

# Temporally and Spatially Resolved Molecular Science

Faraday Discussion 177



**Monday 12 January**

10:00	Registration, Tea and Coffee	
12:00	Lunch	
12.45	<b>Welcome and Introductions</b> Siva Umapathy <i>Chair of Scientific Committee</i>	
12:55	<b>Outline of Discussion Format</b> Emma Cooper and Carla Pegoraro <i>Publishing Editors</i>	
13.00	Introductory Lecture <b>Volker Deckert</b> <i>Jena University</i>	<b>Paper 5020</b>
	<b>Session 1: Dynamics of chemical bond</b> Session Chair: Siva Umapathy	
14:00	<b>Breaking of a bond: when is it statistical?</b> Srihari Keshavamurthy*, Pankaj Yadav <i>Indian Institute of Technology Kanpur</i>	<b>Paper 4575</b>
14:05	<b>Negative hyperconjugation and red-, blue- or zero-Shift in X-Z---Y complexes</b> Eluvathingal Jemmis*, Joy Jyothish, Vidya Kaipanchery <i>Indian Institute of Science, Bangalore</i>	<b>Paper 4431</b>
14:10	<b>Dynamics of the chemical bond: Inter- and intra-molecular hydrogen bond</b> Elangannan Arunan*, Devendra Mani <i>Indian Institute of Science Bangalore</i>	<b>Paper 5022</b>
14:15	Discussion	
15:30	Afternoon Tea/poster session	
	<b>Session 1 resumes: Dynamics of chemical bond</b> Session Chair: Martin Zanni	
16:15	<b>Vibrational Dynamics of the CO Stretching of 9-Fluorenone</b> Keisuke Tominaga*, Yuki Fukui, Kaoru Ohta <i>Kobe University</i>	<b>Paper 4579</b>
16:20	<b>Dynamical, spectroscopic and computational imaging of bond breaking in photodissociation: roaming and role of conical intersections</b> Vincenzo Aquilanti, Masaaki Nakamura, Po-Yu Tsai, Toshio Kasai, King-Chuen Lin*, Federico Palazzetti, Andrea Lombardi <i>National Taiwan University</i>	<b>Paper 4402</b>
16:25	<b>The free-energy barrier to hydride transfer across a dipalladium complex</b> Alison Edwards*, Catriona Vanston, Gordon Kearley, Tamim Darwish, Nicholas DeSouza, Anibal Ramirez-Cuesta, Michael Guy Gardiner <i>Australian Nuclear Science and Technology Organisation</i>	<b>Paper 0182</b>
16:30	<b>Excited state dynamics of organic semiconducting materials</b> Ken Ghiggino*, Andrew Tilley, Ben Robotham, Jonathan M White <i>University of Melbourne</i>	<b>Paper 5024</b>
16:35	Discussion	

18:15-20:00	Poster Session <i>Sponsored by Cogent</i>
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## Tuesday 13 January

	<b>Session 2: Time and Space resolved Methods</b> Session Chair: John Helliwell	
09:00	<b>Pluronic Copolymer Encapsulated SCR7 as a Potential Anticancer Agent</b> Franklin John*, Jinu George, Puthusserickal Hassan, Vinod Aswal, Mrinal Srivastava, Subhas Karki, Sathees Raghavan <i>Biotechnology Laboratory, PG and Research Department of Chemistry, Sacred Heart College</i>	<b>Paper 4398</b>
09:05	<b>The Effect on Structural and Solvent Water Molecules of Substrate Binding to Ferric Horseradish Peroxidase</b> Neil Hunt*, Niall Simpson, Katrin Adamczyk, Gordon Hithell, Daniel Shaw, Gregory Greetham, Michael Towrie, Anthony Parker <i>University of Strathclyde</i>	<b>Paper 4344</b>
09:10	<b>Electronic Excitations in Molecular Solids: Bridging Theory and Experiment</b> Jonathan Skelton*, Estelina da Silva, Rachel Crespo-Otero, Lauren Hatcher, Paul Raithby, Steve Parker, Aron Walsh <i>University of Bath</i>	<b>Paper 4365</b>
09:15	Discussion	
10:30	Morning Tea	
	<b>Session 2 resumes: Time and Space resolved Methods</b> Session Chair: Martin Meedom Nielson	
11:00	<b>Resolution Enhancement through Microscopic Spatiotemporal Control</b> Debabrata Goswami*, Dhiman Das, Soumendra Bandyopadhyay <i>Indian Institute of Technology Kanpur</i>	<b>Paper 4417</b>
11:05	<b>On the photophysics of butadiyne bridged pyrene–phenyl molecular conjugates: multiple emissive pathways through locally excited, intramolecular charge transfer, and excimer states</b> Ashok Kumar Mishra*, Avik Pati, Santosh Gharpure <i>Indian Institute of Technology Madras</i>	<b>Paper 4389</b>
11:10	<b>Time resolved in situ X-ray diffraction study of crystallisation processes of large pore nanoporous aluminophosphate materials</b> Gopinathan Sankar*, Kerry Simmance, Wouter van Beek <i>University College London</i>	<b>Paper 5019</b>
11:15	<b>In-situ characterization of Cu-Co oxides for catalytic application</b> Zhen-Yu Tian*, Henning Vieker, Patrick Mountapmbeme Kouotou, André Beyer <i>Institute of Engineering Thermophysics, Chinese Academy of Sciences</i>	<b>Paper 4338</b>
11:20	Discussion	
13:00	Lunch	
	<b>Session 3: Local and Global Dynamics</b> Session Chair: Euvatingal Jemmis	
14:00	<b>Electron Transfer Quenching in Light Adapted and Mutant Forms of the AppA BLUF Domain</b> Stephen Meech*, Sergey Laptinok, Andras Lukacs, Richard Brust, Allison Haigney, Agnieszka Gil, Mike Towrie, Gregory Greetham, Peter Tonge <i>University of East Anglia</i>	<b>Paper 4325</b>

14:05	<b>Spatio-temporal correlations in aqueous systems: computational studies of static and dynamic heterogeneity by 2D-IR spectroscopy</b> Biman Bagchi*, Rikhia Ghosh, Tuhin Samanta, Saikat Banerjee, Rajib Biswas <i>Indian Institute of Science</i>	<b>Paper 4386</b>
14:10	Discussion	
15:00	Afternoon tea/poster session	
	<b>Session 3 resumes: Local and Global Dynamics</b> Session Chair: Dwayne Miller	
15:45	<b>Vibronic structure in the far-UV electronic circular dichroism spectra of proteins</b> Jonathan Hirst*, Zhuo Li, David Robinson <i>The University of Nottingham</i>	<b>Paper 5025</b>
15:50	<b>Probing deactivation pathways of DNA nucleobases by two-dimensional electronic spectroscopy: first principles simulations</b> Artur Nenov*, Javier Segarra-Martí, Angelo Giussani, Irene Conti, Ivan Rivalta, Elise Dumont, Vishal Jaiswal, Salvatore Altavilla, S Mukamel, M Garavelli <i>Università di Bologna</i>	<b>Paper 4422</b>
15:55	<b>Out-of-equilibrium dynamics of photoexcited spin-state concentration waves</b> Marylise Buron-Le Cointe*, Andrea Marino, Maciej Lorenc, Ioïc Toupet, Robert Henning, Anthony DiChiara, Keith Moffat, Nicolas Bréfuel, Eric Collet <i>University Rennes 1</i>	<b>Paper 4662</b>
16:00	Discussion	
17:15	Close of sessions	
19:00	Pre-Dinner Drinks	
19:30	Conference Dinner	

### Wednesday 14 January

	<b>Session 4: Future challenges</b> Session Chair: Neil Hunt	
09:00	<b>Probing electronic and vibrational dynamics in molecules by time-resolved photoelectron, Auger-electron, and X-ray photon scattering spectroscopy</b> Shaul Mukamel*, Kochise Bennett, Markus Kowalewski <i>University of California, Irvine</i>	<b>Paper 5027</b>
09:05	<b>X-ray diffraction in temporally and spatially resolved biomolecular science</b> John Helliwell*, Alice Brink, Simon Tanley, Surasak Kaenket, Victoria-Laurina Starkey <i>University of Manchester</i>	<b>Paper 4890</b>
09:10	<b>Disentangling detector data in XFEL studies of temporally resolved solution state chemistry</b> Martin Nielson*, Tim van Driel, Kasper Kjær, Elisa Biasin, Martin Haldrup, Henrik Lemke <i>Technical University of Denmark</i>	<b>Paper 4420</b>
09:15	Discussion	
10:30	Morning Tea	

	<b>Session 4 resumes: Future challenges</b> Session Chair: Binman Bagchi	
11:00	<b>Mapping Atomic Motions with Ultrabright Electrons: Towards Fundamental Limits in Space-Time Resolution</b> R. J. Dwayne Miller*, Stephanie Manz, Albert Casandruc, Dongfang Zhang, Yinpeng Zhong, Rolf Loch, Alexander Marx, Taisuke Hasegawaa, Lai Chung Liu, Shima Bayesteh, Hossein Delsim-Hashemi, Matthias Hoffmann, Matthias Felber, Max Hachmann, Frank Mayet, Julian Hirscht, Sercan Keskin, Masaki Hada, Sascha Epp, Klaus Flöttmann <i>Max Planck Institute for the Structure and Dynamics of Matter</i>	<b>Paper 5026</b>
11:05	<b>Two-dimensional sum-frequency generation (2D SFG) spectroscopy: Summary of principles and its application to amyloid fiber monolayers</b> Martin Zanni*, Ayanjeet Ghosh, Jia-Jung Ho, Arnaldo Serrano, David Skoff, Tianqi Zhang <i>University of Wisconsin-Madison</i>	<b>Paper 5029</b>
11:10	<b>Phase modulation nanoscopy: a simple approach to enhanced optical resolution</b> Robert Pal <i>Durham University</i>	<b>Paper 5018</b>
11:15	Discussion	
12:30	<b>Concluding remarks</b> Wolfgang Junge <i>Universität Osnabrück</i>	<b>Paper 5021</b>
13:15	<b>Acknowledgements</b>	