Reaction Rate Theory

Faraday Discussion

19-21 September 2016
Cambridge, UK

Monday 19 September

11:00	Registration, Tea and Coffee	
12:00	Lunch	
12:45	**Welcome and Introductions** Stuart C. Althorpe, *Chair of Scientific Committee*	
12:55	**Outline of Discussion Format** Ruth Zadik and Nicola Convine, *Royal Society of Chemistry Publishing Editors*	
13:00	**Introductory Lecture** (Session Chair: David Clary (University of Oxford)) William H. Miller *University of California, Berkeley*	
	Session 1: Fundamentals (Session Chair: David Clary (University of Oxford)	
14:00	**Low temperature chemistry using the R-matrix method** Jonathan Tennyson, Laura K McKemmish and Tom Rivlin *University College London*	**Paper 11347**
14:05	**Microcanonical and thermal instanton rate theory for chemical reactions at all temperatures** Jeremy O. Richardson *Durham University*	**Paper 11378**
14:10	**Atom tunnelling in the reaction $NH_3^+ + H_2 \rightarrow NH_4^+ + H$ and its astrochemical relevance** Sonia Álvarez-Barcia, Marie-Sophie Russ, Jan Meisner and Johannes Kästner *University of Stuttgart*	**Paper 11245**
14:15	Discussion	
15:30	Afternoon tea	
16:00	**Blip-summed quantum-classical path integral with cumulative quantum memory** Nancy Makri *University of Illinois at Urbana-Champaign*	**Paper 10868**
16:05	**Classical to quantum mechanical tunneling mechanism crossover in thermal transitions between magnetic states** Sergei Vlasov, Pavel F. Bessarab, Valery M. Uzdin and Hannes Jónsson *University of Iceland*	**Paper 11393**
16:10	**Kramers' theory for diffusion on a periodic potential** Reuven Ianconescu and Eli Pollak *Weizmann Institute of Science*	**Paper 11326**
16:15	Discussion	
17:30	Lightning presentations (by invitation of the scientific committee)	
18:00	Poster Session and Wine Reception	
19:30	Close & free evening	

Tuesday 20 September

	Session 2: Non-adiabatic reactions (Session Chair: Scott Habershon)	

09:00	**Proton-coupled electron transfer reactions: analytical rate constants and case study of kinetic isotope effects in lipoxygenase** Alexander V. Soudackov and Sharon Hammes-Schiffer *University of Illinois at Urbana-Champaign*	**Paper 10871**
09:05	**Kinetically-constrained ring-polymer molecular dynamics for non-adiabatic chemistries involving solvent and donor-acceptor dynamical effects** Joshua S. Kretchmer and Thomas F. Miller III *California Institute of Technology*	**Paper 10869**
09:10	**Confronting surface hopping molecular dynamics with Marcus theory for a molecular donor-acceptor system** Jacob Spencer, Laura Scalfi, Antoine Carof and Jochen Blumberger *University College London*	**Paper 11355**
09:15	**Photorelaxation of imidazole and adenine *via* electron-driven proton transfer along H_2O wires** Rafał Szabla, Robert W. Góra, Mikołaj Janicki and Jiří Šponer *Institute of Biophysics, Academy of Sciences of the Czech Republic*	**Paper 11392**
09:20	Discussion	
11:00	Morning Tea	
11:30	**State space path integrals for electronically nonadiabatic reaction rates** Jessica Ryan Duke and Nandini Ananth *Cornell University*	**Paper 10870**
11:35	**Deriving the exact nonadiabatic quantum propagator in the mapping variable representation** Timothy J. H. Hele and Nandini Ananth *Cornell University*	**Paper 11314**
11:40	**Reactive trajectories of the $Ru^{2+/3+}$ self-exchange reaction and the connection to Marcus' theory** Ambuj Tiwari and Bernd Ensing *Van't Hoff Institute for Molecular Sciences*	**Paper 11310**
11:45	Discussion	
13:00	Lunch	
	Session 3: New methods (Session Chair: Peter Bolhuis)	
14:00	**S-shooting: a Bennett–Chandler-like method for the computation of rate constants from committor trajectories** Georg Menzl, Andreas Singraber and Christoph Dellago *University of Vienna*	**Paper 10874**
14:05	**Direct generation of loop-erased transition paths in non-equilibrium reactions** Ralf Banisch and Eric Vanden-Eijnden *New York University*	**Paper 10873**
14:10	**Adaptive free energy sampling in multidimensional collective variable space using boxed molecular dynamics** Mike O'Connor, Emanuele Paci, Simon McIntosh-Smith and David R. Glowacki *University of Bristol*	**Paper 11390**
14:15	**The intrinsic rate constants in diffusion-influenced reactions** Adithya Vijaykumar, Peter G. Bolhuis and Pieter Rein ten Wolde *University of Amsterdam*	**Paper 11356**
14:20	Discussion	
16:00	Afternoon Tea	
16:30	**Effective dynamics along given reaction coordinates, and reaction rate theory** Wei Zhang, Carsten Hartmann and Christof Schütte	**Paper 10875**

	Freie Universität Berlin	
16:35	**Jump Markov models and transition state theory: the quasi-stationary distribution approach** Giacomo Di Gesù, Tony Lelièvre, Dorian Le Peutrec, Boris Nectoux *Ecole des Ponts ParisTech, CERMICS*	**Paper 11308**
16:40	**Uncertainty quantification for quantum chemical models of complex reaction networks** Jonny Proppe, Tamara Husch, Gregor N. Simm and Markus Reiher *ETH Zürich*	**Paper 11126**
16:45	Discussion	
18:00	Poster Session and Pre-Dinner Drinks	
19:30	Conference Dinner	

Wednesday 21 September

	Session 4: Application to large systems (Session Chair: Angelos Michaelides)	
09:00	**A variational approach to nucleation simulation** Pablo M. Piaggi, Omar Valsson and Michele Parrinello *ETH Zurich*	**Paper 10872**
09:05	**Lattice mold technique for the calculation of crystal nucleation rates** Jorge R. Espinosa, Pablo Sampedro, Chantal Valeriani, Carlos Vega and Eduardo Sanz *Universidad Complutense de Madrid*	**Paper 11381**
09:10	**Optical *vs.* chemical driving for molecular machines** R. Dean Astumian *University of Maine*	**Paper 11224**
09:15	Discussion	
10:30	Morning Tea	
11:00	**Unimolecular dissociation of peptides: statistical vs. non-statistical fragmentation mechanisms and time scales** Riccardo Spezia, Ana Martin-Somer, Veronica Macaluso, Zahra Homayoon, Subha Pratihar and William L. Hase *Université Paris Saclay, CEA CNRS*	**Paper 11331**
11:05	**Faraday efficiency and mechanism of electrochemical surface reactions: CO_2 reduction and H_2 formation on Pt(111)** Javed Hussain, Hannes Jónsson and Egill Skúlason *University of Iceland*	**Paper 11384**
11:10	**Pressure-dependent rate constants for PAH growth: formation of indene and its conversion to naphthalene** Alexander M. Mebel, Yuri Georgievskii, Ahren W. Jasper and Stephen J. Klippenstein *Florida International University*	**Paper 11354**
11:15	Discussion	
12:30	**Concluding Remarks Lecture** (Session Chair: Angelos Michaelides) David Chandler *University of California, Berkeley*	
13:10	**Acknowledgements**	
13:15	**Close of meeting and Lunch**	

Presenting authors are indicated in the programme by an underline. The affiliation is for the presenting author. If the presenting author of your paper has changed since abstract selection please email events@rsc.org. Please note that this is a draft programme and timings may change.