

Laboratory Automation and Accelerated Synthesis: Empowering Tomorrow's Chemist--A Workshop

Workshop Speaker and Panelist Biographies

Alan Aspuru-Guzik is a professor of Chemistry and Computer Science at the University of Toronto (UofT) and is the Canada 150 Research Chair in Theoretical Chemistry and a Canada Canadian Institute for Advanced Research (CIFAR) AI Chair at the Vector Institute. He is a CIFAR Lebovic Fellow in the Biologically Inspired Solar Energy program. Aspuru-Guzik holds a Google Industrial Research Chair in Quantum Computing, and is the director of the Acceleration Consortium, a UofT-based strategic initiative. Aspuru-Guzik began his independent career at Harvard University in 2006 where he was a Full Professor from 2013 to 2018. Aspuru-Guzik conducts research in the interfaces of quantum information, chemistry, machine learning and chemistry. He was a pioneer in the development of algorithms and experimental implementations of quantum computers and quantum simulators dedicated to chemical systems. He has studied the role of quantum coherence in the transfer of excitonic energy in photosynthetic complexes and has accelerated the discovery by calculating organic semiconductors, organic photovoltaic energy, organic batteries and organic light-emitting diodes. Currently, Aspuru-Guzik is interested in automation and "autonomous" chemical laboratories for accelerating scientific discovery. He is editor-in-chief of the journal Digital Discovery as well as co-founder of Zapata Computing and Kebotix. He received his B.Sc. from the National Autonomous University of Mexico in 1999 and a PhD from the University of California, Berkeley in 2004, where he was a postdoctoral fellow from 2005-2006.

Nicholas Ball is an Associate Professor of Chemistry at Pomona College. After completing his PhD in 2010, he headed to the California Institute of Technology to pursue his postdoctoral studies with Professor David A. Tirrell as a NIH Postdoctoral Fellow. In the Tirrell laboratory, he studied the role of selenium-based amino acids for the identification of low-abundant proteins. Nicholas was an Assistant Professor at Amherst College from 2013 to 2015. He received his BA in Chemistry at Macalester College and his PhD at the University of Michigan – Ann Arbor.

Matthew Bio is President and CEO at Snapdragon Chemistry. Bio began his career in chemistry in 1993 at Rohm & Haas Company, developing continuous processes for the manufacture and purification of acrylates. After graduating with his doctorate, Bio returned to industry as a process development chemist at Merck Research Laboratories. He moved to Amgen in 2006 where he worked on the development of both batch and continuous manufacturing solutions for synthetic drug substances. He also worked on the development of new manufacturing technologies for synthetic – biologic hybrid molecules. In 2015, Bio joined Snapdragon Chemistry, Inc., a contract development firm specialized in the design of continuous manufacturing technology. Throughout his career, he has been involved in the development of more than 50 clinical candidates and the launch of three new drugs to the market. He is author or inventor on more than 30 peer reviewed publications and patents and numerous regulatory filings. Bio received his PhD in chemistry from Columbia University.

Jin Cha is a program director in the chemical synthesis program at the National Science Foundation. He is on leave from Wayne State University, where he is professor of chemistry. His research interest lies in organic synthesis – methodology development and natural product synthesis. He served on the editorial board of *Organic Reactions*. He obtained his PhD from the University of Oxford.

Andy Cooper is the Academic Director of the Materials Innovation Factory (MIF) via the UK Research Partnerships Infrastructure Fund and the Director of the Leverhulme Centre for Functional Materials Design. His main research interests are organic materials, supramolecular chemistry, and materials for energy production and molecular separation. This is underpinned by a strong technical interest in high-throughput methods and robotics. A unifying theme in his research is the close fusion of computational prediction and experiment to discover new materials with step-change properties. Cooper was elected to the Royal Society in 2015. He has been awarded the Macro Group Young Researchers Award (2002), the RSC Award in Environmentally Friendly Polymers (2005), the McBain Medal (2007), the Corday-Morgan Prize (2009), the Macro Group Award (2010), a Royal Society Wolfson Research Merit Award, the Tilden Prize (2014), the American Chemical Society Doolittle Award (2014), the Hughes Medal (2019) and the RSC Interdisciplinary Prize for combining autonomous robotics (2021). In 2015, he was appointed as a Consultant Professor in Hauzhong University of Science & Technology, China. He was also appointed as Editor-in-Chief of *Chemical Science* in 2019. Cooper obtained his PhD from the University of Nottingham in 1994.

Lee Cronin is the Regius Professor of Chemistry in Glasgow. His research spans many disciplines and has four main aims: the construction of an artificial life form; the digitization of chemistry; the use of artificial intelligence in chemistry including the construction of 'wet' chemical computers; the exploration of complexity and information in chemistry. He has one of the largest multidisciplinary chemistry-based research teams in the world. Lee has given over 300 international talks and has authored over 350 peer reviewed papers with recent work published in *Nature, Science*, and *Proceedings of the National Academy of Sciences of the United States*. He received his Ph.D. in Chemistry from the University of York.

Joseph DeSimone (he/him) is the Sanjiv Sam Gambhir Professor of Translational Medicine and Chemical Engineering at Stanford University. He holds appointments in the Departments of Radiology and Chemical Engineering with courtesy appointments in the Graduate School of Business and in the Departments of Chemistry and of Materials Science & Engineering. Previously, he was a professor at University of North Carolina Chapel Hill and North Carolina State University. He is also Co-founder, Board Chair, and former CEO of the additive manufacturing company, Carbon. DeSimone is responsible for research breakthroughs in areas including green chemistry, medical devices, nanomedicine, and 3D printing, also co-founding several companies based on his research. He has mentored 80 students through PhD completion, half of whom are women and members of underrepresented groups in STEM. DeSimone's recognitions include the U.S. Presidential Green Chemistry Challenge Award; Lemelson-MIT Prize; NIH Director's Pioneer Award; Wilhelm Exner Medal; EY Entrepreneur of the Year Award (U.S.); Harvey Prize; and the U.S. National Medal of Technology and Innovation. He is an elected member of all three branches of the National Academies. He currently serves as a member of the Racial Justice and Equity Subcommittee on National Academy of Engineering Membership and a member of the Committee on Enhancing the U.S. Chemical Economy Through Investments in Fundamental Research in the Chemical Sciences. Previously, he was chair of the Academies' Committee on "Convergence" in Biomedical Research, a member of the Committee on Advancing Institutional Transformation for Minority Women in Academia, co-chair of the Committee on Effectiveness of National Biosurvellience Systems, and co-chair of the

Materials Engineering Section Peer Committee. DeSimone received his PhD in Chemistry in 1990 from Virginia Tech.

Rebecca W. Doerge is the Glen de Vries Dean of the Mellon College of Science at Carnegie Mellon University and a professor in the Dietrich College of Humanities and Social Sciences' Department of Statistics and Data Science and the Mellon College of Science's Department of Biological Sciences. Doerge's research focuses on statistical bioinformatics, which brings together many scientific disciplines for the purpose of asking, answering and disseminating biologically interesting information in the quest to understand the ultimate function of DNA and epigenomic associations. Prior to joining Carnegie Mellon University, Doerge was the Trent and Judith Anderson Distinguished Professor of Statistics at Purdue University. Doerge is a fellow of the American Statistical Association, the American Association for the Advancement of Science, and the Committee on Institutional Cooperation. She is also a member of the Board of Trustees for the National Institute of Statistical Sciences and the Mathematical Biosciences Institute; a member of the Engineering External Review Committee at Lawrence Livermore National Laboratory; and a member of the Global Open-Source Breeding Informatics Initiative Advisory Board. Doerge earned her PhD in statistics from North Carolina State and completed a postdoctoral fellowship at Cornell University.

Spencer Dreher is currently a Senior Principal scientist with 20 years of experience at Merck. Dreher started his career in scale-up Process Chemistry, then moved into the Catalysis Group in the Enabling Technologies group where he learned high-throughput experimentation (HTE) chemistry and automation. He recently moved to Medicinal chemistry and has spent the last several years building and deploying new tools. Dreher served on the American Chemical Society Division of Organic Chemistry board as a member at large, served on the University of Delaware Centers of Biomedical Research Excellence board and is currently on the advisory board for the *Journal of Organic Chemistry* and the Google/ MIT Open Reaction Database board. He has helped to build HTE labs at the University of Pennsylvania and at the Delaware University. Dreher has been active in publication of novel modern chemistry techniques including HTE nanochemistry, use of ultra-HT mass spectroscopic analysis, creation of chemistry informer libraries for standardized comparison of synthetic chemistry methods and use of machine-learning for chemistry reaction prediction. He has mentored over 20 post-docs, graduate students and junior Merck synthetic chemists, many of whom are now leaders in the field of HTE chemistry. Dreher obtained his PhD from Columbia University.

Mimi Hii is currently a Professor of Catalysis in the Department of Chemistry at Imperial College London. Additionally, she serves as Director of the Centre for Rapid Online Analysis of Reactions (ROAR) at the Imperial College London and as Director of the Engineering and Physical Sciences Research CouncilCentre for Doctoral Training in Next Generation Synthesis & Reaction Technology. Her research focuses on the development of catalytic reactions and associated technologies that are relevant to the pharmaceutical and fine chemical industries; particularly on the implementation of flow chemistry in multiphasic catalytic reactions. Hii's contributions to these research areas have been recognized by an 'Asian Rising Star' award in 2013, conferred by the Federation of Asian Chemical Societies; the same year she was elected as a Fellow of The Royal Society of Chemistry. To date, her work has generated >130 peer-reviewed papers, 8 patent applications, and a number of monographs and textbooks in catalysis and flow chemistry. Other notable appointments include Steering group membership of EPSRC's 'Dial-a-Molecule' Grand Challenge Network and serving as an Associate Editor for American Chemical Society *Sustainable Chemistry & Engineering*. Hii received her PhD in chemistry from the University of Leeds in 1994. Klavs F. Jensen is Warren K. Lewis Professor in Chemical Engineering and Materials Science and Engineering at the Massachusetts Institute of Technology (MIT). From 2007- July 2015 he was the Head of the Department of Chemical Engineering. His research interests include methods for automated synthesis, and machine learning techniques for chemical synthesis and interpreting large chemical data sets. He is a co-director of MIT's consortium, Machine Learning for Pharmaceutical Discovery and Synthesis, which aims to bring machine learning technology into pharmaceutical discovery and development. Catalysis, chemical kinetics and transport phenomena are also topics of interest. He is the recipient of several awards, including a Guggenheim Fellowship, the Allan P. Colburn, Richard H. Wilhelm, William H. Walker, and Founders Awards of the American Institute of Chemical Engineers, and the inaugural IUPAC-ThalesNano Prize in Flow Chemistry. Jensen is a member of the National Academy of Sciences, National Academy of Engineering, and the American Academy of Arts and Science. He is a Fellow of the American Association for the Advancement of Science, the American Institute of Chemical Engineers, and the Royal Society of Chemistry. He is a member of the editorial board for *PNAS* and Editor-in-Chief for the Royal Society of Chemistry journal *Reaction Chemistry and Engineering*. He received his MSc in chemical engineering from the Technical University of Denmark and his PhD in chemical engineering from the University of Wisconsin-Madison.

Benji Maruyama works in the Materials and Manufacturing Directorate of the Air Force Research Laboratory. He leads research on the synthesis and processing science of carbon nanotubes. He is also the point of contact for carbon materials for the Materials and Manufacturing Directorate. He serves as technical lead for the RX Electrochemical Energy Storage Materials program. His background and interests include carbon materials, carbon, polymer and metal matrix composites, imaging of complex 3D microstructures and combinatorial experimentation. He is currently involved in the study of growth termination mechanisms for carbon nanotubes, nanostructured materials for battery electrodes, in-situ experimentation and catalyst development. He received his PhD in materials science and engineering from the University of Texas at Austin.

Rachel Switzky is the inaugural director of the Siebel Center for Design. Prior to her current appointment, she has been a global design leader working with Fortune 100 companies over the past 20 years. Most recently, she served as an Executive Director at IDEO, the company who pioneered the concept of design thinking. For the last decade in this role, she helped teams imagine futures and then put them into action, focusing on digital design, emergent technologies and impact at-scale. Her interests also include STEM and Design thinking research. Switzky attended the University of Illinois at Urbana-Champaign, receiving her BFA and MFA in Industrial Design from the College of Fine and Applied Arts.

Ying Wang heads the Advanced Chemistry Technologies group at AbbVie, a centralized chemistry technology group for drug discovery research. From 2006 to 2011, Wang had successfully co-led the File Enhancement Initiative at AbbVie while involved in lead generation and optimization medicinal chemistry programs. In 2013, she spearheaded the multi-function collaboration to evaluate the utility of thermodynamic and kinetic signatures in drug discovery. Wang has augmented the industry leading parallel library synthesis platform at AbbVie. Ying initiated and established the high throughput experimentation platform at AbbVie in 2017, leveraging the proprietary ChemBeads technology she and her coworkers invented. Together with her team members, late-stage functionalization and photoredox drug discovery support were also established at AbbVie recently. She is the leading/corresponding author for more than thirty-five publications and is a key contributor on several patents. Wang received a BS in Chemistry from Nanjing University, a PhD in Organic Chemistry from Iowa State University, and completed a Postdoctoral Fellowship at the University of Chicago.

Planning Committee Biographies

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. Burke also recently helped launch the Carle Illinois College of Medicine and is serving as the inaugural associate dean of research. 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.

Tim Jamison is a professor of Chemistry at the Massachusetts Institute of Technology (MIT). . He was a Damon Runyon-Walter Winchell postdoctoral fellow at Harvard University. In 1999, he began his independent career at MIT, where his research program focuses on the development of new methods of organic synthesis and their implementation in the total synthesis of natural products. Jamison received his PhD from Harvard University.

Shane W. Krska currently serves as Distinguished Scientist in NJ Discovery Chemistry, overseeing new highthroughput experimentation (THE) chemistry capability development and academic collaborations. He began his career at Merck Research Laboratories as a Senior Research Chemist in 1999, where he initially worked in the Reaction Engineering Laboratory in the Department of Chemical Engineering Research and Development (R&D). In 2002, he helped found the Merck Catalysis Laboratory in the Process Research department, whose mission is to develop HTE techniques to enable applications of homogeneous catalysis in pharmaceutical synthesis. In 2012, he helped found the Late-Stage Functionalization group within Discovery Chemistry. He Dr. Krska has authored more than 70 publications and 10 patents. Professional honors he has received include being named an American Chemical Society Young Industrial Investigator (2008), as well as a co-recipient of the R&D Council of N.J. Thomas Alva Edison Patent Award (2009), Environmental Protection Agency Presidential Green Chemistry awards for JANUVIATM (2006) and EMENDTM (2005) and the Catalysis Society of Metropolitan NY Excellence in Catalysis Award (2012). Dr. Krska has served on the industrial advisory board of the National Science Foundation Center for Enabling New Technologies through Catalysis and the Center for Selective C-H Functionalization. He is also a member of the board of the Medicinal and Bioorganic Chemistry Foundation. Krska obtained his PhD in inorganic chemistry from the Massachusetts Institute of Technology.

Anne LaPointe is the director of the Catalyst Discovery and Development Laboratory in the Department of Chemistry and Chemical Biology and has been a professor at Cornell University since 2010. Prior to Cornell, she was a senior staff scientist at Symyx Technologies. While at Symyx, LaPointe developed methods for high-throughput catalyst screening and discovered several new families of olefin polymerization catalysts, which are used commercially. LaPointe's research interests include synthetic and mechanistic inorganic and organometallic chemistry, homogeneous and heterogeneous catalysis, polymer chemistry, sustainable chemistry, and high-throughput experimentation. She is an inventor on more than 40 US and international patents. LaPointe received her PhD in inorganic chemistry from the Massachusetts Institute of Technology.

Robert E. Maleczka, Jr. is a Professor of Chemistry at Michigan State University (MSU). He began his independent career at MSU in 1995. The Maleczka group's research interests include the invention of "green" reactions and strategies for organic synthesis. Honors bestowed on Maleczka include being named an American

Chemical Society (ACS) Fellow, the Merck Technology Collaboration Award, the Environmental Protection Agency's (EPA) 2008 Presidential Green Chemistry Challenge Award, and the Astellas USA Foundation Faculty Award. In 2006, Maleczka co-founded BoroPharm, a Michigan-based company dedicated to the preparation and commercialization of novel chemical building blocks. Among his service and outreach roles, he served as Department Chair from 2010–2021. He has been a Diversity Scholar in the Center for the Integration of Research, Teaching, and Learning, an invited participant ACS/EPA Green Chemistry Market Roundtable and White House Forum, a member and Chair of the ACS Award for Affordable Green Chemistry Selection Committee, and an elected member of the Executive Committee of the ACS Division of Organic Chemistry, where he currently serves as treasurer. He has been a member of the Academies' Chemical Sciences Roundtable since 2018. He earned his BS in chemistry from the University of Illinois his PhD from the Ohio State University.

Arsalan Mirjafari is an Associate Professor in the Department of Chemistry and Physics at Florida Gulf Coast University. His research focuses on development of organic materials, which aims to address key societal challenges such as resources, energy and medicine. Over the past eight years, his undergraduate research group has worked on rational design, synthesis, and applications of functional ionic liquids as a versatile class of organic materials, with a wide array of applications, such as electrolytes for energy storage devices, gene delivery, biomolecules preservation, bio-inspired materials, liquid crystals, catalysis, and carbon dioxide capture. Mirjafari received his PhD in Organic Chemistry from the University of Isfahan, in Iran in 2009 and did his postdoctoral training at the University of South Alabama.

Nicola L. B. Pohl is the Associate Dean for Natural and Mathematical Sciences and Research, College of Arts and Sciences and a Professor of Chemistry and Joan and Marvin Carmack Chair of Bioorganic chemistry at Indiana University-Bloomington. Their research interests include automation and flow chemistry, FAIR (findable, accessible, interoperable, reusable) principles in science, development of methods for the synthesis and analysis of carbohydrates and glycopeptides. Pohl serves as an Advisory Board Member of *Organic Letters* and *The Journal of Organic Chemistry* (American Chemical Society). Pohl has been serving as member of the Academies' Chemical Sciences Roundtable since 2019. Pohl obtained their PhD in Chemistry from the University of Wisconsin-Madison in 1997.

Breakout Session Facilitator Biography

Becky Matz is a Research Scientist on the Research & Development team at the Center for Academic Innovation at the University of Michigan. She directs and supports research projects across Academic Innovation's portfolio of educational technologies and online learning experiences. Becky has research experience in assessing the efficacy of software tools that support student learning and success, analyzing quantitative equity disparities in STEM courses across institutions, and developing interdisciplinary activities for introductory chemistry and biology courses. Becky earned her B.S. in Chemistry from the University of Illinois and her Ph.D. in Chemistry and M.S. in Educational Studies from the University of Michigan.