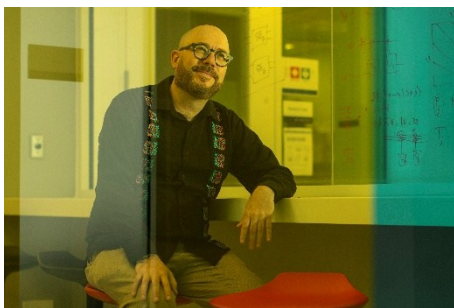


Chemical Science symposium:

Digital chemistry in the age of AI and machine learning

29-30 October 2026, London, UK

Speakers



Alán Aspuru-Guzik

*University of
Toronto, Canada*

Alán Aspuru-Guzik is a professor of Chemistry and Computer Science at the University of Toronto, the Canada 150 Laureate in Theoretical Chemistry, and a Canada CIFAR AI Chair at the Vector Institute for Artificial Intelligence. He is also a CIFAR Fellow and co-directs CIFAR's Accelerated Decarbonization program. Alán also directs the Acceleration Consortium.

Alán's research spans quantum information, machine learning, and chemistry. He pioneered the development of algorithms and experimental implementations of quantum computers and quantum simulators for chemical systems. His work has also examined the role of quantum coherence in excitonic energy transfer in photosynthetic complexes and accelerated discovery through calculations on organic semiconductors, organic photovoltaic materials, organic batteries, and organic light-emitting diodes. He has worked extensively on molecular representations and generative models for learning molecular properties. His current interests include automation and autonomous chemical laboratories for accelerating scientific discovery as well as AI Scientists, in particular the EI Agente project.

Alán has received the Google Focused Award for Quantum Computing, the Sloan Research Fellowship, and the Camille and Henry Dreyfus Teacher-Scholar Award. He won the Heinrich Emanuel Merck Award for Computational Sciences in 2025 and was named a Fellow of the Royal Society of Canada in 2025. He was selected by MIT Technology Review as one of the top innovators under 35 and received the Early Career Award in Theoretical Chemistry from the American Chemical Society. In 2024, Alán received the University of Toronto President's Impact Award and the 2024 PRISM Prize from the Istituto di Struttura della Materia. Alán was named to Maclean's 2024 Power List as one of Canada's 100 most powerful people in the AI category. In 2026, he was featured as a BetaKit Most Ambitious Canadian.

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Andy Cooper

*University of
Liverpool, UK*

Andy is a Royal Society Research Professor and Academic Director of the Materials Innovation Factory (MIF) at the University of Liverpool. He also directs the Leverhulme Centre for Functional Materials Design and pioneered automated, robotics-driven materials discovery, helping establish one of the world's first academic facilities for materials research using automation and robotics. Elected a Fellow of the Royal Society in 2015 and a Foreign Member of the Chinese Academy of Sciences in 2023, he has received numerous honours, including the Hughes Medal (2019), RSC Interdisciplinary Prize (2021), SAIL Award (2021), and Davy Medal (2025). His research focuses on materials chemistry, AI, machine learning, and autonomous robot chemists.

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Fernanda Duarte

*University of
Oxford, UK*

Fernanda Duarte is an Associate Professor in the Department of Chemistry at Oxford. She obtained her PhD from the Pontificia Universidad Católica de Chile in 2012. As a postdoctoral researcher, she trained in biomolecular modelling with Prof. Lynn Kamerlin at Uppsala University and in computational organic chemistry with Prof. Robert Paton at the University of Oxford as a Newton Fellow. After a brief period as a lecturer at the University of Edinburgh, she returned to Oxford in 2018 as an Associate Professor. Her research combines software development (e.g. autodE, Cgbind and mlp-train) with practical applications, from enzymes to small molecules, focusing on mechanistic modelling and molecular design. Fernanda has received several awards, including the MGMS Frank Blaney Award (2020), the OpenEye Outstanding Junior Faculty Award (2021), the Harrison-Meldola Memorial Prize (2021), and the Novartis Early Career Award in Chemistry (2022). She was also selected as a Finalist for Chemical Sciences in the 2024 Blavatnik Award in the UK.

Ganna Gryn'ova

*University of
Birmingham, UK*

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Jun Jiang

*University of
Science and
Technology of
China (USTC),
Hefei, China*

Dr. Jun Jiang is a Distinguished Professor at the University of Science and Technology of China (USTC). He earned his BSc in Theoretical Physics from Wuhan University in 2000 and a PhD in Theoretical Chemistry from the Royal Institute of Technology, Sweden, in 2007. His research focuses on multi-scale modeling, quantum chemistry, molecular mechanics, solid-state physics and biophotonics. His recent work develops the Robotic AI-Chemist, an autonomous platform integrating theoretical computation, wet-lab experiments and automated robotic workflows.

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Michele Ceriotti
EPFL, Switzerland

Michele Ceriotti is a professor at EPFL, where he leads the laboratory for Computational Science and Modeling and directs the Institute of Materials. His research interests are rooted in the atomistic-scale modeling of matter bridging quantum mechanics, statistical physics and machine learning. He has contributed modeling insights into several classes of materials, from water and aqueous systems to molecular crystals, functional materials, metallic alloys and high-entropy compounds. He is a vocal advocate of open science and open software, leading the development of several open-source modeling tools including <http://metatensor.org>, <http://ipi-code.org> and <http://chemiscope.org>.

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Olexandr Isayev

*Carnegie Mellon
University, USA*

Olexandr Isayev is Carl and Amy Jones Professor of Chemistry at Carnegie Mellon University. In 2008, Olexandr received his Ph.D. in computational chemistry. He was a Postdoctoral Research Fellow at Case Western Reserve University and a scientist at the government research lab. Before CMU, he was a faculty at UNC Eshelman School of Pharmacy, the University of North Carolina at Chapel Hill. Olexandr is a 2023 Scialog Fellow and Associate Editor for the ACS Journal of Chemical Information and Modeling. The research in his lab focuses on connecting artificial intelligence (AI) with chemical sciences.

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Peter Seeberger

*Max-Planck
Institute for
Colloids and
Interfaces,
Germany*

Peter H. Seeberger, a chemist, was a tenured professor at MIT and ETH Zurich before becoming director at the Max-Planck Institute in Potsdam in 2009. Since 2021, he is in addition a Vice President of the German Research Foundation (DFG) and since 2023 the Founding Director of the Center for the Transformation of Chemistry (CTC) that received initial funding of €1.25 billion. His research spanning topics from engineering to immunology has been documented in >740 journal articles and >60 patent families and was recognized with >40 international awards.

Peter Seeberger supports diamond open access publishing as the Editor-in-Chief of the Beilstein Journal of Organic Chemistry. He is a co-founder of several successful companies.

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Raghavan B Sunoj

*Indian Institute of
Technology
Bombay*

(IIT Bombay), India

Raghavan B. Sunoj received a PhD in the year 2001 from Indian Institute of Science Bangalore and a postdoctoral training at the Ohio State University (USA) before joining IIT Bombay in 2003. He is currently a professor of chemistry and at the centre for machine intelligence and data science and holds the Google cloud chair in generative-AI. His research interests are in computational chemistry and machine learning as applied to asymmetric catalysis and reaction mechanism.

He is a receipt of prestigious national awards such as the Shanti Swarup Bhatnagar prize (2019) in Chemical Sciences and National Award to Teachers (higher education) (2023). He is an elected fellow of the Indian Academy of Sciences as well as the National Academy of Sciences India. He is an elected member of the board of World Association of Theoretical and Computational Chemists (WATOC), Asia Pacific Association of Theoretical and Computational Chemists (APATCC), and Structural and Mechanistic Chemistry Division of the IUPAC. He is an associate editor of The Journal of Organic Chemistry. He serves on the editorial boards of Chemical Society Reviews (since 2023) and WIREs: computational molecular science (till 2024). He is a member of editorial advisory boards of Chemical Science, Chem, Journal of Computational Chemistry, and Organic Letters.

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Richard Bourne

*University of Leeds,
UK*

Richard A. Bourne is currently a Professor of Digital Chemical Manufacturing at the University of Leeds. He completed a PhD under the supervision of Prof. Martyn Poliakoff, CBE, FRS. He is now a Royal Academy of Engineering Research Chair working on the AI guided development of new sustainable processes with focus on continuous flow routes to pharmaceutical and fine chemical products. His group is based within the Institute of Process Research and Development (IPRD) at the University of Leeds, a joint institute between Chemical Engineering and Chemistry.

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Taylor Sparks

*University of Utah,
USA*

Dr. Sparks is a Professor of Materials Science and Engineering at the University of Utah. He holds a BS in MSE from Utah, an MS in Materials from UCSB, and a PhD in Applied Physics from Harvard. A Royal Society Wolfson Visiting Fellow (University of Liverpool), NSF CAREER Awardee, and TEDxSaltLakeCity speaker, he serves as Editor-in-Chief of IMMI, Director of Graduate Affairs for the John and Marcia Price College of Engineering, and Director of the newly awarded NSF PCL Node AURORA. Outside the lab, he hosts the Materialism podcast, creates materials education videos on YouTube, and goes canyoneering with his four kids in Utah.

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Timothy Noël

*University of
Amsterdam,
Netherlands*

Timothy Noël is Professor and Chair of Flow Chemistry at the University of Amsterdam. His research focuses on the convergence of synthetic organic chemistry with enabling technologies, including flow chemistry, automation, robotics, and artificial intelligence, to accelerate sustainable chemical synthesis. His contributions have been recognized with several international awards, including the DECHEMA Award, the IUPAC-ThalesNano Flow Chemistry Award, the KNCV Gold Medal, an ERC Consolidator Grant, an NWO Vici Grant, and the 2026 Prous Institute-Overton and Meyer Award for New Technologies in Drug Discovery. He serves as Editor-in-Chief of the *Journal of Flow Chemistry* and President of the Flow Chemistry Society.