Molecular excited states theory and experiment

14–16 September 2026 | Cambridge, UK

Faraday Discussions

Monday 14 September 2026

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	**Outline of Discussion format** *Royal Society of Chemistry Publishing Editors*
12:45	**Introductory lecture – Spiers memorial lecture** (Session chair:) Michael A Robb *Imperial College London, UK*
	Session 1: The excited state electronic structure problem: new methods and computer architectures (Session chair:)
13:45	**Title TBC** Katharina Boguslawski *Nicolaus Copernicus University, Poland*
13:50	**Symmetry-projected generalised normal-ordered copuled-cluster theory for excited states** Bang Huynh *University of Oxford, UK*
13:55	**Multireference perturbation theory (MRPT) geometry optimizations with scalar-relativistic effects: Effective core potential (ECP) and spin-free X2C Hamiltonian** Jae Woo Park *Chungbuk National University, South Korea*
14:00	**Ground- and Excited-State Description via a Hybrid Quantum-Classical Method: Case Study of Three States** Benjamin Lasorne *Univ Montpellier, France*
14:05	Discussion
15:45	Refreshments
16:15	**Title TBC** Ksenia Bravaya *University of Boston, USA*
16:20	**Benchmarking electronic-structure methods for nonadiabatic dynamics in a propeller-shaped molecular rotor: Insights into conical intersections** Rachel Crespo-Otero *University College London, UK*
16:25	**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*
16:30	Discussion
17:45	Lightning presentations (by invitation of the Scientific Committee)
18:15	Poster session and wine reception
19:30	Close of sessions

Tuesday 15 September 2026

	Session 2: Non-adiabatic and ultrafast dynamics: models and measurements (Session chair:)
09:00	**Title TBC** Nanna List *KTH Royal Institute of Technology, Sweden and University of Birmingham, UK*
09:05	**Time-resolved extreme ultraviolet photoelectron spectroscopy of 4-bromophenotate anions in a liquid jet** Daniel Neumark *University of California, Berkeley, USA*
09:10	**Modeling the coupled electron-nuclear dynamics following electronic coherences induced by attosecond and few-femtosecond light pulses** Fernando Martin *IMDEA Nanoscience and Universidad Autonoma de Madrid, Spain*
09:15	Discussion
10:30	Refreshments
11:00	**Ultrafast electron diffraction imaging of chemical substitution effects on nonadiabatic nuclear dynamics at conical intersections** Kasra Amini *Max-Born-Institute, Germany*
11:05	**The Information Content in Ultrafast Observables: Spectroscopy and Scattering in Excited Norbornadiene** Adam Kirrander *University of Oxford, UK*
11:10	**Modeling correlation effects in photoionization spectroscopy and photoelectron circular dichroism of ground- and excited-state molecular systems.** Sonia Coriani *Technical University of Denmark, Denmark*
11:15	Discussion
12:30	Lunch
14:00	**Solvent and field effects on photoinduced ring-opening: dynamics of furan as a case study** Lea Ibele *ICR, Aix Marseille University, CNRS, France*
14:05	**Direct dynamics simulation of photochemistry without the Born-Oppenheimer approximation** Ryan MacDonell *Dalhousie University, Canada*
14:10	**Modelling photoelectron spectra in solution: deoxyadenosine as a test case** Roberto Improta *Consiglio Nazionale delle Ricerche, Italy*
14:15	Discussion
15:30	Refreshments
	Session 3: Developing links with large-scale experiments: computing observables and interpreting measurements in new facilities (Session chair:)
16:00	**Real-space imaging of the valence electron density during a photochemical reaction** Thomas Wolf *LCLS and Stanford PULSE Institute, SLAC National Accelerator Laboratory, USA*
16:05	**Understanding Resonant Inelastic X-ray Scattering Experiments of Diazines via Quantum Dynamics Simulation** Antonia Freibert

	Technical University of Munich, Germany
16:10	**Time-Resolved Photoemission Spectroscopy in the X-ray Domain: Opportunities and Challenges with Mixed-Reference Spin-Flip TDDFT** Petr Slavicek *University of Chemistry and Technology, Prague, Czech Republic*
16:15	Discussion
17:30	Close of sessions
18:30	Pre-dinner drinks
19:00	Conference dinner

Wednesday 16 September 2026

	Session 3 continued: Developing links with large-scale experiments: computing observables and interpreting measurements in new facilities (Session chair:)
09:00	**Title TBC** Mary Matthews *Imperial College London, UK*
09:05	**Measurement of Electron Correlations with X-Ray Scattering** Peter M. Weber **Brown University, USA**
09:10	**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*
09:15	Discussion
10:30	Refreshments
	Session 4: AI and data-driven approaches in molecular excited states (Session chair:)
11:00	**Active delta-learning for durface hopping: efficient fitting of potential energy surfaces** Pavlo O. Dral *Xiamen University, China; NCU in Toruń, Poland; Aitomistic, China*
11:05	**Beyond Minimum Energy Conical Intersections: A Data-Driven Reconstruction of the Accessible Intersection Seam** Elisa Pieri *University of North Carolina at Chapel Hill, USA*
11:10	**Machine Learning and Multireference Configuration Interaction for High-Level Nonadiabatic Dynamics Simulation of Hexatriene** Hans Lischka *Texas Tech University, USA*
11:15	Discussion
12:30	**Concluding remarks lecture** (Session chair:) Graham A. Worth *University College London, UK*
13:00	**Acknowledgements**
13:15	**Close of meeting and lunch**

Please note that this is a draft programme and timings may change.