

# SCIENTIFIC PROGRAM

## ICSC30, Perth, Australia, 2007

(Revised 13<sup>th</sup> July)

### Monday, 16<sup>th</sup> July

9.00	<b>OPENING CEREMONY (ECL2)</b>	
9.30	<b>Plenary Lecture</b> Peter Cummings <i>Molecular Simulation and Modelling of Water and Aqueous Solutions in Bulk and at Interfaces: From Ambient To Supercritical Conditions</i>	
10.30	<b>MORNING TEA</b>	
	<b>Theory &amp; Simulation – 1 (ECL2; Chair: Vlachy)</b>	<b>Chemical Speciation – 1 (ECL4; Chair: Persson)</b>
11.00	<b>Keynote Lecture</b> Thomas Hofer <i>Capabilities of Chemical Simulation Methods in the Elucidation of Structures and Dynamics of Solutions</i>	<b>Keynote Lecture</b> Richard Buchner <i>What can be learnt from Dielectric Relaxation Spectroscopy about Ion Solvation and Association?</i>
11.40	Jean-François Dufrêche <i>Dynamics of Ions in Concentrated Electrolyte Solutions</i>	Shin-ichi Ishiguro <i>Solvation Number and Conformation of N,N-Dimethylacrylamide and N,N-Dimethylpropionamide in the Coordination Sphere of the Cobalt(II) Ion in Solution studied by FT-IR and FT-Raman Spectroscopy</i>
12.00	Amalendu Chandra <i>Hydrogen bond dynamics in aqueous solutions and vibrational spectral diffusion</i>	Munetaka Takeuchi <i>Solvation Structure of Li<sup>+</sup> in Concentrated LiPF<sub>6</sub>-Propylene Carbonate Solutions</i> <i>– Time-of-Flight neutron diffraction and MD simulation –</i>
12.20	Michael Probst <i>Interaction of Gold(I) and Gold(III) Ions with Nitromethane</i>	Wolfgang Voigt <i>Thermodynamic properties of CaSO<sub>4</sub> dissolved in concentrated aqueous electrolyte solutions</i>
12.40	<b>LUNCH</b>	

	<b>Nanoparticles &amp; Surfaces – 1 (ECL2; Chair: Pálincás)</b>	<b>Thermodynamics &amp; Kinetics – 1 (ECL4; Chair: Buchner)</b>
14.00	<b>Plenary Lecture</b> Amanda Barnard <i>Modelling the Shape and Phase of Nanoparticles in Solution</i>	<b>Plenary Lecture</b> Peter Williams <i>The Synthesis and Stability of Wroewolfeite, <math>Cu_4SO_4(OH)_6 \cdot 2H_2O</math></i>
15.00	Toshihiro Tominaga <i>Ternary Diffusion Coefficients for Zwitterionic Surfactant-Ionic Surfactant-Water Systems</i>	Tatsuya Urabe Characterization of Aluminum Species in Aqueous Solution by ESI-MS
15.20	Earle Waghorne <i>To Dissolve Or Not To Dissolve: Sticking Coefficients of Organic Solutes at the Water Surface</i>	Nader Hassan <i>Cooperative Effects of Spin-State Transition in Solution</i>
15.40	AFTERNOON TEA	
16.10		Pál Sipos <i>Application of the Specific Ion Interaction Theory (SIT) for the Ionic Products of Highly Concentrated Aqueous Electrolyte Solutions</i>
16.30		Miho Tanaka <i>Chemical Species of Silica in Tokyo Bay: Change of Silica Species Based on the Solution Character</i>
16.50		Anna Płaczek <i>Apparent Molar Volumes and Heat Capacities of Electrolytes and Ions in N,N-dimethylformamide</i>
17.10	FINISH	

# Tuesday, 17<sup>th</sup> July

9.00	<b>Plenary Lecture (ECL2; Chair: Marsh)</b> Doug MacFarlane <i>Ionic Liquids – Novel Solvents for Green Chemistry, Electrochemistry and Biological Chemistry</i>	
	<b>Ionic Liquids – 1 (ECL2; Chair: Marsh)</b>	<b>Chemical Speciation – 2 (ECL4; Chair: Bešter-Rogač)</b>
10.00	Toshiyuki Takamuku <i>X-ray Diffraction Study on Structure of Imidazolium Ionic Liquids</i>	Montserrat Filella <i>NOM and Trace Element Speciation Modelling: a Road Paved with Good Intentions and few Useful Results</i>
10.20	Leslie Glasser <i>Thermodynamics of Ionic Liquids</i>	Clara Magalhães <i>Arsenic and Lead in the System Water – Contaminated Soils from S. Domingos Mine, Portugal</i>
10.40	MORNING TEA	
	<b>Ionic Liquids – 1 (ECL2; Chair: Harris)</b>	<b>Chemical Speciation – 2 (ECL4; Chair: Williams)</b>
11.10	Urszula Domańska-Żelazna <i>Thermodynamic Phase Behavior of Ionic Liquids</i>	Julia Torres <i>Solution Chemistry of Polynuclear Complexes Containing [M<sub>3</sub>Ln<sub>2</sub>(L)<sub>6</sub>] Units (M: 3d transition metal ions, Ln: lanthanide ions, L: oxydiacetate or iminodiacetate)</i>
11.30	Johannes Hunger <i>From Ionic Liquid to Electrolyte Solution – Cooperative Dynamics of Ionic Liquids Mixed with Polar Solvents</i>	Silvia Black <i>Ion Association Effects on the Experimentally Observed Dissociation Constant of Ammonium Ion</i>
11.50	Isabelle Billard <i>Solvation and Complexation of Lathanides and Actinides in Ionic Liquids: Fundamental Aspects and Possible Application for the Nuclear Fuel Cycle</i>	Kavosh Majlesi <i>Complexation of Dioxovanadium(V) and Molybdenum(VI) with NTA and IDA at Different Ionic Strengths Using SIT and Debye-Huckel Models</i>
12.10		Sofia Stepanchikova <i>Experimental Study of Nd, Eu and Ho Hydrolysis at Elevated Temperatures by Spectrophotometric Method</i>
12.30	LUNCH	
14.00	POSTER SESSION	
17.00	FINISH	

# Wednesday, 18<sup>th</sup> July

8.30	<b>Plenary Lecture (ECL2; Chair: Königsberger)</b> Gunnar Eriksson <i>FactSage and ChemApp, Two Tools for the Prediction of Multiphase Chemical Equilibria in Solutions</i>	
	<b>Thermodynamics &amp; Kinetics – 2 (ECL2; Chair: Königsberger)</b>	<b>Theory &amp; Simulation – 2 (ECL4; Chair: Hofer)</b>
9.30	<b>Keynote Lecture</b> Anil Kumar <i>Ionic Interaction in Aqueous Mixtures of Hydrophilic and Hydrophobic Ions</i>	<b>Keynote Lecture</b> Vojko Vlachy <i>Polyelectrolyte Hydration: Theory and Experiment</i>
10.10	MORNING TEA	
	<b>Thermodynamics &amp; Kinetics – 2 (ECL2; Chair: Domańska-Żelazna)</b>	<b>Theory &amp; Simulation – 2 (ECL4; Chair: Hofer)</b>
10.40	Erich Königsberger <i>Thermodynamic Process Simulation of a Bayer Refinery Circuit</i>	Pierre Turq <i>Multiscale Description of Charged Liquids and Confined Media</i>
11.00	Gorazd Vesnaver <i>Kinetics of G-Quadruplex Folding and Unfolding</i>	Clare McCabe <i>A Statistical Associating Fluid Theory for Electrolyte Solutions</i>
11.20	Gavin Hedwig <i>Volumetric Properties of the Glycyl Group of Proteins in Aqueous Solution at High Pressures</i>	
11.40	Gerhard Gritzner <i>A Statistical Approach to Cation - Solvent Interactions</i>	
12.00	LUNCH	
12.50	EXCURSION PICKUP	
13.00-22.00	CONFERENCE EXCURSION + DINNER	

# Thursday, 19<sup>th</sup> July

9.00	<b>Plenary Lecture (ECL2; Chair: Barnard)</b> Geraldine Richmond <i>Combining Surface Nonlinear Spectroscopy and Molecular Dynamics Simulations to Understand Molecular and Ionic Interactions at Liquid-Liquid Interfaces.</i>	
	<b>Nanoparticles &amp; Surfaces – 2 (ECL2; Chair: Barnard)</b>	<b>Solution Structure – 1 (ECL4; Chair: Waghorne)</b>
10.00	<b>Plenary Lecture</b> Nicholas Quirke <i>Interaction of Fluids with Surfaces and Nanoparticles</i>	<b>Keynote Lecture</b> Gábor Pálinkás <i>Structural Characterization of Supramolecular Architectures in Solution</i>
10.40		Hisanobu Wakita <i>Ultra Soft X-ray Spectroscopy for the Structure Analysis of Ions and Molecules in Solution</i>
11.00	MORNING TEA	
	<b>Nanoparticles &amp; Surfaces – 2 (ECL2; Chair: Cummings)</b>	<b>Solution Structure – 1 (ECL4; Chair: Soper)</b>
11.30	Ric Pashley <i>Charging at the Surface of Pure Oil Droplets Dispersed in Water</i>	<b>Keynote Lecture</b> Daniel Bowron <i>Determination of the geometric structure of ion hydration shells within comprehensive solute + solvent models: An approach based on Empirical Potential Structure Refinement of neutron scattering data combined with X-ray absorption spectroscopy</i>
11.50	Marija Bešter-Rogač <i>Thermodynamics of Micellization of Non-Ionic and Ionic Surfactants &amp; Their Structural Properties in Aqueous Solution</i>	
12.10	Wolfgang Wachter <i>How Co-Ions Influence the Stability of Ionic Microemulsions</i>	Natallia Torapava <i>Structure Determination of Hydrated, Hydrolyzed and Solvated Thorium(IV) Ions in Solution and Solid State</i>
12.30		Tünde Megyes <i>X-Ray Diffraction Characterization of Metallocyclic Complexes in Solution</i>
12.50	LUNCH	

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**Ohtaki Symposium (ECL2; Chair: Ishiguro)**

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14.00

**Dedication**

Toshiyuki Takamuku

*Fifty Years of Professor Hitoshi Ohtaki's Dedication to  
Solution Chemistry*

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14.20

**Keynote Lecture**

Toshio Yamaguchi

*On the Role of Solvent Environment in Alcohol-induced  $\alpha$ -  
Helix Formation of Model Peptides*

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15.00

Ingmar Persson

*Structure of the Hydrated Lanthanoid(III) Ions in Aqueous  
Solution Determined by EXAFS Spectroscopy*

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15.20

Alan Soper

*Structure Refinement Methods Applied to Neutron and X-Ray  
Diffraction Data on Water and Aqueous Solutions*

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15.40

**AFTERNOON TEA**

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16.00

Magnus Sandström

*Sulfur X-ray Absorption and Vibrational Spectroscopy of  
Sulfite, Sulfur dioxide and Sulfonate Solutions, and of  
Substituted Sulfonates  $X_3CSO_3^-$  ( $X=H, Cl, F$ ).*

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16.30

Yasunori Tominaga

*Low-frequency Depolarized Raman Scattering of Supercritical  
Water*

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16.50

**FINISH**

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# Friday, 20<sup>th</sup> July

9.00	<b>Plenary Lecture (ECL2; Chair: Yamaguchi)</b> Ken Marsh <i>Ionic Liquids: Are they Salts or High Boiling Organic Liquids?</i>	
	<b>Ionic Liquids – 2 (ECL2; Chair: Yamaguchi)</b>	<b>Thermodynamics &amp; Kinetics – 3 (ECL4; Chair: Magalhães)</b>
10.00	Yasuhiro Umebayashi <i>Lithium Ion Solvation in Bis-(trifluoromethanesulfonyl) Imide type Room Temperature Ionic Liquids: DFT Calculations and Raman Spectroscopic Study</i>	<b>Plenary Lecture</b> Erik Nibbering <i>Ultrafast Proton Transfer in Aqueous Acid-Base Neutralization</i>
10.20	Thomas Ruether <i>A new family of ionic liquids based on a new N-heterocyclic motive as the cationic component: physico-chemical properties and plastic crystal behaviour</i>	
10.40	Ken Harris <i>Transport Properties of Ionic Liquids at High Pressure</i>	
11.00	<b>MORNING TEA</b>	
	<b>Ionic Liquids – 2 (ECL2; Chair: Takamuku)</b>	<b>Thermodynamics &amp; Kinetics – 3 (ECL4; Chair: Sandström)</b>
11.30	Kenta Fujii <i>Conformational Equilibrium of Bis(fluorosulfonyl) Imide Anion in Room-Temperature Ionic Liquid</i>	Masaaki Tabata <i>Solvent Composition Effects on Relaxation of Bulk Water Molecules and on Water Molecule Exchange Reaction of Aquanickel(II) in Aqueous Mixed Solvents with 2-Propanol or 1-Propanol</i>
11.50	Ryo Kanzaki <i>Acidity and Basicity of Ionic Liquids of Onium Salt</i>	Imre Tóth <i>Naked Tl-Pt Bonded Cyano Complexes: New Results</i>
12.10	Ika Oktavianawati <i>Xylanase-Hydrolyzed Reaction on Xylan in Ionic Liquids</i>	Masahide Terazima <i>Time-Resolved Enthalpies, Heat Capacities and Translational Diffusion of Reaction Intermediates of Biological Proteins</i>
12.30	Junhua Huang <i>Analysis of Ionic Motions in Plastic Crystals by Dielectric Response</i>	Deresh Ramjugernath <i>Estimation of the Vapour Pressure of Organic Compounds by a Group Contribution Method</i>
12.50	<b>CLOSING CEREMONY (ECL2)</b>	
13.15	<b>FINISH</b>	