# Automating Chemical Laboratories

The First Annual Scialog Conference
April 11-14, 2024

scialog2024®

ARNOLD & MABEL BECKMAN FOUNDATION

WALDER FOUNDATION

RESEARCH CORPORATION *for* SCIENCE ADVANCEMENT

THE FREDERICK GARDNER COTTRELL FOUNDATION

# 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.

## Diversity, Inclusion and No Harassment

Research Corporation for Science Advancement fosters an inclusive 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 2024 ***Scialog: Automating Chemical Laboratories*** meeting, cosponsored by Research Corporation, the Beckman Foundation, and the Frederick Gardner Cottrell Foundation. This is the first 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 first 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 dialog, 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 two outstanding keynote speakers **Sarah Reisman** (Caltech) and **Klavs Jensen** (MIT) to set the stage for breakout discussions. They will be joined by 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)
**Nikki Pohl**, (Indiana University, Bloomington)
**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 dialogue. 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**
Program Director
Research Corporation for Science Advancement

## Conference Agenda

### Thursday, April 11

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|---|---|---|
| 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 | **Welcome**<br>Dan Linzer, President, RCSA<br>Anne Hultgren, Director, Arnold & Mabel Beckman Foundation<br>**Conference Overview, Outcomes and Proposal Guidelines**<br>Andrew Feig, Senior Program Director, RCSA<br>**Introductions/Ice Breakers** | Sonoran Ballroom |
| 8:30 – 11:00 pm | **Starlight Cafe** | Sonoran Rooftop Patio |

### Friday, April 12

| | | |
|---|---|---|
| 7:00 – 8:00 am | **Breakfast** | Sonoran Rooftop Patio |
| 8:00 – 8:45 am | **Keynote Presentation**<br>*Data-Driven Tools for Synthetic Organic Chemistry*<br>Prof. Sarah Reisman, California Institute of Technology | Sonoran Ballroom |
| 8:45 – 9:00 am | **Breakout Session Overview and Instructions** | Sonoran Ballroom |
| 9:00 – 10:15 am | **Breakout Session I** | Wayne, Mesa, Canyon, Desert or Vigas Patio, 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)<br>**Facilitator Meeting** | All Spaces<br>Sonoran Ballroom |
| 11:45 – 1:00 pm | **Lunch** | Sonoran Rooftop Patio |
| 1:00 – 2:15 pm | **Breakout Session II** | Wayne, Mesa, Canyon, Desert or Vigas Patio, 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 – 8:15 pm | **Keynote Presentation**<br>*Accelerating Chemical Discovery and Development with Automation and Machine Learning*<br>Prof. Klavs Jensen, Massachusetts Institute of Technology | Sonoran Ballroom |
| 8:15 – 11:00 pm | **Starlight Cafe** | Sonoran Rooftop Patio |

## Saturday, April 13

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|---|---|---|
| 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 | **Large Group Discussion: Local, Regional, National?**<br>Dr. Anne Lapointe & Dr. Karl Mueller | 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, Mesa, Canyon, Desert or Vigas Patio, Sonoran Ballroom |
| 11:00 – 11:20 am | **Report Out** | Sonoran Ballroom |
| 11:20 – 11:50 am | **Mini Breakout Session IV** (Fellows)<br><br>**Facilitator and Funding Partners Discussion** | All Spaces<br><br>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 14

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

## Keynote Presentations

### Data-Driven Tools for Synthetic Organic Chemistry

**Sarah E. Reisman**
*California Institute of Technology*

**Abstract:**
Research in the Reisman lab centers on the synthesis of complex natural products, with a particular focus on the development of new convergent fragment coupling and annulation strategies. The densely packed arrays of heteroatoms and stereogenic centers present in natural product targets challenge the limits of current technology and inspire the development of new synthetic strategies and tactics. In concert with our total synthesis efforts, we have an active program on the development of new reductive coupling reactions, including Ni-catalyzed asymmetric reactions of C($sp^3$) electrophiles. This presentation will focus on our recent efforts developing data science and machine learning workflows that can help guide synthetic strategy planning and reaction performance optimization.

### Accelerating Chemical Discovery and Development with Automation and Machine Learning

**Klavs Jensen**
*Massachusetts Institute of Technology*

**Abstract**:
I highlight opportunities and challenges for automation and machine learning to advance chemical discovery and development through selected examples from the literature and my own laboratory. Examples include automation considerations for Bayesian optimization of well-defined chemical spaces and autonomous discovery of new molecules guided by machine learning predictions of physical properties and synthesis steps and conditions.

## 2024 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 **6:30 a.m. PST Sunday, April 14, 2024**. Instructions for submission will be provided at the meeting.

10. Awards are anticipated to start around **July 1, 2024**.

## Scialog Fellows

**Milad Abolhasani** abolhasani@ncsu.edu
Chemical & Biomolecular Engineering, North Carolina State University
*My broad research interests lie at the intersection of flow chemistry, microreaction engineering, lab automation, and data science to accelerate materials and molecular discovery and development via self-driving fluidic labs by leveraging process and data intensification.*

**Laura Ackerman-Biegasiewicz** laura.ackerman@emory.edu
Chemistry, Emory University
*Discovery of sustainable chemistry and base metal catalyzed reactions utilizing high-throughput experimentation, diverse analytical techniques, and emerging technology.*

**Zak Al Balushi** albalushi@berkeley.edu
Materials Science and Engineering, University of California, Berkeley
*Our research concerns the creation of novel synthesis, processing and integration schemes for emerging electronic materials, and the development of new in-situ characterization instrumentation that will ultimately aid in the discovery of new materials for device technologies.*

**Oceane Bel** obel@pnnl.gov
PCSD, Pacific Northwest National Laboratory
*My research interests include network simulation, performance enhancement of networks and systems and Artificial Intelligence (AI). In the past 2 years I also started tackling security issues such as modeling attack on networks.*

**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.*

**Pieremanuele Canepa** pcanepa@central.uh.edu
Electrical and Computer Engineering, University of Houston
*Leveraging the synergy of powerful high-performance computers, advanced algorithms, and large data sets generated via modeling, my laboratory (https://caneparesearch.org) draws direct links between the atomistic structure of energy materials and their macroscopic properties.*

**Gaurav Chopra** gchopra@purdue.edu
Chemistry, Computer Science (by courtesy), Purdue University
*We work on molecular artificial intelligence architectures, develop large language models for privacy-preserving closed-loop laboratory automation applied to experimental immunology, mass spectrometry and chemical synthesis to translate therapies for cancer and neurodegeneration.*

**Connor Coley** ccoley@mit.edu
Chemical Engineering & Electrical Engineering and Computer Science, Massachusetts Institute of Technology
*We work on both computational and experimental techniques (with a strong emphasis on the former) to enable autonomous molecular discovery at the intersection of chemistry, data science, machine learning, and laboratory automation with an emphasis on small molecule drug discovery.*

## Scialog Fellows Continued

**Stacy Copp** stacy.copp@uci.edu
Materials Science and Engineering, University of California, Irvine
*I study novel photonic nanomaterials templated by DNA and synthetic polymers. A major research thrust in my lab centers on understanding and designing fluorescent DNA-stabilized silver nanoclusters by using high-throughput experiments together with machine learning approaches.*

**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.*

**Gabe Gomes** gabegomes@cmu.edu
Chemistry and Chemical Engineering, Carnegie Mellon University
*The Gomes group integrates state-of-the-art machine learning into chemical sciences and engineering by developing intelligent agents that autonomously design, plan, and execute experiments on automated labs for reaction discovery and optimization.*

**Jim Grinias** grinias@rowan.edu
Chemistry & Biochemistry, Rowan University
*The Grinias Lab focuses on fundamental research in chemical separations. Specific interests include instrument miniaturization and high-throughput methodology. Application areas of interest include (bio)pharmaceutical characterization and the analysis of biological systems.*

**Mengyang Gu** mengyang@pstat.ucsb.edu
Statistics and Applied Probability, University of California, Santa Barbara
*My research team develops probabilistic models and fast algorithms with uncertainty quantification, to accelerate simulations and automate inverse estimation from experiments, such as innovating microscopy and scattering analysis for characterizing soft and active matter systems.*

**Shuo Han** hanshuo@uic.edu
Electrical and Computer Engineering, University of Illinois Chicago
*I work on the algorithmic foundation of interactive data-driven decision-making, where data are collected online for optimizing a given objective. My current focus in to develop algorithms that can 1) handle large decision spaces; 2) ensure safety; 3) integrate human feedback.*

## Scialog Fellows Continued

**Mark Hendricks** hendrimp@whitman.edu
Chemistry, Whitman College
*The Hendricks Lab is interested in the synthesis of metallic and semiconducting nanocrystals, particularly in the underlying mechanisms through which they form. We are also interested in laboratory automation and how automation is taught in the undergraduate chemistry curriculum.*

**Oles Isayev** olexandr@olexandrisayev.com
Chemistry, Carnegie Mellon University
*Since 2016, my work has pioneered research at the interface between ML and QM. These studies resulted in developing several families of atomistic molecular ML potentials. All methods were implemented in open-source software and have been made freely available via GitHub.*

**Nick Jackson** jacksonn@illinois.edu
Chemistry, University of Illinois at Urbana-Champaign
*Automated modular synthesis, Bayesian Optimization, generative molecular modeling, polymer synthesis*

**Vida Jamali** vjamali3@gatech.edu
Chemical and Biomolecular Engineering, Georgia Institute of Technology
*My research interest lies at the intersection of nanoscience, in situ transmission electron microscopy, and AI. By bringing AI in the loop for microscopy we aim to develop microscopes as experimentation tools for material design.*

**Haegyum Kim** haegyumkim@lbl.gov
Materials Sciences Division, Lawrence Berkeley National Laboratory
*AI-driven autonomous laboratory for accelerated materials discovery.*
*Inorganic materials synthesis and characterization for energy storage application.*
*Fundamental understanding of material synthesis mechanisms to realize "synthesis by design".*

**Aditi Krishnapriyan** aditik1@berkeley.edu
Chemical Engineering; Electrical Engineering and Computer Sciences, University of California, Berkeley
*My research interests include physics-inspired machine learning methods; geometric deep learning; inverse problems; and development of general learning strategies informed by physical sciences applications including molecular dynamics, and fluid mechanics.*

**Sebastian Kube** sebastian.kube@wisc.edu
Materials Science and Engineering, University of Wisconsin - Madison
*High-throughput and autonomous experiments to accelerate the discovery of new alloys and understand their complex behavior, with a focus on alloys for extreme environments as in applications with high temperatures or radiation levels.*

**Sten Lambeets** sten.lambeets@pnnl.gov
Physics and Computers Sciences Directorate, Pacific Northwest National Laboratory
*I am a specialist in Atom Probe Microscopy and focus my research efforts on the development of Operando Atom Probe Microscopy to study the influence of intense electric fields on chemical reaction mechanisms, most particularly in the case at the solid-gas interfaces.*

## Scialog Fellows Continued

**Dave Leitch** dcleitch@uvic.ca
Chemistry, University of Victoria
*We in the Leitch lab are chemical cartographers, striving to map chemical reaction space in the realm of organic synthesis/catalysis. We use a mix of traditional and modern techniques, including HTE and automation, to impact real-world problems in chemical synthesis predictions.*

**Chong Liu** chongliu@chem.ucla.edu
Chemistry and Biochemistry, University of California, Los Angeles
*Machine-learning and automated experimentation in electrochemistry.*

**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
*Construction of automated virtual high-throughput screening tools for low-dimensional carbon materials; computational database for carbon-based molecules and materials; robust infrastructure for data-driven models.*

**Jeff Lopez** jlopez@northwestern.edu
Chemical and Biological Engineering, Northwestern University
*I study charge transport processes and reactions at electrochemical interfaces to inform the design of new materials for energy storage applications. My group uses automated experimentation and high throughput analysis to accelerate materials discovery and development.*

**Long Luo** long.luo@wayne.edu
Chemistry, Wayne State University
*We want to develop an autonomous reaction optimization system for alternating current (AC) electrolysis for organic synthesis, which has a much larger reaction parameter space than conventional electrolysis due to the two additional parameters of AC frequency and waveform.*

**Marilyn Mackiewicz** marilyn.mackiewicz@oregonstate.edu
Chemistry, Oregon State University
*The research performed by the Mackiewicz Lab develops nanomaterials for clinical use. To further advance materials discovery and design we are interested in using artificial intelligence, machine learning, and continuous flow chemistry to advance materials design and discovery.*

**Arun Mannodi Kanakkithodi** amannodi@purdue.edu
Materials Engineering, Purdue University
*I am a computational materials scientist applying density functional theory (DFT) simulations and machine learning (ML) to drive materials discovery. My research group is primarily working on composition- and defect-engineering of semiconductors for optoelectronic applications.*

## Scialog Fellows Continued

**Mike McGuirk** cmmcguirk@mines.edu
Chemistry, Colorado School of Mines
*Our group seeks to realize new families of permanently porous organic frameworks, in which the crystalline order of molecular building blocks is constructed through directional non-covalent interactions.*

**Melody Morris** melodymorris@umass.edu
Polymer Science & Engineering, University of Massachusetts Amherst
*The Morris group leverages accessible high-throughput tools to enable connections between macromolecular sequence and properties for advanced materials. Initial thrusts include automated syntheses for biomaterials and high-throughput assay development for polymer degradation.*

**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
*My group is interested in developing new analytical methods using 3D printing and photoelectrochemistry.*

**Andrea Pickel** apickel@ur.rochester.edu
Mechanical Engineering, University of Rochester
*My group develops optical metrology to probe temperature in challenging environments. We use luminescent materials to create thermometry techniques with sub-diffraction limited spatial resolution, and we apply these tools to areas such as catalysis and device thermal management.*

**Jolene Reid** jreid@chem.ubc.ca
Chemistry, University of British Columbia
*Our research aims to invent new strategies for developing efficient chemical reactions that generate important compounds with high yields and selectivity. We approach this by using selective catalysis based on small organic molecules developed through machine learning.*

**Trevor David Rhone** rhonet@rpi.edu
Physics, Rensselaer Polytechnic Institute
*My research is on emergent phenomena in materials, with a focus on electronic spin and charge degrees of freedom. I use artificial intelligence (AI) for materials discovery and creating physical insight. AI identifies materials that spark technological innovation.*

**Nicholas Riley** nmriley@uw.edu
Chemistry, University of Washington
*We leverage state-of-the-art mass spectrometry and chemical glycobiology to develop innovative technologies for investigating essential principles of glycoprotein regulation and dysregulation.*

## Scialog Fellows Continued

**Grant Rotskoff** rotskoff@stanford.edu
Chemistry, Stanford University
*My work focuses on controllable and rigorous machine learning for biophysical dynamics, nonequilibrium statistical mechanics, and materials design. Much of our recent work aims to integrate generative models with conventional computational techniques to accelerate modeling.*

**Jessica Sampson** jrsampso@udel.edu
Chemistry and Biochemistry, University of Delaware
*My interests are the development of new reactions using high throughput experimentation. I work to do this by developing tools that increase the technique's accessibility, by collaborating with academic and industry groups, and by development of new analytical workflows.*

**Christopher Sandford** christopher.sandford@dartmouth.edu
Chemistry, Dartmouth College
*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
*My research seeks to accelerate materials design by integrating high-performance computing, machine learning, literature data, and atomistic simulations, bridging the gap between computational predictions and experiments using data-driven synthesis recipes.*

**Martin Seifrid** m_seifrid@ncsu.edu
Materials Science and Engineering, North Carolina State University
*My group is interested in precise control of structure and function in organic conductors bottom-up (synthesis, molecular design) and from top-down (formulation, processing). We develop tools for self-driving laboratories (SDLs) – ML-guided automation – and materials informatics.*

**Amir Sheikhi** sheikhi@psu.edu
Chemical Engineering, Pennsylvania State University
*We are interested in automating biomaterial design, synthesis, and in vitro/in vivo characterizations. The automation of chemical laboratories for biomaterials has the potential to have a significant impact on the field of regenerative medicine by overcoming these challenges.*

**Cory Simon** cory.simon@oregonstate.edu
Chemical Engineering, Oregon State University
*Designing and implementing Bayesian optimization algorithms for adaptive experimental design---specifically, to be experiment-efficient in the search for an optimal molecule, material, operating condition for a chemical reactor, etc.*

## Scialog Fellows Continued

**Nairiti Sinha** njs6356@psu.edu
Materials Science and Engineering, Pennsylvania State University
*My group is exploring high throughput tools for screening and optimizing the sequence of monomers in a synthetic biomimetic polymer (a sequence-defined polymer) for fabrication & assembly of next generation smart biomaterials.*

**Siddharth Srivastava** siddharths@asu.edu
Computing and Augmented Intelligence, Arizona State University
*I am interested in developing AI systems such as lab-assistant robots that can plan and learn to solve complex tasks reliably. I am particularly interested in developing well-founded approaches that are safe and reliable for use in the real-world, even in sparse-data settings.*

**Daniel Tabor** daniel_tabor@tamu.edu
Chemistry, Texas A&M University
*Our research group is developing new methods for integrating reinforcement learning methods for molecular and materials design and developing chemically meaningful representations for molecular materials.*

**Bex Taylor** bex@andrew.cmu.edu
Mechanical Engineering, Carnegie Mellon University
*The Taylor lab research focuses on nucleic acid nanotechnology in the following three areas: (1) Molecular and cellular mechanobiology, (2) Bio-inspired Micro- and Nanosystems and (3) Advanced Manufacturing. We are working to automate the production of DNA nanotechnology.*

**Helen Tran** tran@utoronto.ca
Chemistry, University of Toronto
*We leverage the rich palette of polymer chemistry to design materials encoded with information for self-assembly, degradability, and electronic transport. We are interested in conjugated polymers for transient electronics and peptoids for self-assembled nanomaterials.*

**Allison Walker** allison.s.walker@vanderbilt.edu
Chemistry, Vanderbilt University
*My lab focuses on the development of artificial intelligence and other computational tools for the discovery and biosynthesis of natural products. In particular we are developing tools for genome mining for novel bioactive natural products and for designing biosynthetic pathways.*

**Yinan Wang** wangy88@rpi.edu
Industrial and Systems Engineering, Rensselaer Polytechnic Institute
*My research focuses on engineering-driven machine-learning methodologies for intelligent decision-making. The objective is to propose interpretable machine learning models by fusing data-driven and physical models to enable system automation and intelligent decision-making.*

## Scialog Fellows Continued

**Andrew Zahrt** zahrt@sas.upenn.edu
Chemistry, University of Pennsylvania
*My interests involve developing new machine learning and automation tools to accelerate discovery in organic chemistry. This includes streamline characterization and synthesis, as well as automating experimentation with "intelligent" systems.*

**Yan Zeng** yan.zeng.helen@gmail.com
Chemistry and Biochemistry, Florida State University
*The Zeng Lab combines robotics, materials synthesis and characterizations (chemical, structural, electrochemical), and advanced modeling methods (chemical thermodynamics, machine learning) to develop novel materials with outstanding electrochemical and catalytical performance.*

## 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
*Broadly interested in electrochemistry. (i) Electrochemical sanned probe microscopies. (ii) Electrospray from nanoscale pipettes. (iii) Electrochemistry in small domains. (iv) High-throughput electrochemical measurement.*

**Malika Jeffries-EL** malikaj@bu.edu
Chemistry, Boston University
*The Jeffries-EL group focuses on synthesizing novel organic semiconductors for various optoelectronic applications. Their current efforts aim to expedite the discovery of emissive materials for use in OLEDs by utilizing machine-learning approaches and automated synthesis.*

**Klavs Jensen** kfjensen@mit.edu
Chemical Engineering, Massachusetts Institute of Technology
*Research interests span thermal--, electro-, and photo-chemistry in batch and flow, kinetics and optimization, automation and robotics, and machine learning with the aim of developing new methods that accelerate chemical discovery and development.*

**Anne LaPointe** lapointe@cornell.edu
Chemistry and Chemical Biology, Cornell University
*My research interests include organometallic chemistry, homo- and heterogenous catalysis, lab automation, high throughput screening, and polymer synthesis, recycling and upcycling.*

**Philip LeDuc** prl@andrew.cmu.edu
Mechanical Engineering, Biological Sciences, Computational Biology, Biomedical Engineering, and Electrical and Computer Engineering Departments of Mechanical Engineering, Biological Sci, 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
*Working at the interface of program development and fundamental research, I am involved in the exploration of novel materials and chemicals through automated/autonomous workflows. Recent work has focused on the science of solvation and the prediction of new materials with AI.*

## Discussion Facilitators Continued

**Nikki Pohl** npohl@iu.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

**Chris Welch** chris.welch@icase.center
ICASE, Indiana Consortium for Analytical Science and Engineering
*Measurements, Separations, Chirality, Stereochemistry, High Throughput Experimentation, Pharmaceutical Process R&D, Commercialization & Startups, New Research Technologies, Strategic Planning, Scientific Publication and Communication Strategy*

## Guests

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

**Ruoming Gong** ruoming.gong@northwestern.edu
Applied Math, Northwestern University
*I am interested in the conversation dynamics and the formation of scientific collaborations.*

**Anne Hultgren** ahultgren@beckman-foundation.org
Arnold and Mabel Beckman Foundation
*The Arnold and Mabel Beckman Foundation funds innovative research in chemistry and life sciences, broadly defined, and especially those projects that create new materials, methods, and avenues of enquiry.*

**Naoko Tanese** ntanese@curcifoundation.org
Leadership, The Shurl and Kay Curci Foundation
*I serve as the first Chief Science Officer for The Shurl and Kay Curci Foundation, supporting basic science research.*

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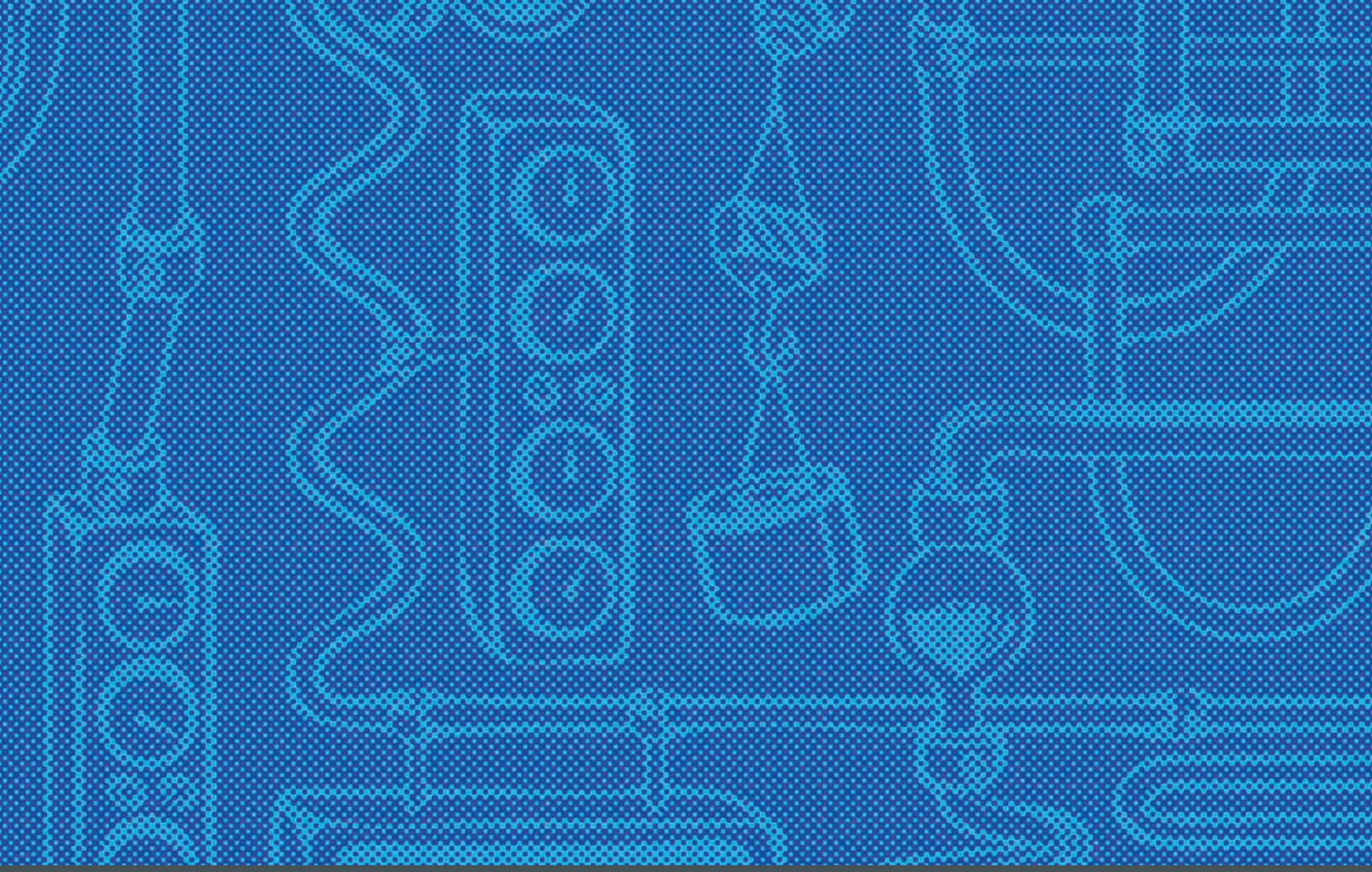

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