Mesostructure and Dynamics in Liquids and Solutions

www.rsc.org/faraday_d

A General Discussion on Mesostructure and Dynamics in Liquids and Solutions was held in Bristol, UK on the 18th, 19th and 20th of September 2013.

RSC Publishing is a not-for-profit publisher and a division of the Royal Society of Chemistry. Any surplus made is used to support charitable activities aimed at advancing the chemical sciences. Full details are available from www.rsc.org

CONTENTS


INTRODUCTORY LECTURE

9 Importance of many-body orientational correlations in the physical description of liquids
Hajime Tanaka

PAPERS AND DISCUSSIONS

77 The liquid-liquid transition in supercooled ST2 water: a comparison between umbrella sampling and well-tempered metadynamics
Jeremy C. Palmer, Roberto Car and Pablo G. Debenedetti

95 The thermodynamical response functions and the origin of the anomalous behavior of liquid water
Francesco Mallamace, Carmelo Corsaro, Domenico Mallamace, Cirino Vasi and H. Eugene Stanley

Cover

Nucleation and growth of ice in water-salt solutions is preceded by the formation of nanodomains of pure, four-coordinated water molecules within the mixture.

109 General discussion

145 Fluctuations and micro-heterogeneity in mixtures of complex liquids
Aurélien Perera and Bernarda Kežić

159 What happens to the structure of water in cryoprotectant solutions?
James J. Towey, Alan K. Soper and Lorna Dougan

177 Distinguishing aggregation from random mixing in aqueous t-butyl alcohol solutions
David S. Wilcox, Blake M. Rankin and Dor Ben-Amotz

191 Linking molecular/ion structure, solvent mesostructure, the solvophobic effect and the ability of amphiphiles to self-assemble in non-aqueous liquids
Emmy C. Wijaya, Tamar L. Greaves and Calum J. Drummond

217 Mesoscale inhomogeneities in aqueous solutions of small amphiphilic molecules
Deepa Subramanian, Christopher T. Boughter, Jeffery B. Klauda, Boualem Hammouda and Mikhail A. Anisimov

239 General discussion

263 Exploring the behaviour of the hydrated excess proton at hydrophobic interfaces
Revati Kumar, Chris Knight and Gregory A. Voth

279 Monolayer and bilayer structures in ionic liquids and their mixtures confined to nano-films
Alexander M. Smith, Kevin R. J. Lovelock and Susan Perkin

293 A comparative study on bulk and nanoconfined water by time-resolved optical Kerr effect spectroscopy
Andrea Taschin, Paolo Bartolini, Agnese Marcelli, Roberto Righini and Renato Torre

309 Liquid organization and solvation properties at polar solid/liquid interfaces
Eric A. Gobrogge, B. Lauren Woods and Robert A. Walker

329 Dynamics and vibrational spectroscopy of water at hydroxylated silica surfaces
Prashant Kumar Gupta and Markus Meuwly

347 General discussion

371 Low-density liquid water is the mother of ice: on the relation between mesostructure, thermodynamics and ice crystallization in solutions
Griffin Bullock and Valeria Molinero

389 The microscopic features of heterogeneous ice nucleation may affect the macroscopic morphology of atmospheric ice crystals
Stephen J. Cox, Zamaan Raza, Shawn M. Kathmann, Ben Slater and Angelos Michaelides

405 Lifetimes and lengthscales of structural motifs in a model glassformer
Alex Malins, Jens Eggers, Hajime Tanaka and C. Patrick Royall

425 Population and size distribution of solute-rich mesospecies within mesostructured aqueous amino acid solutions
Anna Jawor-Baczynska, Barry D. Moore, Han Seung Lee, Alon V. McCormick and Jan Sefcik
Second-harmonic scattering in aqueous urea solutions: evidence for solute clusters?
Martin R. Ward, Stanley W. Botchway, Andrew D. Ward and Andrew J. Alexander

Corresponding states for mesostructure and dynamics of supercooled water
David T. Limmer and David Chandler

Mesoscopic structural organization in triphilic room temperature ionic liquids
Olga Russina, Fabrizio Lo Celso, Marco Di Michiel, Stefano Passerini, Giovanni Battista Appetecchi, Franca Castiglione, Andrea Mele, Ruggero Caminiti and Alessandro Triolo

Individual gold nanorods report on dynamical heterogeneity in supercooled glycerol
Haifeng Yuan, Saumyakanti Khatua, Peter Zijlstra and Michel Orrit

Water's non-tetrahedral side
Richard H. Henchman and Stuart J. Cockram

The study of correlations between hydrogen bonding characteristics in liquid, sub- and supercritical methanol. Molecular dynamics simulations and Raman spectroscopy analysis
Abdenacer Idrissi, Roman D. Oparin, Sergey P. Krishtal, Sergey V. Krupin, Evgeny A. Vorobiev, Andrey I. Frolov, Leo Dubois and Mikhail G. Kiselev

A mesoscopic model for the rheology of soft amorphous solids, with application to microchannel flows
Alexandre Nicolas and Jean-Louis Barrat

CONCLUDING LECTURE

Fluctuations, clusters, and phase transitions in liquids, solutions, and glasses: from metastable water to phase change memory materials
C. Austen Angell and Zuofeng Zhao

ADDITIONAL INFORMATION

Poster titles
List of participants
Index of contributors