

## Faraday Discussion 154: Ionic Liquids

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

### Provisional Programme

#### Monday 22 August

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

**Tuesday 23 August**

<b>Session 2</b>	<b>Structure: experiments and simulations</b>
09:00 <b>Paper 6</b>	<b>New experimental evidences supporting the mesoscopic segregation model in room temperature ionic liquids</b> Alessandro Triolo* <i>Istituto per i Processi Chimico-Fisico, Pisa, Italy</i>
<b>Paper 7</b>	<b>Ionic liquids studied across different scales: a computational perspective</b> K Scholze, F Dommert, Y Y Zhao, R Berger, C Holm and L Delle Site* <i>University of Stuttgart, Germany</i>
<b>Paper 8</b>	<b>Temperature-dependent structure of ionic liquids - x-ray scattering and simulations</b> 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	<b>Morning coffee</b>
<b>Session 2</b>	
11:00 <b>Paper 9</b>	<b>Mesoscopic structure in ionic liquids: A combined ultrafast optical Kerr-effect (OKE) &amp; dielectric relaxation study</b> David A. Turton*, Thomas Sonnleitner, Johannes Hunger, Alexander Stoppa, Glenn Hefter, Andreas Thoman, Markus Walther, Richard Buchner, and Klaas Wynne <i>University of Strathclyde, UK</i>
<b>Paper 10</b>	<b>2D or not 2D: The flexible nano-structures of ionic liquids</b> Karina Shimizu, Alfonso Pensado, Agílio A. H. Pádua and José N. Canongia Lopes <i>Instituto Superior Técnico, Portugal</i>
<b>Paper 11</b>	<b>From molten salts to room temperature ionic liquids: Simulation studies on chloroaluminate systems</b> 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	<b>Lunch and poster session</b>

**Tuesday 23 August**

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

Wednesday 24 August

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

\* Denotes presenting author to whom affiliation applies