

Chemical Science symposium:

Digital chemistry in the age of AI
and machine learning

29-30 October 2026, London, UK



ROYAL SOCIETY
OF CHEMISTRY



Thursday 29 October (timings are GMT)

09:00	Registration and refreshments
10:00	Welcome and introductions Rebecca Campbell, Executive Editor, <i>Chemical Science</i>
	Session 1 (Session chair: Graeme Day)
10:20	Reaction modelling and synthesis planning: from mechanistic insights to data-driven exploration Fernanda Duarte <i>University of Oxford, UK</i>
11:05	Automated Synthesis Provides Reliable Data for Machine Learning – Towards the Autonomous Laboratory Peter Seeberger <i>Max-Planck Institute for Colloids and Interfaces, Germany</i>
11:50	Rewards as a conditioning mechanism for new materials Taylor Sparks <i>University of Utah, USA</i>
12:35	Lunch and posters
	Session 2 (Session chair: Tanja Junkers)
14:00	RoboChem and the Rise of Intelligent (Flow) Chemistry Timothy Noël <i>University of Amsterdam, The Netherlands</i>
14:45	Self-optimising Flow Reactors for Sustainable Process Development Richard Bourne <i>University of Leeds, UK</i>
15:30	Refreshments
	2026 Chemical Science Lectureship session (Session chair: Andy Cooper)
16:00	El Agente está Presente: Theoretical and Computational chemistry has changed forever Alán Aspuru-Guzik <i>University of Toronto, Canada</i>
16:45	Flash poster presentations (by invitation)
17:15	Poster session
19:00	Close of sessions



Friday 30 October (timings are GMT)

09:00	Welcome
	Session 4 (Session chair: Graeme Day)
09:10	Machine Learning and Generative-AI for Chemical Reaction Development Raghavan B Sunoj <i>IIT Bombay, India</i>
09:55	Building a Global Infrastructure for AI-Driven Innovation Jun Jiang <i>University of Science and Technology of China, China</i>
10:40	Refreshments
	Session 5 (Session chair: Tanja Junkers)
11:10	Title - TBC Andy Cooper <i>Institute, country</i>
11:55	Accelerating molecular design with autonomous AI agents Olexandr Isayev <i>Carnegie Mellon University, USA</i>
12:40	Publishing Q&A - Introduction – Rebecca Campbell - RSC editor panel discussion (<i>Journals</i>)
13:25	Lunch and photo
	Session 6 (Session chair: Andy Cooper)
14:45	Errors that matter: Uncertainty-aware universal machine-learning potentials calibrated on experiments Michele Ceriotti <i>EPFL, Switzerland</i>
15:30	Physics-rich machine learning and design of functional organic molecules and materials Ganna Gryn'ova <i>University of Birmingham, UK</i>
16:15	Poster prizes and concluding remarks
16:30	Close of sessions