Faraday Division 145: Physical Organic Chemistry
2 – 4 September 2009
Cardiff (UWIC Llandaff Campus), UK

Wednesday 2 September 2009

11:30	**Registration**
12.30	**Lunch** (tickets required)
13:30	**Welcome and Introductions:** Colin Bain, *Durham University, UK*
Session 1	**Reaction Mechanisms 1** Session Chair: Colin Bain
13.45 **Paper 1**	**Introductory Lecture & Spiers Memorial Lecture** **Interplay of theory and computation in chemistry --- examples from on-water organic catalysis, enzyme catalysis, and single-molecule fluctuations** Rudolph A Marcus* *California Institute of Technology, USA*
14.45 **Paper 2**	**The kinetics and mechanisms of organic reactions in liquid ammonia** Mike Page*, John H Atherton and Pengju Ji *University of Huddersfield, UK*
Paper 3	**Interrogation of dynamic multi-catalyst ensemble in asymmetric catalysis** Guy Lloyd-Jones*, Julian Eastoe, Ian J S Fairlamb, Jesus M Fernández-Hernández, Emane Filali, John C Jeffery, Aina Martorell, Anthony Meadowcroft, Per-Ola Norrby, Thomas Riis-Johannessen, David A Sale and Paula M Tomlin *University of Bristol, UK*
15.45	**Afternoon Tea**
Session 2	**Theory and Simulation 1** Session Chair: Ian Williams
16.15 **Paper 4**	**Valence bond modelling and density functional theory calculations of reactivity and mechanism of Cytochrome P450 enzymes; thioether sulfoxidation** Sason Shaik*, Yong Wang, Hui Chen, Jinshuai Song and Rinat Meir *Hebrew University, Israel*
Paper 5	**The EVB as a quantitative tool for formulating simulations and analyzing biological and chemical reactions** Arieh Warshel* and Shina Caroline Lynn Kamerlin *University of Southern California, USA*
Paper 6	**On the catalytic role of structural fluctations in enzyme reactions: computational evidences in the formation of compound 0 in horseradish peroxidase** Massimiliano Aschi*, Andrea Amadei, Costantino Zazza, Amedeo Palma, Nico Sanna and Simone Tatoli *Universita di l'Aquila, Italy*
17.45	**Close of Session**
18:30	**Dinner** (all delegates invited - sponsored by Syngenta) syngenta
19:30	**Poster Session and Wine Reception** (all delegates invited sponsored by Syngenta) syngenta

RSC | Advancing the Chemical Sciences

Thursday 3 September 2009

Session 3	**Dynamics 1** Session Chair: Peter Chen
09:00 **Paper 7**	**Methylene-transfer reactions of benzylium/tropylium ions with neutral toluene studied by means of ion-trap mass spectroscopy** Detlef Schröder*, Emilie-Laure Zins and Claude Pepe *Academy of Sciences, Czech Republic*
Paper 8	**Ultrafast time-resolved transient infrared and resonance Raman spectroscopy study of the photo-deprotection and rearrangement reactions of *p*-hydroxyphenacyl caged phosphates** Qian Cao,Yong Du, Michael W George*, Xiangguo Guan, Jiadon Xue, David Lee Phillips*, Wai Ming Kwok, Mingde Li, Chensheng Ma and Xue-Zhong Sun *University of Nottingham, UK*
Paper 9	**Ultrafast reaction dynamics in nanoscale water droplets confined by ionic surfactants** Minako Kondo, Ismael A Heisler and Stephen R Meech* *University of East Anglia, UK*
10:30	**Morning Coffee**
Session 4	**Self-assembly and Recognition** Session Chair: Chris Hunter
11:00 **Paper 10**	**New Host-guest chemistry of supramolecular nanotubes** Jeremy K M Sanders*, Emiliano Tamanini, Nandhini Ponnuswamy and G Dan Pantos *University of Cambridge, UK*
Paper 11	**The effect of multivalent binding on the lateral phase separation of adhesive lipids** Kwan Ping Liem, Gavin T Noble, Sabine L Flitsch and Simon J Webb* *University of Manchester, UK*
Paper 12	**Designing instructable networks using synthetic replicators** Douglas Philp* *University of St Andrews, UK*
12:30	**Lunch** (all delegates invited)

RSC | Advancing the Chemical Sciences

Session 5	**Reaction Mechanisms 2** Session Chair: Michael Page
13:30 **Paper 13**	**Phosphate ester analogues as probes for understanding enzyme catalysed phosphoryl transfer** Nicholas H Williams*, Abdulfattah alkherraz, Shina C L Kamerlin, Guoqiang Feng, Qaiser I Sheik and Arieh Warshel *University of Sheffield, UK*
Paper 14	**Radicals in enzymatic catalysis – a thermodynamic perspective** Johnny Hioe and Hendrik Zipse* *LMU München, Germany*
Paper 15	**The application of No Barrier Theory to the aldol addition reaction** J Peter Guthrie*, Alexander R Bannister and Sriyawathie Peiris *University of Western Ontario, Canada*
Paper 16	**Dynamic path bifurcation for the Beckmann reaction: observation and implication** Hiroshi Yamataka*, Makoto Sato, Hiroto Hasegawa and Salai Cheettu Amma*l* *Rikkyo University, Japan*
15.30	**Afternoon Tea**
Session 6	**Interfaces** Session Chair: Jay Seigel
16.00 **Paper 17**	**Oxidation of alcohols using supported gold and gold palladium nanoparticles** Peter J Miedziak, David W Knight, Donald Bethell, Meenakshisundaram Sankar, Ewa Nowicka, Gemma L Brett, Robert L Jenkins, Nikolaos Dimitratos and Graham J Hutchings* *University of Cardiff, UK*
Paper 18	**Structure and dynamics of phospholipid bilayer films under electrochemical control** A Robert Hillman*, Karl S Ryder, Andrew W Burley, Richard J Wiltshire, James Merotra, Michaela Grau, Sarah I Horswell, Andrew Glidle, Robert M Dalgliesh, Arwel Hughes and Andrew Wildes *University of Leicester, UK*
17:00	**Close of Session**
18.45	Coach transfer to Angel Hotel
19:15	Pre-Dinner Drinks, Angel Hotel (all delegates invited)
19.30	Conference Dinner (all delegates invited)
22.30	Coach transfer to UWIC Llandaff

RSC | Advancing the Chemical Sciences

Friday 4 September 2009

Session 7	**Dynamics 2** Session Chair: Barry Carpenter
09:00 **Paper 20**	**Ultrafast dynamics of malachite green at the air/water interface studied by femtosecond time-resolved sum frequency generation (TR-ESFG): An indicator for local viscosity** Tahei Tahara*, Pratik Sen and Shoichi Yamaguchi *RIKEN, Japan*
Paper 21	**Probing the effect of the solution environment on the vibrational dynamics of an enzyme model system with ultrafast 2D-IR spectroscopy** G M Bonner, A R Ridley, S K Ibrahim, C J Pickett and N T Hunt* *University of Strathclyde, UK*
Paper 22	**Understanding solvent effects on structure and reactivity of organic intermediates: a Raman study** G Balakrishnan, S Sahoo, B K Chowdhury and Siva Umapathy* *Indian Institute of Science, India*
10:30	**Morning Coffee**
Session 8	**Theory and Simulation 2** Session Chair: Rory More O'Ferrall
11:00 **Paper 23**	**Entropic trends in aqueous solutions of the common functional groups** Richard H Henchman*, Sheeba Jem Irudayam and Richard D Plumb *University of Manchester, UK*
Paper 24	**Ab initio transition state theory for polar reactions in solution** Jeremy Harvey* *University of Bristol, UK*
Paper 25	**Electronic Structures of [n]-Cyclacenes (n = 6–12) and Short, Hydrogen-Capped, Carbon Nanotubes** Christopher Cramer*, Daniel Sadowsky and Kristopher McNiell *University of Minnesota, USA*
12:30 **Paper 26**	**Concluding Remarks** Josef Michl* *University of Colorado, USA*
13:00	**Acknowledgements:** Colin Bain, *University of Durham, UK*
13:15	**Close of Meeting**
13.15	**Lunch** (tickets required)

* denotes presenting author to whom affiliation applies