Quantum effects in small molecular systems

Faraday Discussion

10–12 September 2018, Edinburgh, UK

Monday 10 September

11:30	Registration and Lunch	
12:45	**Welcome and Introductions** Majdi Hochlaf *Chair of Scientific Committee*	
12:55	**Outline of Discussion Format** Lynn Murphy and Thomas Foley, *Royal Society of Chemistry Publishing Editors*	
13:00	**Introductory Lecture** (Session Chair: Majdi Hochlaf) Sir David Clary *University of Oxford*	
	Session 1: Precise characterisation of isolated molecules (Session Chair: Ad van der Avoird)	
THEME: Accurate rovibronic spectroscopy of isolated molecular systems		
14:00	**Quantum and classical IR spectra of $(HCOOH)_2$, $(DCOOH)_2$ and $(DCOOD)_2$ using *ab initio* potential energy and dipole moment surfaces** Joel Bowman and Chen Qu *Emory University, USA*	**Paper** 19612
14:05	**Disentangling the complex spectrum of the ethynyl cation** Roberto Linguerri, B. Mehnen, S. Ben Yaghlane, M. Mogren Al Mogren and M. Hochlaf *Université Paris-Est Marne-la-Vallée, France*	**Paper** 20023
14:10	**Teaching vibrational spectra to assign themselves** Paul Houston, Brian L. Van Hoozen, Jr., Chen Qu, Qi Yu and Joel M. Bowman *Cornell University, USA*	**Paper** 20386
14.15	**Excited state dynamics and time-resolved photoelectron spectroscopy of para-xylylene** Ingo Fischer, Kevin Issler, Anja Röder, Florian Hirsch, Lionel Poisson, Roland Mitrić and Jens Petersen *University of Wuerzburg, Germany*	**Paper** 19993
14:20	Discussion	
16:00	Afternoon tea	
THEME: State-to-state bimolecular quantum collisions		
16:30	**On the gas-phase formation of the HCO^- anion: accurate quantum study of the H^- + CO radiative association and HCO radiative electron attachment** Thierry Stoecklin, Philippe Halvick, Miguel Lara-Moreno, Tarek Trabelsi and Majdi Hochlaf *Université de Bordeaux, France*	**Paper** 19615
16:35	**Collisional relaxation kinetics for ortho and para $NH2^-$ under photodetachment in cold ion traps** Francesco Gianturco, Olga Y. Lakhmanskaya, Mario Hernández Vera, Ersin Yurtsever and Roland Wester *University of Innsbruck, Austria*	**Paper** 19968
16:40	Discussion	
17:30	**The funding opportunities of the European Research Council** *Monica Favaro, European Research Council Executive Agency*	
17:50	Lightning presentations – (by invitation of the scientific committee)	
18:00	Poster Session and Wine Reception	
19:15	Close of sessions	

Tuesday 11 September

	Session 2: Quantum dynamics of isolated molecules (Session Chair: Sir David Clary)	
THEME: Exotic molecular systems quantum dynamics at different timescales		
09:00	**Multiple pulse coherent dynamics and wave packet control of the N2 a" $^1\Sigma_g^+$ dark state by attosecond four-wave mixing** Stephen R. Leone, Erika R. Warrick, Ashley P. Fidler, Wei Cao, Etienne Bloch and Daniel M. Neumark *University of California, Berkeley, USA*	**Paper** 19614
09:05	**Heavy Rydberg states: large amplitude vibrations** Adam Kirrander, Christian Jungen, Robert Donovan and Kenneth Lawley *University of Edinburgh, UK*	**Paper** 20030
09:10	**Curve crossing in a manifold of coupled electronic states: direct quantum dynamics simulations of formamide** Graham Worth, K. Eryn Spinlove, Gareth W. Richings, Michael A. Robb *University College London, UK*	**Paper** 19983
09:15	Discussion	
10:30	Morning Tea	
THEME: Manifestation of quantum effects on bimolecular reactions		
11:00	**Natural reaction channels in H + CHD_3 → H_2 + CD_3** Uwe Manthe and Roman Ellerbrock *Universitaet Bielefeld, Germany*	**Paper** 19994
11:05	**Ab initio instanton rate theory made efficient using Gaussian process regression** Jeremy Richardson, Gabriel Laude, Danilo Calderini and David P. Tew *ETH Zurich, Switzerland*	**Paper** 19932
11:10	**Properties of Feshbach and "shape"-resonances in ozone and their role in recombination reactions and anomalous isotope effects** Alexander Teplukhin and Dmitri Babikov *Marquette University, USA*	**Paper** 19984
11:15	Discussion	
12:30	Lunch	
	Session 3: Molecules in confinement in liquid solvents (Session Chair: Gilberte Chambaud)	
THEME: Solvent effects on the spectroscopy and dynamics of molecules		
13:30	**On the importance of initial conditions for excited-state dynamics** Petr Slavíček, Jiří Suchan, Daniel Hollas and Basile F. E. Curchod *Institute of Chemical Technology Prague, Czech Republic*	**Paper** 19616
13:35	**Proton transfer in guanine–cytosine base pair analogues studied by NMR spectroscopy and PIMD simulations** Martin Dračínský, Radek Pohl, Ondřej Socha, Petr Slavíček, Michal Šála, Paul Hodgkinson *IOCB Prague, Czech Republic*	**Paper** 20012
13:40	**Electron-driven proton transfer enables nonradiative photodeactivation in microhydrated 2-aminoimidazole** Mikołaj Janicki, Rafał Szabla, Jiří Šponer and Robert W. Góra *Wroclaw University of Science and Technology, Poland*	**Paper** 19997
13:45	**The influence of aqueous solvent on the electronic structure and non-adiabatic dynamics of indole explored by liquid-jet photoelectron spectroscopy** Stephen E Bradforth, Gaurav Kumar, Anirban Roy, Ryan S. McMullen and Shanmukh Kutagulla *University of Southern California, USA*	**Paper** 19617

13.50	Discussion	
15:30	Afternoon Tea	
	Session 4: Molecules in confinement in clusters, quantum solvents and matrices (Session Chair: Joseph S. Francisco)	
	THEME: Large molecular systems	
16:00	**Stereochemistry-dependent hydrogen bonds stabilise stacked conformations in jet-cooled cyclic dipeptides: (LD) vs. (LL) cyclo tyrosine–tyrosine** Anne Zehnacker, Feriel BenNasr, Ariel Pérez-Mellor, Ivan Alata, Valeria Lepere and Nejm-Eddine Jaïdane *Université Paris-Sud, France*	**Paper** 19619
16:05	**Theoretical studies of atmospheric molecular complexes interacting with NIR to UV light** Malgorzata Biczysko, Justyna Krupa and Maria Wierzejewska *Shanghai University, International Center for Quantum and Molecular Structures, China*	**Paper** 19999
16:10	Discussion	
17:00	Close of sessions	
18:30	**Pre-Dinner Drinks**	
19:00	**Conference Dinner – South Hall Dining Room, John McIntyre Conference Centre**	

Wednesday 12 September

	Session 4 (continued): Molecules in confinement in clusters, quantum solvents and matrices (Session Chair: Joel Bowman)	
	THEME: Multiscale quantum effects	
09:00	**Spectral signatures of proton delocalization in $H^+(H_2O)_{n=1-4}$ ions** Anne B. McCoy, Laura C. Dzugan, Ryan J. DiRisio and Lindsey R. Madison *University of Washington, USA*	**Paper** 19618
09:05	**Fully quantum calculation of the second and third virial coefficients of water and its isotopologues from ab initio potentials** Krzysztof Szalewicz, Piotr Jankowski, Krzysztof Szalewicz and Allan H. Harvey *University of Delaware, USA*	**Paper** 19623
09:10	**Large amplitude motion of molecules trapped in solid parahydrogen** Claudine Crépin, Alejandro Gutiérrez-Quintanilla, Michèle Chevalier, Justinas Ceponkus, Rolando R. Lozada-García and Jean-Michel Mestdagh *CNRS – ISMO, France*	**Paper** 19954
09:15	Discussion	
10:30	Morning Tea	
	THEME: Molecules embedded into fullerenes and clathrates	
11:00	**Alignment of ^{17}O-enriched water-endofullerene $H_2O@C_{60}$ in a liquid crystal matrix** Karel Kouřil, Benno Meier, Shamim Alom, Richard J. Whitby and Malcolm H. Levitt *University of Southampton, UK*	**Paper** 19910
11:05	**Does cage quantum delocalisation influence the translation–rotational bound states of molecular hydrogen in clathrate hydrate?** David Benoit, David Lauvergnat and Yohann Scribano *University of Hull, UK*	**Paper** 20039

11:10	**Effects of symmetry breaking on the translation-rotation eigenstates of H_2, HF, and H_2O inside the fullerene C_{60}** Zlatko Bačić, Vojtěch Vlček, Daniel Neuhauser and Peter M. Felker *New York University, USA*	**Paper** 20312
11:15	Discussion	
12:30	**Concluding Remarks Lecture** (Session Chair: Majdi Hochlaf) Ad van der Avoird *Radboud University Nijmegen, The Netherlands*	
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.