, long duration energy storage (LDES). I also have an interest in technoeconomic and life cycle assessment modeling.

Pieremanuele Canepa pcanepa@central.uh.edu
Electrical and Computer Engineering, University of Houston
We apply computational methods to advance understanding materials properties for energy storage. Our research leverages the synergy between materials science, thermodynamics, electrochemistry, and the power of supercomputers to discover novel materials and molecules.

Luis De Jesús Báez ldjesus@buffalo.edu
Chemistry, University at Buffalo SUNY
We are an all solid-state synthetic lab that navigates the intersection between materials, physical, and inorganic chemistry to furnish a fundamental understanding of the morphology–composition–entropy relationship to tailor properties.

Scialog Fellows Continued

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 macromolecules and materials to control chemistry, especially under external stimuli. We develop computational methods for both classical and quantum computers to accelerate chemical discovery.

Yu Gan ygan5@stevens.edu
Biomedical Engineering, Stevens Institute of Technology
My research interest involves developing AI tools (e.g., computer vision, generative model) for characterizations of tissue and materials. My research includes image analytic tools to automatically identify nano-material morphology, fiber trace, and tissue classification, etc.

Victor García-López vglopez@lsu.edu
Chemistry, Louisiana State University
We synthesize light-activated molecular switches and machines that can control the structure and dynamics of biological membranes. This enables drug delivery, ion transport, and modulation of membrane protein function, providing a powerful tool to influence cellular processes.

Gabe Gomes gabegomes@cmu.edu
Chemistry, Chemical Engineering, Machine Learning, Carnegie Mellon University
Machine learning, computational chemistry, and automation for reaction discovery and optimization. Integration of foundation models into chemical sciences and engineering with agents that can autonomously design, plan, and execute experiments on automated and cloud labs.

Jim Grinias grinias@rowan.edu
Chemistry & Biochemistry, Rowan University
My research interests primarily focus on liquid-phase separations, especially the fundamentals of column and instrument design in liquid chromatography. Our group has also focused on miniaturization, two-dimensional separation techniques, and microfluidic platforms.

Mark Hendricks hendrimp@whitman.edu
Chemistry, Whitman College
Metallic and semiconductor nanocrystal synthesis, automated science, pedagogy of lab automation

Nick Jackson jacksonn@illinois.edu
Chemistry, University of Illinois at Urbana-Champaign
AI-driven theoretical chemistry for soft materials design, closed-loop optimization, generative polymer models, organic semiconductors

Aditi Krishnapriyan aditik1@berkeley.edu
Chemical Engineering; Electrical Engineering and Computer Sciences, University of California, Berkeley
Machine learning methods development for applications in chemistry and physics, including as related to molecular simulation.

Scialog Fellows Continued

Sten Lambeets sten.lambeets@pnnl.gov
Physics and Computers Sciences Directorate, Pacific Northwest National Laboratory
As an expert in atom probe tomography and surface science, I explore how intense electric fields control surface chemistry. Currently, I am integrating the Operando atom probe with AI algorithms to explore and optimize field-assisted chemical reactions autonomously.

Zhou Lin zhoulin@umass.edu
Chemistry, University of Massachusetts Amherst
Development of computational models based on quantum mechanics, chemical informatics, and machine learning to decode and predict electronic structures and optical properties for complex systems, such as molecular clusters, heterogeneous catalysts and optoelectronic devices.

Fang Liu fang.liu@emory.edu
Chemistry, Emory University
My research group aims to tackle the challenges in data-driven design and discovery for chemistry in the solution phase from two aspects: (1) automated and accurate computational data generation and (2) machine learning models for in situ analysis of spectroscopy

Mingjie Liu mingjieliu@ufl.edu
Chemistry, University of Florida
My research group uses data-driven methods to design sustainable materials for energy and environmental applications. We focus on building computational databases, automating workflows, and training ML models to address carbon neutrality, water treatment, and energy storage.

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
Using predictive modeling using AI/machine learning to innovate materials discovery for their translation to clinical applications

Arun Mannodi Kanakkithodi amannodi@purdue.edu
Materials Engineering, Purdue University
I use first principles simulations and machine learning to study the structure and properties of sold-state materials. My primary current projects involve composition-engineering and defect-engineering of semiconductors for solar absorption and photocatalysis.

Scialog Fellows Continued

Mike McGuirk cmmcguirk@mines.edu
Chemistry, Colorado School of Mines
Organic and hybrid materials, supramolecular assembly, and environmental sustainability, leveraging expertise in non-covalent interactions, structural order, and chemical reactivity to develop synthetic tools for the construction and destruction of functional materials

Melody Morris melodymorris@umass.edu
Polymer Science & Engineering, University of Massachusetts Amherst
The Morris group develops low-cost, automated strategies to identify heterologous hybrid protein and cell-containing materials to improve the sustainability, assembly, and physical properties of soft materials, enabling materials design cycle implementation.

Badri Narayanan badri.narayanan@louisville.edu
Mechanical Engineering, University of Louisville
We integrate materials modeling at electronic to mesoscopic scales, data-science, and machine learning to gain fundamental understanding of electrochemical phenomena in materials relevant for energy storage, brain-like computing, and catalysts.

Glen O'Neil oneilg@montclair.edu
Chemistry & Biochemistry, Montclair State University
Automated fabrication of analysis tools using 3D printing; high throughput electrochemistry.

Jin Qian jqian2@lbl.gov
Chemical Sciences Division, Lawrence Berkeley National Laboratory
We develop and apply new theoretical/computational chemistry tools (Digital Twin & Real-space KS-DFT) to tackle complexity challenges in renewable energy systems.

Jolene Reid jreid@chem.ubc.ca
Chemistry, University of British Columbia
Our research develops strategies for efficient, selective chemical reactions to create valuable compounds. Using small organic molecules, we focus on predictable catalyst design. We combine synthesis, computation, and statistical modeling to advance reactions and catalysts.

Trevor David Rhone rhonet@rpi.edu
Physics, Rensselaer Polytechnic Institute
Materials discovery and knowledge discovery accelerated by physics inspired artificial intelligence.

Grant Rotskoff rotskoff@stanford.edu
Chemistry, Stanford University
My current research interests include uncovering design principles for large-scale machine learning models for physical and chemical systems, understanding transfer learning and the role of simulated data, and sampling / optimal data-acquisition.

Scialog Fellows Continued

Jessica Sampson jrsampso@udel.edu
Chemistry and Biochemistry, University of Delaware
I am interested in the application of high throughput experimentation (HTE) to the development and study of reactions for the synthesis of small molecule and organometallic compounds, including through the development of improved data and analytical workflows.

Christopher Sandford christopher.sandford@utsa.edu
Chemistry, University of Texas at San Antonio
Research in the Sandford Lab is focused on methods employing switchable catalysts that can control iterative reaction sequences, and on developing sustainable catalytic methodologies using physical organic and data science tools

Daniel Schwalbe-Koda dskoda@ucla.edu
Materials Science and Engineering, University of California, Los Angeles
We seeks to accelerate materials design 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
As a synthetic organic polymer chemist at LLNL, my research interests are centered in: Polymer chemistry, Automated high throughput screening and characterization, Additive manufacturing, Photopolymerization, Energy production and storage, and Polymer lifetime and sustainability.

Martin Seifrid m_seifrid@ncsu.edu
Materials Science and Engineering, North Carolina State University
My group develops self-driving laboratories – automated experiments guided by machine learning – to design precisely controlled organic mixed ionic-electronic conducting materials with applications in sensing, energy storage, healthcare, and neuromorphic computing.

Cory Simon cory.simon@oregonstate.edu
Chemical Engineering, Oregon State University
I am interested in designing and implementing Bayesian optimization algorithms to constitute data-driven, automated decision-making algorithms for "self-driving" labs.

Shijing Sun shijing@uw.edu
Mechanical Engineering, University of Washington
My research focuses on autonomous labs for clean energy. I develop self-driving modular lab workflows for solar energy conversion and Li-ion storage, using robotics, AI, and human-machine collaboration.

Daniel Tabor daniel_tabor@tamu.edu
Chemistry, Texas A&M University
Our group works in the area of theoretical chemistry. The most relevant areas for this conference are our interests in high-throughput computational molecular design, the development of reinforcement learning methods for chemistry, and the development of new representations.

Scialog Fellows Continued

Allison Walker allison.s.walker@vanderbilt.edu
Chemistry, Vanderbilt University
My lab develops machine learning and other computational tools to aid in natural product and drug discovery and to engineer the biosynthesis of natural products to produce new natural product-like compounds. I am interested in automating data collection and model validation.

Yinan Wang wangy88@rpi.edu
Industrial and Systems Engineering, Rensselaer Polytechnic Institute
My research focuses on engineering-driven machine learning and automation with applications to complex physical systems. The objective is to propose novel interpretable machine learning models by fusing data-driven models and physical models to improve system automation.

Jie Xu xuj@anl.gov
Nanoscience and Technology Division, Argonne National Laboratory
I lead the development of Polybot that combines artificial intelligence with modular robotics, designed as an autonomous discovery platform to accelerate research at Argonne. Her research focuses on polymer-based materials for future electronics and energy applications.

Andrew Zahrt zahrt@sas.upenn.edu
Chemistry, University of Pennsylvania
I am interested in synthetic organic chemistry, automated synthesis, high-throughput experimentation, applied computational chemistry, and machine learning.

Yan Zeng yan.zeng.helen@gmail.com
Chemistry and Biochemistry, Florida State University
The Zeng Lab utilizes robotics and AI to develop advanced energy materials and green chemical processes for critical materials extraction and conversion.

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
Electrochemistry, imaging, mass spectrometry, high throughput measurements

Malika Jeffries-EL malikaj@bu.edu
Chemistry, Boston University
The Jeffries-EL group specializes in synthesizing novel organic semiconductors for optoelectronic applications. They focus on accelerating the discovery of emissive materials for organic light-emitting diodes through machine learning and automated synthesis methods.

Anne LaPointe lapointe@cornell.edu
Chemistry and Chemical Biology, Cornell University
Synthetic and mechanistic inorganic and organometallic chemistry, homogeneous and heterogeneous catalysis, polymer chemistry, sustainable chemistry and high throughput experimentation

Philip LeDuc prl@andrew.cmu.edu
Mechanical Engineering, Biological Sciences, Computational Biology, Biomedical Engineering, Electrical and Computer Engineering, Carnegie Mellon University
I work 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 looking for unifying principles.

Karl Mueller drktmueller@gmail.com
Physical and Computational Sciences, Pacific Northwest 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.

Nancy Washton nancy.washton@pnnl.gov
Computing and Information Technology, Pacific Northwest National Laboratory
Research leader with a Ph.D. in Chemistry specializing in integrating generative AI, advanced LLM Agents, and cloud computing to accelerate discovery. Expertise in developing innovative workflows, deploying scalable AI solutions, and advancing in-silico technologies.

Discussion Facilitators Continued

Chris Welch chris.welch@icase.center
ICASE, Indiana Consortium for Analytical Science and Engineering
Organic Chemistry, Analytical Chemistry, Biochemistry, Stereochemistry, Instrumentation

Guests

Catrina Bryant cbryant@beckman-foundation.org
Arnold and Mabel Beckman Foundation
Automation and AI in laboratories.

Anne Hultgren ahultgren@beckman-foundation.org
Arnold and Mabel Beckman Foundation
The Arnold and Mabel Beckman Foundation provides funding for basic research projects in chemistry and life sciences.

Anastasiya Salova anastasiya.salova@northwestern.edu
Engineering Sciences & Applied Mathematics, Northwestern University
Networks, dynamics, science of science, synchronization, connectomics

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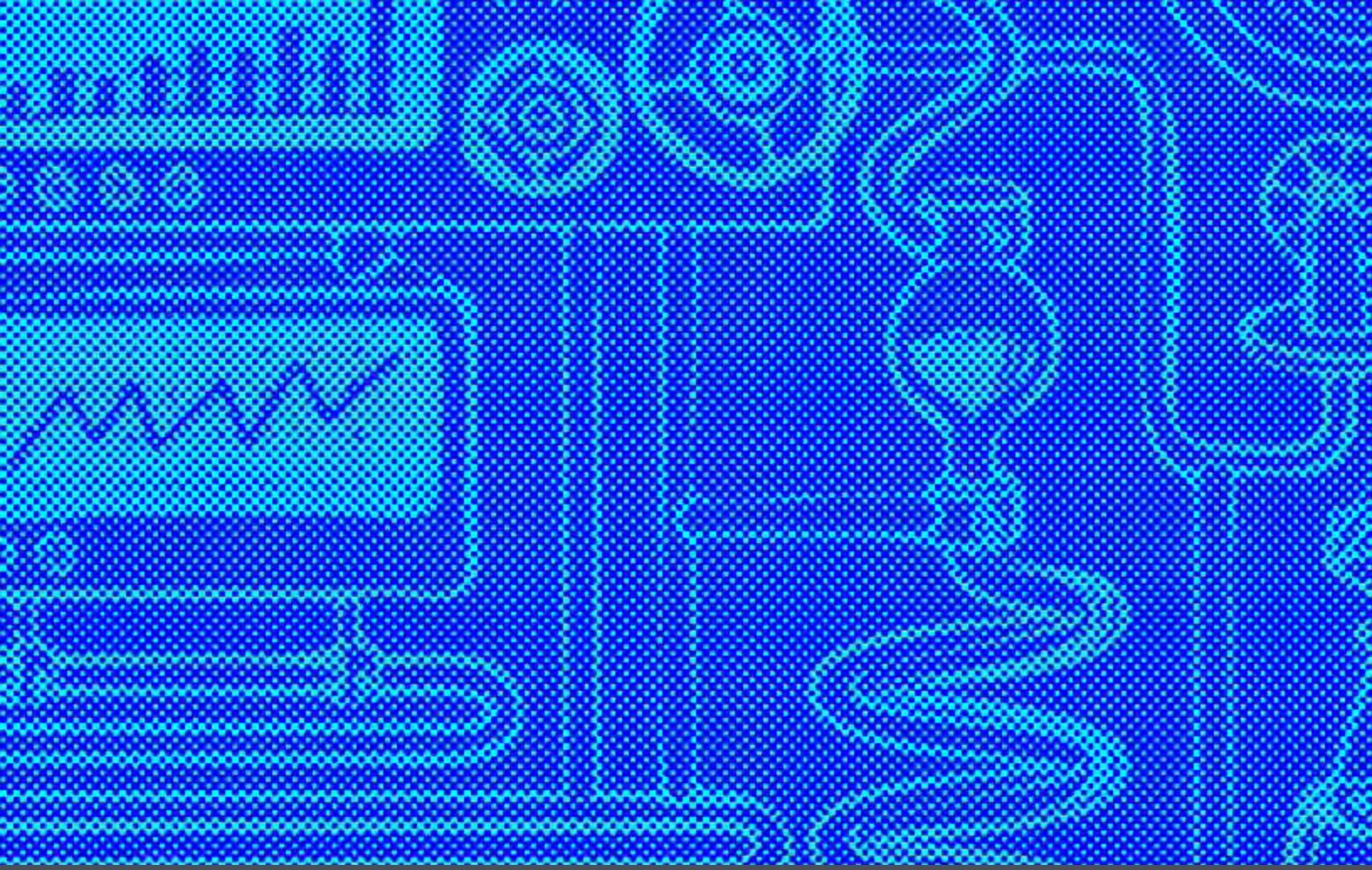
Richard Wiener rwiener@rescorp.org
Senior Program Director



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