

Programme

Faraday Discussion 163: Photo-initiated quantum molecular dynamics 15-17 April 2013 Nottingham, UK

15 April

11:00	Registration, tea and coffee
12.45	Welcome and Introductions Helen Fielding
13.00 Paper 1	Introductory Lecture: Albert Stolow* <i>National Research Council, Canada</i>
Session 1	Single molecules: photochemistry and photophysics in isolated molecular systems Session chair: Helen Fielding
14:00 Paper 2	A New approach towards transition state spectroscopy Kirill Prozument, Rachel Glyn Shaver, Monika Ciuba, John S. Muentner, G. Barratt Park, John F. Stanton, Hua Guo, Bryan M. Wong, David S. Perry and Robert W. Field* <i>Massachusetts Institute of Technology, USA</i>
Paper 3	Time-resolved imaging of the iodide-thymine and iodide-uracil binary cluster systems Sarah B. King, Margaret A. Yandell and Daniel M. Neumark* <i>University of California, Berkeley, USA</i>
15:00	Afternoon Tea Session chair: Katharine Reid
15:30 Paper 4	A multi-sheeted three-dimensional potential energy surface for the H-atom photodissociation of phenol Sai G. Ramesh and Wolfgang Domcke* <i>Technische Universität München, Germany</i>
Paper 5	Probing ultrafast dynamics in photoexcited pyrrole: timescales for $1\pi\sigma^*$ mediated H-atom elimination Gareth M. Roberts, Craig A. Williams, Hui Yu, Adam S. Chatterley, Jamie D. Young, Susanne Ullrich and Vasilios G. Stavros* <i>University of Warwick, UK</i>
16:30	Close of Sessions
16:30 – 18:00	Poster Session and Wine Reception
19:00	Dinner (dinner tickets only)

16 April

Session 2	Extended systems: photochemistry and photophysics of chromophores in proteins, solution or clusters Session Chair: Andrew Orr-Ewing
09:00 Paper 6	Electronic transient spectroscopy from the deep UV to the NIR: unambiguous disentanglement of complex processes Eberhard Riedle*, Maximilian Bradler, Matthias Wenninger, Christian F. Sailer and Igor Pugliesi <i>Ludwig-Maximilians-Universität, Germany</i>
Paper 7	Ultrafast ring-opening reactions: a comparison of α-terpinene, α-phellandrene, and 7-dehydrocholesterol with 1,3-cyclohexadiene Brenden C. Arruda, Broc Smith, Kenneth G. Spears and Roseanne J. Sension* <i>University of Michigan, USA</i>
Paper 8	Ultrafast photo-initiated molecular quantum dynamics in the DNA dinucleotide d(ApG) revealed by broadband transient absorption spectroscopy Mayra C. Stuhldreier and Friedrich Temps* <i>Christian-Albrechts-University Kiel, Germany</i>
10:30	Morning Coffee Session Chair: Graham Worth
11:00 Paper 9	Photodynamics of Lys+-Trp Protein Motifs: Hydrogen Bonds Ensure Photostability Matteo Guglielmi, Manuel Doemer, Ivano Tavernelli and Ursula Rothlisberger* <i>Swiss Federal Institute of Technology EPF Lausanne, Switzerland</i>
Paper 10	Coherent exciton transport driven by torsional dynamics: a quantum dynamical study of phenylene-vinylene type conjugated systems R. Binder, J. Wahl, S. Römer and Irene Burghardt* <i>Goethe University Frankfurt, Germany</i>
Paper 11	Quantum-classical effective-modes dynamics of the $\pi\pi^* \rightarrow n\pi^*$ decay in 9H-adenine. A quadratic vibronic coupling model David Picconi, Francisco José Avila Ferrer, Roberto Improta, Alessandro Lami and Fabrizio Santoro* <i>ICCOM-CNR</i>
12:30	Lunch Session Chair: Mike Bearpark
14:00 Paper 12	Ultrafast excited state dynamics of the green fluorescent protein chromophore and its kindling fluorescent protein analogue Steve Meech*, Kiri Addison, Ismael Heisler, Jamie Convard, Tara Dixon and Philip Page <i>University of East Anglia, UK</i>
Paper 13	Ultrafast dual photoresponse of isolated biological chromophores: link to the photoinduced mode-specific non-adiabatic dynamics in proteins Anastasia V. Bochenkova* and Lars H. Andersen <i>Aarhus University, Denmark</i>
Paper 14	Excited-state dynamics of Photoactive Yellow Protein

	chromophores elucidated by high-resolution spectroscopy and <i>ab initio</i> calculations Eric M. M. Tan, Saeed Amirjalayer, Bert H. Bakker and Wybren J. Buma* <i>University of Amsterdam, the Netherlands</i>
15:30	Close of Session & Afternoon Tea
Session 3	Applications of molecular dynamics to global challenges: photovoltaic cells, photodynamic therapy, imaging, ... Session Chair: Jan Verlet
16:00 Paper 15	Designs for molecular circuits that use electronic coherence Francesca Fassioli, Daniel G. Oblinsky and Gregory D. Scholes* <i>University of Toronto, Canada</i>
Paper 16	Time-resolved photoemission on the attosecond scale: opportunities and challenges Renate Pazourek, Stefan Nagele and Joachim Burgdörfer* <i>Vienna University of Technology, Austria</i>
Paper 17	How quasi-free holes and electrons are generated in organic photovoltaic interfaces Alessandro Troisi* <i>University of Warwick, UK</i>
17:30	Close of sessions
19:00	Pre-Dinner Drinks
19:30	Conference Dinner

17 April

Session 4	Controlling molecular dynamics: controlling photochemistry using sequences of light pulses, shaped light pulses or bond selection prior to photoexcitation Session chair: Christoph Meier
09:00 Paper 18	Active and passive control of zinc phthalocyanine photodynamics Divya Sharma, Annemarie Huijser, Janne Savolainen, Gerwin Steen and Jennifer Herek* <i>Universiteit Twente, the Netherlands</i>
Paper 19	Strong field control of predissociation dynamics María E. Corrales, Garikoitz Balerdi, Vincent Lorient, Rebeca de Nalda and Luis Bañares* <i>Universidad Complutense de Madrid, Spain</i>
Paper 20	Formation of fragment ions (H^+, H_3^+, CH_3^+) from ethane in intense femtosecond laser fields—from understanding to control Nora Schirmel, Nicola Reusch, Philipp Horsch and Karl-Michael Weitzel* <i>Philipps-Universität Marburg, Germany</i>
10:30	Morning Coffee Session chair: Ben Whitaker
11:00	On the possibility of enhanced multiple ionization near conical

Paper 21	intersections Phil H. Bucksbaum* and V. Petrovic <i>Stanford University, USA</i>
Paper 22	Coherent one-photon phase control in closed and open quantum systems: A general master equation approach Leonardo A. Pachón, Li Yu and Paul Brumer* <i>University of Toronto, Canada</i>
Paper 23	Photophysics of fulvene under the non-resonant Stark effect. Shaping the conical intersection seam Sergi Ruiz-Barragan and Lluís Blancafort* <i>University of Girona, Spain</i>
	Chair: Helen Fielding
12:30	Concluding Remarks Lecture Mike Ashfold* <i>University of Bristol, UK</i>
13:30	Acknowledgements
13:45	Close of Meeting