

Faraday Discussion 154: Ionic Liquids

22 – 24 August 2011
Queen's University, Belfast, UK

Provisional Programme

Monday 22 August

| | |
|-------------------------|--|
| 12:00 | Registration |
| 13:00 | Welcome and introductions |
| Session 1 | Thermodynamics and phase behaviour |
| 13:15 Paper 1 | Introductory lecture Austen Angell* <i>Arizona State University, USA</i> |
| 14:15 Paper 2 | Simulations of structure and dynamics of nanoparticle-based ionic liquids Athanasios Panagiotopoulos* <i>Princeton University, USA</i> |
| Paper 3 | Using ethane and butane as probes to the molecular structure of 1-alkyl-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]imide ionic liquids Margarida Costa Gomes* <i>Université Blaise-Pascal, France</i> |
| 15:15 | Afternoon tea |
| 15:45 Paper 4 | Critical behaviour and vapour-liquid coexistence of 1-alkyl-3-methylimidazolium bis(trifluoromethylsulfonyl)amide ionic liquids via Monte Carlo simulations Edward Maginn* <i>University of Notre Dame, USA</i> |
| Paper 5 | Phase behaviour, transport properties, and interactions in Li-salt doped ionic liquids Aleksander Matic* and Jagath Pitawala <i>Chalmers University of Technology, Sweden</i> |
| 16:45 | Close of session |
| 16:45 – 18:00 | Poster session |

Tuesday 23 August

| | |
|-------------------------|--|
| Session 2 | Structure: experiments and simulations |
| 09:00 Paper 6 | New experimental evidences supporting the mesoscopic segregation model in room temperature ionic liquids Alessandro Triolo* <i>Istituto per i Processi Chimico-Fisico, Pisa, Italy</i> |
| Paper 7 | Ionic liquids studied across different scales: a computational perspective K Scholze, F Dommert, Y Y Zhao, R Berger, C Holm and L Delle Site* <i>University of Stuttgart, Germany</i> |
| Paper 8 | Temperature-dependent structure of ionic liquids - x-ray scattering and simulations Cherry S Santos, Hemant K Kashyap, Harsha V R Annapureddy, N Sanjeev Murthy, Claudio J Margulis and Edward W Castner* <i>Rutgers University, USA</i> |
| 10:30 | Morning coffee |
| Session 2 | |
| 11:00 Paper 9 | Mesoscopic structure in ionic liquids: A combined ultrafast optical Kerr-effect (OKE) & dielectric relaxation study David A. Turton*, Thomas Sonleitner, Johannes Hunger, Alexander Stoppa, Glenn Hefter, Andreas Thoman, Markus Walther, Richard Buchner, and Klaas Wynne <i>University of Strathclyde, UK</i> |
| Paper 10 | 2D or not 2D: The flexible nano-structures of ionic liquids Karina Shimizu, Alfonso Pensado, Agílio A. H. Pádua and José N. Canongia Lopes <i>Instituto Superior Técnico, Portugal</i> |
| Paper 11 | From molten salts to room temperature ionic liquids: Simulation studies on chloroaluminate systems M. Salanne*, M.J.A. Siqueira, A.P. Seitsonen, P.A. Madden, C. Simon and B. Kirchner <i>Université Pierre et Marie Curie, France</i> |
| 12:30 | Lunch and poster session |

Tuesday 23 August

| | |
|--------------------------|--|
| Session 3 | Interfacial behaviour |
| 14:00 Paper 12 | The interface ionic liquid(s)/electrode(s): in situ STM and AFM measurements Frank Endres* <i>Clausthal University of Technology, Germany</i> |
| Paper 13 | Molecular-scale insights into the mechanisms of ionic liquids interactions with carbon nanotubes Kathleen Kirchner, Andrey Frolov*, Tom Kirchner and Maxim V Fedorov <i>Max Planck Institute for Mathematics in the Sciences, Germany</i> |
| Paper 14 | Graphene-Based Supercapacitors in the Parallel-Plate Electrode Configuration: Ionic Liquid versus Organic Electrolyte Youngseon Shim, Hyung J. Kim, and YounJoon Jung* <i>Seoul National University, South Korea</i> |
| 15:30 | Afternoon tea |
| Session 3 | |
| 16:00 Paper 15 | Adsorption, absorption and desorption of gases at liquid surfaces: water on [C8C1Im][BF4] and [C2C1Im][Tf2N] Alexey Deyko and Robert G. Jones* <i>University of Nottingham, UK</i> |
| Paper 16 | Nonlinear vibrational spectroscopic studies on the ionic liquid/molecular liquid interfaces T. Iwahashi, Y. Sakai, D. Kim, T. Ishiyama, A. Morita and Y. Ouchi* <i>Nagoya University, Japan</i> |
| Paper 17 | Slow and fast capacitive process taking place at the ionic liquid / electrode interface Bernhard Roling*, Marcel Drüscher, Thomas Jänsch <i>University of Marburg, Germany</i> |
| 17:30 | Close of session |
| 19:00 | Pre-dinner drinks |
| 19:30 | Conference dinner |

Wednesday 24 August

| | |
|--------------------------|---|
| Session 4 | Chemical reactivity and dynamics |
| 09:00 Paper 18 | Protonics in ionic liquids and plastic solids Douglas MacFarlane* <i>Monash University, Australia</i> |
| Paper 19 | Electron solvation dynamics and reactivity in ionic liquids observed by picosecond radiolysis techniques James Wishart* <i>Brookhaven National Lab, USA</i> |
| Paper 20 | Investigating the origin of entropy-derived rate accelerations in ionic liquids Hon Man Yau, Anna K. Croft and Jason B. Harper* <i>University of New South Wales, Australia</i> |
| 10:30 | Morning coffee |
| 11:00 Paper 21 | Ab initio simulations of thermal decomposition and of electron transfer reactions in room temperature ionic liquids Pietro Ballone* <i>Queens University Belfast, UK</i> |
| Paper 22 | The Ion Speciation of Ionic Liquids in Molecular Systems of Low and Medium Polarity Hermann Weingärtner* <i>Ruhr-Universität Bochum, Germany</i> |
| Paper 23 | Measurements of the Complete Solvation Response of Coumarin 153 in Ionic Liquids and the Accuracy of Simple Dielectric Continuum Predictions Mark Maroncelli*, Durba Roy, Xinxing Zhang, Min Liang and Nikolaus P Ernsting <i>Pennsylvania State University, USA</i> |
| Paper 24 | High pressure studies of the transport properties of ionic liquids Kenneth R Harris* and Mitsuhiro Kanakubo <i>University of New South Wales, Australia</i> |
| 13:00 Paper 25 | Concluding remarks Ruth Lynden-Bell* <i>University of Cambridge, UK</i> |
| 13:30 | Acknowledgements |
| 13:45 | Close of meeting |

* Denotes presenting author to whom affiliation applies