

Quantum Effects in Complex Systems

Faraday Discussion



11–13 September 2019
Coventry
United Kingdom

Wednesday 11 September

11:30	Registration, Tea and Coffee	
12:00	Lunch	
12:45	Welcome and Introductions Scott Habershon, <i>Chair of Scientific Committee</i>	
12:55	Outline of Discussion Format Ruth Zadik and Laura Smith, <i>Royal Society of Chemistry Publishing Editors</i>	
13:00	Introductory Lecture (Session Chair: Scott Habershon) David Manolopoulos <i>University of Oxford, UK</i>	
	Session 1: Quantum coherence in complex environments (Session Chair: Garth Jones)	
14:00	Time-resolved spectra of I₂ in a krypton crystal by G-MCTDH simulations: nonadiabatic dynamics, dissipation and environment driven decoherence David Picconi and Irene Burghardt <i>University Frankfurt, Germany</i>	Paper 25981
14:05	Variety, the spice of life and essential for robustness in excitation energy transfer in light-harvesting complexes David Hutchinson, Sue Ann Oh and David F. Coker <i>University of Otago, New Zealand</i>	Paper 25691
14:10	How quantum is radical pair magnetoreception? Peter J Hore, Thomas P. Fay, Lachlan P. Lindoy and David E. Manolopoulos <i>University of Oxford, UK</i>	Paper 25962
14.15	OLEDs as models for bird magnetoreception: detecting electron spin resonance in geomagnetic fields Tobias Grünbaum, Sebastian Milster, Hermann Kraus, Wolfram Ratzke, Simon Kurrmann, Viola Zeller, Sebastian Bange, Christoph Boehme and John M. Lupton <i>Universität Regensburg, Germany</i>	Paper 25979
14.20	Discussion	
16:00	Afternoon tea	
16.30	Towards a spectroscopic protocol for unambiguous detection of quantum coherence in excitonic energy transport Animesh Datta, Max Marcus and George C. Knee <i>University of Warwick, UK</i>	Paper 25966
16:35	On the arrangement of chromophores in light harvesting complexes: chance versus design Alessandro Troisi, Kirsten Claridge and Daniele Padula <i>University of Liverpool, UK</i>	Paper 25994
16:40	Improved population operators for multi-state nonadiabatic dynamics with the mixed quantum-classical mapping approach Maximilian Saller, Aaron Kelly and Jeremy O. Richardson <i>ETH Zurich, Switzerland</i>	Paper 25995
16:45	Discussion	
18.00	Lightning presentations (by invitation of the scientific committee)	

18:15	Poster Session and Wine Reception
19.45	Evening Meal (Rootes Restaurant) – open to all delegates

Thursday 12 September

Session 2: Spectroscopic signatures of quantum effects (Session Chair: Gabriella Schlau-Cohen and Alex Jones)		
09:00	An experimental and computational study of the effect of aqueous solution on the multiphoton ionisation photoelectron spectrum of phenol <u>Helen Fielding</u> , Alice Henley, Jamie W. Riley and Bingxing Wang <i>University College London, UK</i>	Paper 25688
09:05	Using spectroscopy to probe relaxation, decoherence, and localization of photoexcited states in π-conjugated polymers <u>William Barford</u> , John L. A. Gardner and Jonathan R. Mannouch <i>University of Oxford, UK</i>	Paper 25949
09:10	Exploring the capabilities of optical pump X-ray probe NEXAFS spectroscopy to track photo-induced dynamics mediated by conical intersections <u>Francesco Segatta</u> , Artur Nenov, Silvia Orlandi, Alberto Arcioni, Shaul Mukamel and Marco Garavelli <i>University of Bologna, Italy</i>	Paper 25999
09:15	Discussion	
10:30	Morning Tea	
11:00	Limits of exciton delocalization in molecular aggregates <u>Greg Scholes</u> <i>Princeton University, USA</i>	Paper 25686
11:05	Modeling multidimensional spectral lineshapes from first principles: application to water-solvated adenine <u>Javier Segarra Martí</u> , Francesco Segatta, Tristan A. Mackenzie, Artur Nenov, Ivan Rivalta, Michael J. Bearpark and Marco Garavelli <i>Imperial College London, UK</i>	Paper 26031
11:10	Vibrational coherence and quantum yield of retinal-chromophore-inspired molecular switches <u>Jérémie Léonard</u> , Moussa Gueye, Marco Paolino, Etienne Gindensperger, Stefan Haacke and Massimo Olivucci <i>IPCMS; CNRS-Université de Strasbourg, France</i>	Paper 25993
11:15	Discussion	
12:30	Lunch	
Session 3: Zero-point energy and tunnelling (Session Chair: Graham Worth and David Tew)		
13:30	Which quantum statistics-classical dynamics method is best for water? <u>Stuart Althorpe</u> , Raz L. Benson and George Trenins <i>University of Cambridge, UK</i>	Paper 25690
13:35	What are the signatures of tunnelling in enzyme-catalysed reactions? <u>Sam Hay</u> , Linus O. Johannissen, Andreea I. Iorgu and Nigel S. Scrutton <i>University of Manchester, UK</i>	Paper 25980
13:40	Challenges in constructing accurate methods for hydrogen transfer reactions in large biological assemblies: rare events sampling for mechanistic discovery and tensor networks for quantum nuclear effects <u>Srinivasan Iyengar</u> and Nicole DeGregorio <i>Indiana University, USA</i>	Paper 26111
13:45	Discussion	

15:00	Afternoon Tea	
15:30	First-principles quantum simulations of exciton diffusion on a minimal oligothiophene chain at finite temperature Irene Burghardt and Robert Binder <i>Goethe University Frankfurt, Germany</i>	Paper 25689
15:35	Quantum proton tunneling in multi-electron/-proton transfer electrode processes Ken Sakaushi <i>National Institute for Materials Science, Japan</i>	Paper 25947
15:40	Classical and nonclassical effects in surface hopping methodology for simulating coupled electronic-nuclear dynamics Craig Martens <i>University of California, Irvine, USA</i>	Paper 25986
15:45	Discussion	
17:00	Close of sessions	
18:30	Pre-Dinner Drinks – Chancellors Suite, Rootes Building	
19:00	Conference Dinner – Chancellors Suite, Rootes Building	

Friday 13 September

	Session 4: Emerging opportunities and future directions (Session Chair: Scott Habershon)	
09:00	Nonadiabatic dynamics with quantum nuclei: simulating charge transfer with ring polymer surface hopping Soumya Ghosh, Samuele Giannini, Kevin Lively and Jochen Blumberger <i>Ruhr Universitaet Bochum, Germany</i>	Paper 25990
09:05	Temperature dependence of the vibrational spectrum of porphycene: a qualitative failure of classical-nuclei molecular dynamics Mariana Rossi, Yair Litman and Jörg Behler <i>Fritz Haber Institute of the Max Planck Society, Germany</i>	Paper 25989
09:10	Exciton dissociation and charge separation at donor-acceptor interfaces from quantum-classical dynamics simulations Aaron Kelly <i>Dalhousie University, Canada</i>	Paper 25961
09:15	Discussion	
10:30	Morning Tea	
11:00	Concluding Remarks Lecture (Session Chair: Scott Habershon) Sharon Hammes-Schiffer <i>Yale University, USA</i>	
11:45	Acknowledgements	
12:00	Close of meeting and lunch	

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