NATIONAL ACADEMIES Sciences Engineering Medicine

CHEMICAL SCIENCES ROUNDTABLE | BOARD ON CHEMICAL SCIENCES AND TECHNOLOGY

Building Access to Tomorrow's Medicines: bringing together humans, robots, and artificial intelligence - A Workshop

Hosted by the Chemical Sciences Roundtable

AI + Y 2024 Series

Keck Center (K100)

500 Fifth Street NW, Washington, DC

THURSDAY, FEBRUARY 20, 2025 – FRIDAY, FEBRUARY 21, 2025

The workshop will discuss role of artificial intelligences in expanding research capacity, particularly for rare diseases, while exploring critical challenges such as preventing healthcare disparities and ensuring the availability and affordability of advanced technological resources. Panel discussions and a foresight exercise will feature thought leaders examining the integration of AI, laboratory automation, and robotics to advance the chemical sciences' role in traditional drug discovery.

DAY 1: THURSDAY, FEBBRUARY 20, 2025 (ALL TIMES ARE US EASTERN)

Breakfast is available for purchase in the cafeteria (3rd Floor)

08:00AM–09:00AM **Optional: Early Morning Coffee**
Provided by the Academies for registered in-person attendees

09:00AM–09:05AM **Opening Remarks**
Michael Janicke, Chemical Sciences Roundtable, National Academies of Sciences, Engineering, and Medicine

Session One | Drug Discovery: "The Future is Now"
This panel will focus on how advanced tools like AI/ML, robotics, and automation are transforming the chemical laboratories to efficiently progress the drug discovery process.

09:05AM–09:10AM **Session Introduction and Overview**
Andrew White, CSR and University of Rochester

(15 minutes per speaker for background and opening remarks)

09:10AM–10:10AM
Alexandra Snyder Charen, Generate Biomedicines
James Li, GondolaBio
Nicolò Fusi, Microsoft Research
Jesse Kirkpatrick, George Mason University

10:10AM–10:20AM **Break (10 minutes)**

10:20 AM–11:30AM **Session One | Panel Discussion**

11:30 PM **Lunch**
Lunch is available for purchase in the cafeteria (3rd Floor)

Session Two | Expanding Access: "Removing the Biases from Drug Discovery"
Discussions will shift to emphasize how investments into the advanced tools used in and the data generated from the drug discovery process contributes collectively to the affordability and availability of patient care across a broad spectrum of diseases.

12:30PM–12:40PM **Session Introduction and Overview**
Nikki Pohl, CSR and Indiana University Bloomington

(15 minutes per speaker for background and opening remarks)

12:40PM–01:30PM
Lynda Chin, Apricity Health
Sanmi Koyejo, Stanford University
Nick Davis, Changer

01:30PM–02:30PM **Session Two | Panel Discussion**

02:30PM–02:45PM **Break (15 minutes)**

Session Three | Foresight Activity: "Imagining the Future" (interactive breakout sessions)

02:45PM–02:50PM **Session Introduction and Overview**
Laurel Royer, CSR and Carinalis Consulting and Research

02:50PM–03:30PM
Erran Carmel, American University
Apurva Dave, National Academies of Sciences, Engineering, and Medicine

03:30PM–03:35PM **End-of-day Remarks**
Laurel Royer, CSR and Carinalis Consulting and Research

03:50PM–04:45PM **Session Three | Panel Discussion Foresight Activity**
Moderated Breakout Sessions (In-person attendees and CSR Roundtable Members)
- **Keck 104 – Positive Future**
- **Keck 102 – Negative Future**
- **Keck 100 – Middle Ground Future**

05:00PM **Adjourn | End of Day 1 workshop**

DAY 2: FRIDAY, FEBRUARY 21, 2025 (ALL TIMES ARE US EASTERN)

12:00PM–12:05PM **Welcome and Workshop Overview for Day 2**
Michael Janicke, Chemical Sciences Roundtable, National Academies of Sciences, Engineering, and Medicine

12:05PM–12:50PM **Readouts from Foresight Activity (from Breakout Rooms)**
Moderated by Laurel Royer

Session Four | Building the Community: "Out of the Box Success Stories"
Closing this exciting meeting, we will explore on how collaboration between citizen scientists and other relevant groups can contribute to shared responsibilities, open communication, and access to advanced technological resources to maximize innovations in the drug discovery process that facilitate the highest delivery of patient care.

12:50PM–01:00PM **Session Introduction and Overview**
Marty Burke, CSR and University of Illinois Urbana-Champaign

(15 minutes per speaker for background and opening remarks)

01:00PM–01:45PM
Emily Kramer-Golinkoff, Emily's Entourage (virtual)
Margaret Honey, Scratch Foundation (virtual)
Rob Zellem, NASA Goddard Space Flight Center

01:45PM–02:45PM **Session Four | Panel Discussion**

02:45PM–03:00PM **Break (15 minutes)**

03:00PM–03:15PM **Reflection on Session Three Breakout Sessions and Closing Remarks on Workshop**
Marty Burke and Nikki Pohl, CSR co-chairs

03:15PM **Adjourn workshop | End of Day 2 workshop**

BIOGRAPHIES ON SPEAKERS AND PLANNERS

Milad Abolhasani (Workshop Organizer and Chemical Sciences Roundtable)

Milad Abolhasani, PhD, serves as the ALCOA Professor and a University Faculty Scholar in the Department of Chemical and Biomolecular Engineering at North Carolina State University (NCSU). Prior to joining NCSU, Dr. Abolhasani was an NSERC Postdoctoral Fellow in the Department of Chemical Engineering at MIT (2014-2016). He leads a diverse research group that studies self-driving labs tailored toward accelerated discovery, development, and manufacturing of advanced functional materials and molecules using fluidic micro-processors at NCSU. Dr. Abolhasani has received numerous awards and fellowships, including NSF CAREER Award, AIChE 35 Under 35, Dreyfus Award for Machine Learning in the Chemical Sciences & Engineering, AIChE CRE Early Career Investigator Award, Scialog Fellowship, AIChE NSEF Young Investigator Award, I &EC Research 2021 Class of Influential Researchers, AIChE Futures Scholar, ALCOA Research Achievement Award, ACS-PRF Doctoral New Investigator Award, and Emerging Investigator recognition from Nanoscale, Lab on a Chip, Reaction Chemistry & Engineering, and Journal of Flow Chemistry. He holds a PhD in Mechanical Engineering from the University of Toronto, a MS in Chemical Engineering from the University of British Columbia, and a BS in Mechanical Engineering from Sharif University of Technology.

Martin Burke (Workshop Organizer and Chemical Sciences Roundtable)

Martin Burke is the May and Ving Lee Professor of Chemical Innovation at University of Illinois at Urbana-Champaign. The Burke research group is pioneering the development of "molecular prosthetics"—small molecules that mimic the functions of deficient proteins that underlie a wide range of human diseases. The group has also created an automatable lego-like platform for synthesis that is broadly enabling and expanding access to the molecule-making process. The Burke group has harnessed this platform to advance molecular prosthetics for treating cystic fibrosis into clinical trials and to enable preclinical testing of molecular prosthetics for anemia and a new class of nontoxic fungicidal agents. Dr. Burke also recently helped launch the Carle Illinois College of Medicine and is serving as the inaugural associate dean of research. Dr. Burke has received the American Chemical Society Nobel Laureate Signature Award for Graduate Education in Chemistry and is a founder of four biotechnology companies. He received his PhD from Harvard University and an MD from Harvard Medical School.

Erran Carmel

Professor Erran Carmel is a tenured full Professor at the Information Technology department and was the interim Dean (2014-2016) at the Kogod School of Business at American University. He is currently working on a number of research areas: Digital identity; Crypto ethics; Future of work. During the early decades of the rise of the global internet, Carmel studied the globalization of technology work and wrote three books in this domain. Carmel's 1999 book "Global Software Teams" was the first on this topic—and is considered a landmark in the field, helping many organizations take their first steps into distributed tech work. His second book "Offshoring Information Technology" came out in 2005 and became popular as

outsourcing began to be taught in business schools around the world. His 2011 book is about the special issues that time zone separation imposes on global coordination of work. "I'm Working While They're Sleeping: Time Zone Separation Challenges and Solutions" is co-authored with his AU colleague Alberto Espinosa. He has written over 100 articles, reports, and manuscripts. He consults and speaks to industry and professional groups. In the 1990s he co-founded and led AU's program in Management of Global Information Technology. He has been a Visiting Professor at Haifa University (Israel), University College Dublin (Ireland), at Universidad Adolfo Ibáñez (Chile), Beijing Normal University (China), and Ca' Foscari University of Venice (Italy).

Alexandra Snyder Charen

Alex Snyder is the Head of Research and Development at Generate Biomedicines, a biotechnology company that uses artificial intelligence, machine learning and protein engineering to create novel medicines. Prior to joining Generate in 2022, Dr. Snyder was a Principal at the biotech incubator Two River, following her role as Associate Vice President and Head of Translational Oncology at Merck. She previously was Translational Medicine Lead at Adaptive Biotechnologies, and started her career as faculty and federally-funded Principal Investigator at Memorial Sloan Kettering Cancer Center. Dr. Snyder is a Cancer Steering Committee (CSC) Biomedical Co-Chair for the Executive Committee of the FNIH and co-leads the SITC Biomarker Working Group. She is a Clinical Assistant Professor of Medicine at NYU and Bellevue Hospitals, Section Editor for the Journal for the Immunotherapy of Cancer, and was a member of the board of Navigating Cancer. Dr. Snyder received her medical degree and internal medicine training at the Icahn School of Medicine at Mount Sinai and Mount Sinai Hospital, followed by medical oncology fellowship at Memorial Sloan Kettering Cancer Center (MSKCC).

Lynda Chin (Workshop Organizer)

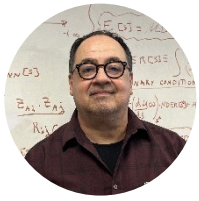
Dr. Lynda Chin, M.D. is a physician, scientist, and entrepreneur, currently serving as CEO of Apricity Health, a company she founded to harness dynamic patient data to enhance care and accelerate precision drug discovery. Previously, she was the Chief Innovation Officer for Health at the UT System and the founding Chair of Department of Genomic Medicine at MD Anderson Cancer Center, following a distinguished research career at Dana-Farber/Harvard and the Broad Institute. Dr. Chin has a proven track record of building innovative models that bridge research and patient care, integrating science, technology, and data to accelerate therapeutic development. She pioneered the Applied Cancer Science model, bringing industry-seasoned drug developers into academia, first at Dana-Farber and later at MD Anderson, to create innovative partnerships with biopharma in drug discovery. This work laid the foundation for Apricity Health's platform that connects care delivery and drug discovery verticals to unlock the value of dynamic data from every patient in precision drug discovery. An elected member of the National Academy of Medicine, Dr. Chin has received numerous honors for her contributions to precision medicine. She earned her M.D. from Albert Einstein College of Medicine, with clinical training at Columbia Presbyterian and Montefiore Medical Centers.

Nick Davis

Nick Davis is an engineer working to build the future of human health. As Managing Partner of Changer, a family office, Nick collaborates with medicine companies to build intelligence platforms that revolutionize SG&A and R&D capabilities. Over the past 15 years, he has partnered with institutions like Bristol Myers Squibb, Dana Farber, Flagship Pioneering, Sands Capital and Santander to drive innovation at the intersection of science, engineering and computing. Previously, Nick served as Chief Executive Officer of Theonys, a pioneering RNA-focused therapeutics company co-founded with Professors Peter C. Dedon at MIT and Richard I. Gregory at Harvard. With support from Bayer, Temasek and Emerson Collective, Theonys advanced groundbreaking RNA therapeutics capabilities, pushing the boundaries of precision medicine in solid tumors. Nick earned his Doctor of Science in Biological Engineering from MIT, where he developed machine learning tools for multiscale analysis of disease processes as a Sloan Research Fellow. He also holds a Bachelor of Science in Bioengineering from Stanford, where he advanced tools for quantitative systems biology as a Bio-X Research Fellow.

Nicolò Fusi

Nicolò Fusi is a General Manager at Microsoft Research (MSR) in Cambridge, MA, where he leads multidisciplinary teams on artificial intelligence, biomedical machine learning, and statistics to accelerate scientific discovery through generative AI. Fusi received a Ph.D. from the University of Sheffield and Bachelor's and Master's degrees in Computer Science from the University of Milan.



Carlos Gonzalez (Workshop Organizer and Chemical Sciences Roundtable)

Carlos Gonzalez has been the Chief of the Chemical Sciences Division of the National Institute of Standards and Technology (NIST) since 2012. Dr. Gonzalez joined NIST in 1997 as a member of the Computational Chemistry Group within the Physical and Chemical Properties Division. He was appointed to the position of Chief, Chemical and Biochemical Reference Data Division in 2008. Previously, Dr. Gonzalez was a Postdoctoral Scholar at Carnegie Melon University under the mentorship of Prof. John A. Pople, a 1998 Nobel Laureate in Chemistry. Dr. Gonzalez received his Ph.D. in Chemistry from Wayne State University.

Margaret Honey

Dr. Margaret Honey became President and CEO of the Scratch Foundation in January 2024, bringing over 30 years of experience in advancing digital learning for children. Known for her work at the intersection of technology and education, Dr. Honey is dedicated to expanding access to high-quality, creative learning opportunities through for young people everywhere.
Before joining Scratch, Dr. Honey was the CEO of the New York Hall of Science (NYSCI), where she championed the Design-Make-Play approach to STEM education. Her efforts transformed NYSCI into an incubator of for creative STEM learning and bringing to the NYC area the annual World Make Faire event. Additionally, she fostered strong community partnerships in Queens, opening a STEAM-focused preschool that serves over 300 children annually. Prior to NYSCI, Dr. Honey led the Center for Children and Technology at the Education Development Center, where she managed several large-scale projects funded by

the National Science Foundation and the U.S. Department of Education. She co-directed the Northeast and Islands Regional Education Laboratory, a $40 million initiative dedicated to improving educational outcomes through research.
Dr. Honey holds a Ph.D. in developmental psychology from Columbia University and has contributed significantly to discussions on learning, technology, and access to educational opportunities for all young people. Her early work includes the acclaimed public television series The Voyage of the Mimi and a decade-long school reform project in Union City, New Jersey. A respected thought leader, she has testified before Congress and contributed to numerous publications on STEM education and policy. She currently serves on the boards of Bank Street College of Education, Gulf of Maine Research Institute, Post University, and Sphero, and is a member of the National Academy of Education.

Jesse Kirkpatrick

Jesse Kirkpatrick is a research associate professor in George Mason University's College of Engineering and Computing and Co-Director of the Mason Autonomy and Robotics Center. He has led numerous initiatives to advance Responsible AI in education, research, and policy. He regularly consults on ethical, legal, and societal implications of AI for government and industry. He has played a pivotal role in developing responsible innovation frameworks and practices in the commercial tech sector and for defense contexts. He has received various honors and awards and is an official "Mad Scientist" for the U.S. Army.

Sanmi Koyejo (Workshop Organizer)

Sanmi Koyejo is an assistant professor in the Department of Computer Science at Stanford University. Koyejo leads the Stanford Trustworthy Artificial Intelligence (STAIR) lab, which works to develop the principles and practice of trustworthy machine learning, focusing on applications to science and healthcare. Koyejo has been the recipient of several awards, including a Skip Ellis Early Career Award, a Sloan Fellowship, a Terman faculty fellowship, an NSF CAREER award, a Kavli Fellowship, and an IJCAI early career spotlight. Koyejo serves on the Neural Information Processing Systems Foundation Board, the Association for Health Learning and Inference Board, and as president of the Black in AI organization.

Emily Kramer-Golinkoff

Emily Kramer-Golinkoff, MBE is Co-Founder of Emily's Entourage, an innovative 501(c)3 that accelerates research for individuals in the final 10% of the cystic fibrosis (CF) population that do not benefit from existing mutation-targeted therapies. She is also an internationally recognized patient advocate and speaker. Since 2011, Emily's Entourage has awarded millions of dollars in research grants, launched a now-clinical stage CF gene therapy company, developed a patient database and clinical trial matchmaking program to accelerate clinical trial recruitment, and led worldwide efforts to drive high-impact research and drug development. The organization has been featured in media outlets, including New York Times, STAT, CNN, Yahoo, AOL, People, The Philadelphia Inquirer and more. Emily has a master's degree in bioethics and certification in clinical ethics mediation from the University of Pennsylvania, where she also completed her undergraduate degree. She has given talks at The White House, TEDx, University of Pennsylvania's Annenberg School for Communication Commencement, Stanford University's

Medicine X Conference, and more. Emily was named a "Champion of Change" for President Obama's Precision Medicine Initiative and is the recipient of the 2024 Personalized Medicine Coalition's Award in Leadership in Personalized Medicine, 2020 Philadelphia Magazine Luminary Award, and the 2016 Global Genes Rare Champion of Hope for Advocacy Award. Learn more at emilysentourage.org.

James Li

James Li, Ph.D., is President of GondolaBio, LLC, a biotechnology company dedicated to developing life-changing medicines that address well-characterized genetic diseases at their source. Originally established as BridgeBioX, a subsidiary of BridgeBio Pharma, GondolaBio secured $300 million in private financing from external investors in 2024 and became an independent company. Before leading GondolaBio, Dr. Li served as Chief Business Officer at BridgeBioX, where he oversaw research and early development programs and drove new company formation and due diligence efforts. Previously, he was an engagement manager at McKinsey & Company, advising pharmaceutical clients on strategic initiatives and leading asset optimization projects. Dr. Li holds B.S. degree in Molecular Biophysics and Biochemistry from Yale University. He received his Ph.D. in Biochemistry, with a minor in Management Science and Engineering, from Stanford University.

Nicola Pohl (Workshop Organizer and Chemical Sciences Roundtable)

Nicola Pohl is professor of chemistry, the Joan and Marvin Carmack Chair in Bioorganic Chemistry, and the Associate Dean of Natural and Mathematical Sciences and Research for the College of Arts and Sciences at Indiana University Bloomington. She was a professor of chemistry and of chemical and biological engineering and held the Wilkinson Professor of Interdisciplinary Engineering at Iowa State University before moving to Indiana University. The Pohl research group works to find new ways to make and analyze sugars to dissect their important roles in plant, animal, and human biology and to design therapeutics. One major long-term goal of the group is to develop rational designs of therapeutic interventions, such as vaccines and glycoproteins, on the basis of a deeper knowledge of the role of carbohydrates. Her research group created the first automated solution-phase method for readily synthesizing oligosaccharides and is now working to expand the scope of those methods to tackle the equal challenge of providing building blocks to feed their automated oligosaccharide synthesis machines. Dr. Pohl received her PhD in chemistry from the University of Wisconsin-Madison and completed a National Institutes of Health Postdoctoral Fellowship in the Department of Chemical Engineering at Stanford University.

Laurel Royer (Workshop Organizer and Chemical Sciences Roundtable)

Laurel Royer, PhD, is the Founder and Chief Scientific Officer of Carinalis Consulting and Research. Dr. Royer has more than 15 years of combined research, scientific, technical advising expertise. She has developed and built an inter- and trans-disciplinary consultancy focused on evaluating the balance between innovation and detrimental impact. She applies the fundamentals of the chemical and related sciences to evaluate manufacturing/production and application, disposal, contamination, and exposure issues via the use cycle to support stakeholders in achieving an overall positive impact. To that cause, she supports clients and partners across a myriad of sectors addressing both proactive and reactive

responses at the intersection of the built and natural environments. Dr. Royer is keenly aware that the consequences of chemical contamination and exposure unequally impact communities across the globe. To that end, she works with these communities in technical advisory roles and is an ardent advocate of addressing the disproportionate burdens and consequences of our anthropogenic footprint. She holds a PhD in Environmental Organic Chemistry and a MS in Medicinal Chemistry and Molecular Pharmacology from Purdue University, a BS in Chemistry from the University of the Virgin Islands.

Robert T. Zellem

Dr. Rob Zellem is an astrophysicist at NASA's Goddard Space Flight Center. His research focuses on the characterization of the atmospheres of exoplanets using both the transit and direct imaging methods. Rob is the Deputy Project Scientist for Communications for NASA's Nancy Grace Roman Space Telescope where he is the primary liaison between the Roman Project Science team and Goddard's Office of Communications. He is also a member of the Roman Coronagraph Project Science team where he led the development of the science calibration plan. He is the Project Scientist and Lead for Exoplanet Watch, a citizen science project to observe transiting exoplanets to update their ephemerides to ensure the efficiency use of large telescope time. He is the Ground-Based Sub-working Group co-lead for Pandora, whereby he is coordinating ground-based observations to support both the operations and scientific interpretation of Pandora data. He is also a co-lead for NASA's Nexus for Exoplanet System Science (NExSS) and a science team member for the NASA's CASE contribution to ESA's Ariel mission.