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, *Imperial College London, UK* Javier Segarra Martí, *Universitat de València, Spain* *Co-chairs of Scientific Committee*
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, *Royal Society of Chemistry Publishing Editors*
12:50	(Session chair: Michael Bearpark) **Introductory lecture – Spiers memorial lecture** Michael A Robb *Imperial College London, UK*
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 *Nicolaus Copernicus University, Poland*
14:05	**Symmetry-adapted generalised normal-ordered coupled-cluster theory for excited states** Bang Huynh *University of Oxford, UK*
14:10	**Multireference perturbation theory (MRPT) geometry optimisations with scalar-relativistic effects: effective core potential (ECP) and spin-free X2C Hamiltonian** Jae Woo Park *Chungbuk National University, South Korea*
14:15	**Unified adiabatic and diabatic excited-state description *via* the ensemble-variational quantum eigensolver** Benjamin Lasorne *Univ Montpellier, France*
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 *Xiamen University, China; NCU in Toruń, Poland; Aitomistic, China*
16:35	**Beyond minimum energy conical intersections: a data-driven reconstruction of the accessible intersection seam** Elisa Pieri *University of North Carolina at Chapel Hill, USA*
16:40	**A data-efficient machine-learning approach for modeling the photodynamics of all-trans hexatriene based on multireference configuration interaction calculations** Hans Lischka *Texas Tech University, USA*
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

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 *University of Boston, USA*
09:05	**Benchmarking electronic-structure methods for nonadiabatic dynamics in a propeller-shaped molecular rotor: Insights into conical intersections** Rachel Crespo-Otero *University College London, UK*
09:10	**Modular integration of MRSF-TDDFT, NAMD, and QM/MM for excited-state dynamics on the OpenQP platform** Cheol Ho Choi *Kyungpook National University, South Korea*
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 *KTH Royal Institute of Technology, Sweden and University of Birmingham, UK*
11:05	**Time-resolved extreme ultraviolet photoelectron spectroscopy of 4-bromophenolate anions in a liquid jet** Daniel Neumark *University of California, Berkeley, USA*
11:10	**Advances in the projected forces and momenta decoherence method for attosecond nonadiabatic molecular dynamics** Fernando Martín *IMDEA Nanoscience and Universidad Autonoma de Madrid, Spain*
11:15	Discussion
12:30	Lunch
	Session 3 continued: Non-adiabatic and ultrafast dynamics: models and measurements (Session chair: Rocío Borrego-Varillas)
14:00	**Towards few-femtosecond and frequency-resolved ultrafast electron diffraction: visualizing conical intersection vibrational dynamics in real and frequency space** Kasra Amini *Max-Born-Institute, Germany*
14:05	**The information content in ultrafast observables: spectroscopy and scattering in excited norbornadiene** Adam Kirrander *University of Oxford, UK*
14:10	Discussion
15:00	Refreshments

	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 *ICR, Aix Marseille University, CNRS, France*
15:35	**Towards direct dynamics simulation of photochemistry without the Born-Oppenheimer approximation** Ryan MacDonell *Dalhousie University, Canada*
15:40	**Modelling photoelectron spectra in solution: adenosine as a test case** Roberto Improta *Consiglio Nazionale delle Ricerche, Italy*
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

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 *LCLS and Stanford PULSE Institute, SLAC National Accelerator Laboratory, USA*
09:05	**Understanding resonant inelastic X-ray scattering experiments of diazines *via* quantum dynamics simulation** Antonia Freibert *Technical University of Munich, Germany*
09:10	**Time-resolved photoemission with mixed-reference spin-flip TDDFT** Petr Slavicek *University of Chemistry and Technology, Prague, Czech Republic*
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 *Imperial College London, UK*
11:05	**Spectrally resolved X-ray scattering** Peter M. Weber *Brown University, USA*
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 *Paul Scherrer Institute, Switzerland*
11:15	Discussion
12:30	(Session chair: Javier Segarra Martí) **Concluding remarks lecture** Graham A. Worth *University College London, UK*
13:00	**Acknowledgements**
13:15	**Close of meeting and lunch**