

ScotChem Computational Chemistry Symposium 2026

University of Edinburgh
16th June 2026

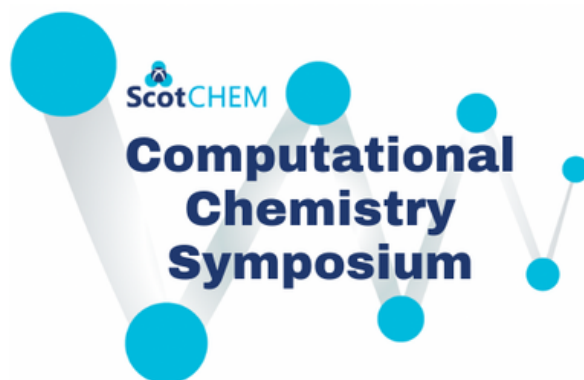


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Programme

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
10:25 – 10:50	Scott Cockroft - <i>Transmembrane Transport: Simulation-Guided Discovery</i>
10:50 – 11:15	Laia Vila Nadal – <i>From Molecular Electronic Structure to Inverse Design</i>
11:15 – 11:40	Connor Macdonald – <i>Machine Learning for Supramolecular Design</i>
11:40 – 12:05	Malin Zollner – <i>Multireference Excited-State Screening Reveals Hidden Candidate Space in Organic Semiconductors</i>
12:05 – 13:20	Lunch and Poster Session
	Session 2
13:20 – 13:30	Magdalena Drafi-McHugh (Edinburgh International Data Facility)
13:30 – 13:55	Ross Urquhart – <i>Peptides at the interface – A study on TIP4P water models</i>
13:55 – 14:20	Ben Connaughton – <i>Computational Explorations of Halogenase Substrate Scope</i>
14:20 – 14:45	Hrithik Manojkumar – <i>Exploration of computational protocols for the study of Cu-catalysed reactions</i>
14:45 – 15:15	Coffee Break
	Session 3
15:15 – 15:40	Gagan Preet – <i>TBD</i>
15:40 – 16:05	Cecilia Hong – <i>Conformational isomerism tunes refrigeration potential in MOFs</i>
	Keynote Lecture
16:05 – 17:05	Natalie Fey – <i>Computational Chemistry x Data Science</i>
17:05 – 17:45	Posters, Drinks and Networking
17:45 – 18:00	Announcement of Poster Prizes, Closing Remarks