ScotChem Computational Chemistry Symposium 2026

University of Edinburgh
16th June 2026

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School of Chemistry

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Computational Chemistry Symposium

Programme

Venue:
Joseph Black Building, David Brewster Road, King's Buildings, Edinburgh EH9 3FJ

9:45 – 10:15	Arrival + Registration and Poster Mounting
10:15 – 10:25	Welcome and Announcements
	Session 1 (Chair- Michael Bühl)
10:25 – 10:50	Scott Cockroft - *Transmembrane Transport: Simulation-Guided Discovery*
10:50 – 11:15	Laia Vila Nadal – *From Molecular Electronic Structure to Inverse Design*
11:15 – 11:40	Connor Macdonald – *Machine Learning for Supramolecular Design*
11:40 – 12:05	Malin Zollner – *Multireference Excited-State Screening Reveals Hidden Candidate Space in Organic Semiconductors*
12:05 – 13:20	Lunch and Poster Session
	Session 2 (Chair- Tanja van Mourik)
13:20 – 13:30	Magdalena Drafi-McHugh (Edinburgh International Data Facility)
13:30 – 13:55	Ross Urquhart – *Peptides at the Interface – A Study on TIP4P Water Models*
13:55 – 14:20	Ben Connaughton – *Computational Explorations of Halogenase Substrate Scope*
14:20 – 14:45	Hrithik Manojkumar – *Exploration of Computational Protocols for the Study of Cu-catalysed Reactions*
14:45 – 15:15	Coffee Break
	Session 3 (Chair- Hans Senn)
15:15 – 15:40	Kade Spicer – *Differential Ionisation in Proton-Helium Collisions*
15:40 – 16:05	Cecilia Hong – *Conformational Isomerism Tunes Refrigeration Potential in MOFs*
	Keynote Lecture
16:05 – 17:05	Natalie Fey – *Computational Chemistry x Data Science*
17:05 – 17:45	Posters, Drinks and Networking
17:45 – 18:00	Announcement of Poster Prizes, Closing Remarks