

Molecular excited states theory and experiment

14–16 September 2026 | Cambridge, UK



Faraday
Discussions

Monday 14 September 2026 (All timings are BST)

11:30	Registration and lunch
12:30	Welcome and introductions Michael Bearpark, <i>Imperial College London, UK</i> Javier Segarra Martí, <i>Universitat de València, Spain</i> <i>Co-chairs of Scientific Committee</i>
12:40	Build on software – Sponsor flash talk Nisha Patel Director of Developer Tools Customer Engineering, Intel
12:45	Outline of Discussion format Amy Lucas, Evie Karkera, <i>Royal Society of Chemistry Publishing Editors</i>
12:50	(Session chair: Michael Bearpark) Introductory lecture – Spiers memorial lecture Michael A Robb <i>Imperial College London, UK</i>
13:50	Short break (water available)
	Session 1: The excited state electronic structure problem: new methods and computer architectures (Session chair: Basile Curchod)
14:00	EOM-fpCCSD: an accurate alternative to EOM-CCSD for doubly excited and charge-transfer states Katharina Boguslawski <i>Nicolaus Copernicus University, Poland</i>
14:05	Symmetry-adapted generalised normal-ordered coupled-cluster theory for excited states Bang Huynh <i>University of Oxford, UK</i>
14:10	Multireference perturbation theory (MRPT) geometry optimisations with scalar-relativistic effects: effective core potential (ECP) and spin-free X2C Hamiltonian Jae Woo Park <i>Chungbuk National University, South Korea</i>
14:15	Unified adiabatic and diabatic excited-state description via the ensemble-variational quantum eigensolver Benjamin Lasorne <i>Univ Montpellier, France</i>
14:20	Discussion
16:00	Refreshments
	Session 2: AI and data-driven approaches in molecular excited states (Session chair: Michael Bearpark)
16:30	Active delta-learning for surface hopping: efficient fitting of potential energy surfaces Pavlo O. Dral <i>Xiamen University, China; NCU in Toruń, Poland; Aitomistic, China</i>
16:35	Beyond minimum energy conical intersections: a data-driven reconstruction of the accessible intersection seam Elisa Pieri <i>University of North Carolina at Chapel Hill, USA</i>
16:40	A data-efficient machine-learning approach for modeling the photodynamics of all-trans hexatriene based on multireference configuration interaction calculations Hans Lischka <i>Texas Tech University, USA</i>
16:45	Discussion
18:00	Lightning poster presentations (odds) (by invitation of the Scientific Committee)
18:15	Poster session (odds) and wine reception
19:30	Close of sessions

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Tuesday 15 September 2026 (All timings are BST)

	Session 1 continued: The excited state electronic structure problem: new methods and computer architectures (Session chair: Javier Segarra Martí)
09:00	Shake-up resonances in dissociative electron attachment of formamide Ksenia Bravaya <i>University of Boston, USA</i>
09:05	Benchmarking electronic-structure methods for nonadiabatic dynamics in a propeller-shaped molecular rotor: Insights into conical intersections Rachel Crespo-Otero <i>University College London, UK</i>
09:10	Modular integration of MRSF-TDDFT, NAMD, and QM/MM for excited-state dynamics on the OpenQP platform Cheol Ho Choi <i>Kyungpook National University, South Korea</i>
09:15	Discussion
10:30	Refreshments
	Session 3: Non-adiabatic and ultrafast dynamics: models and measurements (Session chair: Oksana Plekan)
11:00	From reproducibility to comparability in computational photochemistry: lessons from the PhotoChem explorer prototype Nanna H. List <i>KTH Royal Institute of Technology, Sweden and University of Birmingham, UK</i>
11:05	Time-resolved extreme ultraviolet photoelectron spectroscopy of 4-bromophenolate anions in a liquid jet Daniel Neumark <i>University of California, Berkeley, USA</i>
11:10	Advances in the projected forces and momenta decoherence method for attosecond nonadiabatic molecular dynamics Fernando Martín <i>IMDEA Nanoscience and Universidad Autonoma de Madrid, Spain</i>
11:15	Discussion
12:30	Lunch
	Session 3 continued: Non-adiabatic and ultrafast dynamics: models and measurements (Session chair: Caroline Dessent)
14:00	Frequency-resolved ultrafast electron diffraction: visualizing vibrational dynamics in frequency- and real-space Kasra Amini <i>Max-Born-Institute, Germany</i>
14:05	The information content in ultrafast observables: spectroscopy and scattering in excited norbornadiene Adam Kirrander <i>University of Oxford, UK</i>
14:10	Discussion
15:00	Refreshments

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	Session 3 continued: Non-adiabatic and ultrafast dynamics: models and measurements (Session chair: Basile Curchod)
15:30	Solvent and field effects on photoinduced ring-opening: dynamics of furan as a case study Lea Ibele <i>ICR, Aix Marseille University, CNRS, France</i>
15:35	Towards direct dynamics simulation of photochemistry without the Born-Oppenheimer approximation Ryan MacDonell <i>Dalhousie University, Canada</i>
15:40	Modelling photoelectron spectra in solution: adenosine as a test case Roberto Improta <i>Consiglio Nazionale delle Ricerche, Italy</i>
15:45	Discussion
17:00	Lightning poster presentations (evens) (by invitation of the Scientific Committee)
17:15	Poster session (evens) and wine reception
18:30	Close of sessions
19:30	Conference dinner

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Wednesday 16 September 2026 (All timings are BST)

	Session 4: Developing links with large-scale experiments: computing observables and interpreting measurements in new facilities (Session chair: Adam Kirrander)
09:00	Real-space imaging of valence-electron bonding dynamics with ultrafast hard X-Ray scattering Thomas Wolf <i>LCLS and Stanford PULSE Institute, SLAC National Accelerator Laboratory, USA</i>
09:05	Understanding resonant inelastic X-ray scattering experiments of diazines via quantum dynamics simulation Antonia Freibert <i>Technical University of Munich, Germany</i>
09:10	Time-resolved photoemission with mixed-reference spin-flip TDDFT Petr Slavicek <i>University of Chemistry and Technology, Prague, Czech Republic</i>
09:15	Discussion
10:30	Refreshments
	Session 4 continued: Developing links with large-scale experiments: computing observables and interpreting measurements in new facilities (Session chair: Daniel Neumark)
11:00	Optimisation of measurement and data analysis of time-resolved X-ray absorption spectroscopy of thin film organic semiconductors Belen Alonso Garcia <i>Imperial College London, UK</i>
11:05	Spectrally resolved X-ray scattering Peter M. Weber <i>Brown University, USA</i>
11:10	Time-resolved core-level photoelectron spectroscopy of glycine fragmentation: a case study on the capabilities and limitations of site-selective probes at XFELs Andre Al-Haddad <i>Paul Scherrer Institute, Switzerland</i>
11:15	Discussion
12:30	(Session chair: Javier Segarra Martí) Concluding remarks lecture Graham A. Worth <i>University College London, UK</i>
13:00	Acknowledgements
13:15	Close of meeting and lunch