

Programme

Faraday Discussion 157: Molecular Reaction Dynamics in Gases, Liquids and Interfaces

25 – 27 June, 2012

Assisi, Italy

Monday 25 June

12:45	Pre-Lunch Drink
13:00	Lunch
14:00	Welcome and Introductions Piergiorgio Casavecchia <i>University of Perugia, Italy</i>
14.10 Paper 1	Introductory Lecture: F. Fleming Crim <i>University of Wisconsin, USA</i>
Session 1	Bimolecular Reaction Dynamics in the Gas Phase Session Chair: Piergiorgio Casavecchia, <i>University of Perugia, Italy</i>
15:10 Paper 2	Three-state surface hopping calculations of acetaldehyde photodissociation to CH₃+HCO on <i>ab initio</i> potential surfaces Bina Fu, Yongchang Han and Joel M Bowman* <i>Emory University, USA</i>
15:15 Paper 3	Reaction dynamics of temperature-variable anion water clusters studied with crossed beams and by direct dynamics R Otto, J Xie, J Brox, S Trippel, M Stei, T Best, M R Siebert, W L Hase and R Wester* <i>Universität Innsbruck, Austria</i>
15:20 Paper 4	Multi-path variational transition state theory for chemical reaction rates of complex polyatomic species: ethanol + OH reaction Jingjing Zheng and Donald G Truhlar* <i>University of Minnesota, USA</i>
16:40	Coffee break
17:10 Paper 5	Imaging the effects of the antisymmetric stretch excitation of CH₄ in the reaction with F atom Hiroshi Kawamata, Weiqing Zhang and Kopin Liu* <i>IAMS, Academia Sinica, Taiwan</i>
17:15 Paper 7	The dynamics of the D₂+OH → HOD+D reaction: A combined theoretical and experimental study Shu Liu, Chunlei Xiao, Tang Wang, Jun Chen, Tiangang Yang, Xin Xu, Dong H Zhang* and Xueming Yang <i>Chinese Academy of Sciences, China</i>
18:10	Poster Session
20:10	Dinner

Tuesday 26 June

Session 2	Photodissociation Dynamics in the Gas and Liquid-Phase Session Chair: Andrew J. Orr-Ewing, <i>University of Bristol, UK</i>
09:30 Paper 8	Contrasting excited state reaction pathways of phenol and para-methylthiophenol in the gas and liquid phases Yuyuan Zhang, Thomas A A Oliver, Michael N R Ashfold and Stephen Bradforth* <i>University of Southern California, USA</i>
09:35 Paper 10	Ultrafast dynamics of aniline following 269-238nm excitation and the role of the S2($\pi 3s/\pi\sigma^*$) state Roman Spesyvtsev, Oliver M Kirkby and Helen H Fielding* <i>University College London, UK</i>
09:40 Paper 9	Reaction dynamics of Cl + butanol isomers by crossed-beam sliced ion imaging Armando D Estillore, Laura M Visger-Kiefer, and Arthur G Suits* <i>Wayne State University, USA</i>
11:00	Coffee break
11:30 Paper 11	Between ethylene and polyenes – the non-adiabatic dynamics of cis-dienes Thomas S Kuhlman, William J Glover, Toshifumi Mori, Klaus B Møller and Todd J Martinez* <i>Stanford University, USA</i>
11:35 Paper 12	Infrared driven CO oxidation reactions on isolated platinum cluster oxides $Pt_nO_m^+$ Alexander C Hermes, Suzanne M Hamilton, Graham A Cooper, Christian Kerpel, Dan J Harding, Gerard Meijer, André Fielicke and Stuart R Mackenzie* <i>University of Oxford, UK</i>
11:40 Paper 13	Product state and speed distributions in photochemical triple fragmentations G de Wit, B R Heazlewood, M S Quinn, A T Maccarone, K Nauta, S A Reid, M J T Jordan and S H Kable* <i>University of Sydney, Australia</i>
13:00	Lunch

Session 3	Reaction Dynamics at Interfaces Session Chair: Alec M. Wodtke, <i>Max Planck Institute for Biophysical Chemistry, Germany</i>
14:30 Paper 14	Vibrationally bond-selected chemisorption of methane isotopologues on Pt(111) studied by reflection absorption infrared spectroscopy Li Chen, Hirokazu Ueta, Régis Bisson and Rainer D Beck* <i>École Polytechnique Fédérale de Lausanne, Switzerland</i>
14:35 Paper 15	On probing ions at the gas-liquid interface by quantum state-resolved molecular beam scattering: The curious incident of the cation in the night-time Andrew W Gisler and David J Nesbitt* <i>JILA and University of Colorado, Boulder, USA</i>
14:40 Paper 16	Dynamics of molecular and polymeric interfaces probed with atomic beam scattering and scanning probe imaging Ryan D Brown, Qianqian Tong, James S Becker, Miriam A Freedman, Nataliya A Yufa, and S J Sibener* <i>University of Chicago, USA</i>
16:00	Coffee break
16:30 Paper 17	Nonadiabatic dynamics of metal surfaces: Independent electron surface hopping with phenon and electron thermostats Neil Shenvi and John C Tully*, <i>Yale University, USA</i>
16:35 Paper 18	Reaction dynamics at a metal surface; Halogenation of Cu(110) A Eisenstein, L Leung, T Lim, Z Ning and J C Polanyi* <i>University of Toronto, Canada</i>
16:40 Paper 19	Kinematics and dynamics of atomic-beam scattering on liquid and self-assembled monolayer surfaces William A Alexander, Lihnan Shen, Jianming Zhang, Gilbert M Nathanson, and Timothy K Minton* <i>Montana State University, USA</i>
20:00	Pre-Dinner Drink
20:30	Conference Dinner

Wednesday 27 June

Session 4	Ultrafast Reaction Dynamics Session Chair: Peter Hamm, <i>University of Zurich, Switzerland</i>
09:30 Paper 20	Vibrationally resolved transition state spectroscopy of the F + H₂ and F + CH₄ reactions Tara I Yacovitch, Etienne Garand, Jongjim B Kim, Christian Hock, Thomas Theis and Daniel M Neumark* <i>University of California, Berkeley, USA</i>
09:35 Paper 21	The last mile of molecular reaction dynamics virtual experiments: The case of the OH(N=1-10)+CO(j=0-3) reaction Antonio Laganà,* Ernesto Garcia, Alessandra Paladini, Piergiorgio Casavecchia and Nadia Balucani <i>University of Perugia, Italy</i>
09:40 Paper 22	Surface-aligned femtochemistry: Real-time investigation of photoinduced bimolecular reaction dynamics at oxide surfaces Mihai E Vaida and Thorsten M Bernhardt* <i>University of Ulm, Germany</i>
11:00	Coffee break
11:30 Paper 23	Crowding effects on the small, fast-folding protein λ6-85 Sharlene Denos, Apratim Dharb and Martin Gruebele* <i>University of Illinois At Urbana-Champaign, USA</i>
11:35 Paper 24	Ligand-field symmetry effects in Fe(II) polypyridyl compounds probed by transient x-ray absorption spectroscopy Hana Cho, Matthew L Strader, Kiryong Hong, Lindsey Jamula, Tae Kyu Kim, James K McCusker Robert W Schoenlein and Nils Huse* <i>University of Hamburg, Germany</i>
12:30	Concluding Remarks Lecture: Richard N. Zare <i>Stanford University, USA</i>
13:15	Acknowledgements and Close of Meeting
13:30	Lunch

*Presenting author to whom affiliation applies