

Faraday Division 141: Water – From Interfaces to the Bulk
27 – 29 August 2008
Heriot-Watt University, Edinburgh, UK

Wednesday 27 August

11:00	Registration Foyer outside Lecture Theatre 1
12:30	Lunch Middle Floor Mezzanine Dining Room (<i>tickets only</i>)
13:15	Welcome and Introductions: Martin McCoustra, <i>Heriot-Watt University, UK</i>
Session 1	Surface Charge of the Liquid Water Surface
	Session Chair: Martin McCoustra, <i>Heriot-Watt University, UK</i>
13.30 Paper 1	Introductory Lecture & Winner of Spiers Memorial Lecture 2008 Ions at aqueous interfaces Pavel Jungwirth* <i>Academy of Sciences of the Czech Republic</i>
14.30 Paper 2	The surface of neat water is basic James K Beattie*, Alex M Djerdjev and Gregory G Warr <i>University of Sydney, Australia</i>
Paper 3	Negative charges at the air/water interface and their consequences for aqueous wetting films containing surfactants Katarzyna Hänni-Ciunel, Natascha Schelero and Regine von Klitzing* <i>Technical University Berlin, Germany</i>
15.30	Afternoon Tea – Microbyte
	Session Chair: Colin Bain, <i>University of Durham, UK</i>
16.00 Paper 5	Water-mediated ordering of nanoparticles in an electric field Dusan Bratko, Christopher D Daub and Alenka Luzar* <i>Virginia Commonwealth University, USA</i>
Paper 6	Ultrafast phase transitions in metastable water near liquid interfaces Oliver Link, Esteban Vohringer-Martinez, Eugen Lugovoj , Yaxing Liu, Katrin Siefermann, Manfred Faubel, Helmut Grubmuller, R Benny Gerber, Yifat Miller and Bernd Abel* <i>Universität Göttingen, Germany</i>
17.00	Close of Session
18.30/19:30	Dinner - Middle Floor Mezzanine Dining Room (<i>tickets only</i>)
19:30/20:30	Poster Session and Wine Reception - Microbyte & Bridge Link Walkway

Thursday 28 August

Session 2	Biological Interfaces and Non-linear Optical Tools
	Session Chair: Michael E Paulaitis, <i>John Hopkins University, USA</i>
09:00 Paper 7	Hydration dynamics of purple membranes Douglas J Tobias*, Neelanjana Sengupta and Mounir Tarek <i>University of California, Irvine, USA</i>
Paper 8	From shell to cell: neutron scattering studies of biological water dynamics and coupling to activity A Frölich, F Gabel, M Jasnin, U Lehnert, D Oesterhelt, A Sadler, M Tehei, M Weik, K Wood and G Zaccai* <i>Institut Laue Langevin, France</i>
Paper 9	Time scales of water dynamics at biological interfaces: peptides, proteins and cells Johan Qvist, Erik Persson, Carlos Mattea and Bertil Halle* <i>Lund University, Sweden</i>
10:30	Morning Coffee – Microbyte
	Session Chair: Kohei Uosaki, <i>Hokkaido University, Japan</i>
11:00 Paper 10	Structure and dynamics of interfacial water in model lung surfactants Avishek Ghosh, Maria Sovago, R. Kramer Campen, Maria Sovago and Mischa Bonn* <i>FOM – Institute for Atomic and Molecular Physics, The Netherlands</i>
Paper 11	The THz dance of water with the proteins: The effect of protein flexibility on the dynamical hydration shell of ubiquitin Benjamin Born, Seung Joong Kim, Martin Gruebele and Martina Havenith* <i>Ruhr-Universität Bochum, Germany</i>
12:00	Close of Session and Lunch - Middle Floor Mezzanine Dining Room <i>(all invited, no tickets required)</i>

Session 3	Ice Interfaces
	Session Chair: Georg Held, <i>University of Reading, UK</i>
13.30 Paper 12	Coarse grained modelling of the interface between water and heterogeneous surfaces Amish Patel**, Adam P Willard** and David Chandler* (<i>work being presented by **</i>) <i>University of California, Berkeley, USA</i>
Paper 13	Water growth on metals and oxides: binding, dissociation and role of hydroxyl groups Miquel Salmeron*, H Bluhm, M Tatarkhanov, G Ketteler, T K Shimizu, A Mugarza, X Deng and T Herranz <i>University of California, Berkeley, USA</i>
Paper 14	Order and disorder in the wetting layer on Ru(0001) Mark Gallagher, Ahmed Omer, George R Darling and Andrew Hodgson* <i>University of Liverpool, UK</i>
15.00	Afternoon Tea – Microbyte
	Session Chair: Regine von Klitzing, <i>Technical University Berlin, Germany</i>
15.30 Paper 15	What ice can teach us about water interactions: a critical comparison of the performance of different water models Carlos Vega*, J L F Abascal, M M Conde and J L Aragonés <i>Universidad Complutense de Madrid, Spain</i>
Paper 16	On thin ice: surface order and disorder during pre-melting C L Bishop, D Pan, L M Liu, G A Tribello, A Michaelides, E G Wang and B Slater* <i>University College London, UK</i>
Paper 17	Reactivity of water-electron complexes on crystalline ice surfaces Mathieu Bertin, Michael Meyer, Julia Stähler, Cornelius Gahl, Martin Wolf and Uwe Bovensiepen* <i>Freie Universität Berlin, Germany</i>
17:00	Close of Session
18:45	Coach transfer to Novotel Edinburgh Park Hotel from Heriot Watt campus
19:15	Pre-Dinner Drinks Novotel Edinburgh Park Hotel (<i>all invited</i>)
20:00	Conference Dinner Novotel Edinburgh Park Hotel (<i>all invited</i>)
23:00	Coach transfer back from Novotel Edinburgh Park Hotel to Heriot-Watt campus

Friday 29 August 2008

Session 4	Nanoscale, Confined Interfaces and Electrochemical Systems
	Session Chair: John Finney, <i>University College London, UK</i>
09:00 Paper 18	“Similarities” between confined and supercooled water Maria Antonietta Ricci*, Fabio Bruni and Alessia Giuliani <i>Università degli Studi "Roma Tre", Italy</i>
Paper 19	Structural and mechanical properties of confined glassy water in nanoscale confinement Thomas G Lombardo, Nicolás Giovambattista and Pablo G Debenedetti* <i>Princeton University, USA</i>
Paper 20	Water nanodroplets confined in zeolite pores Francois-Xavier Coudert**, Fabien Cailliez, Rodolphe Vuilleumier, Alain H Fuchs and Anne Boutin* (<i>work being presented by **</i>) <i>Université de Paris-Sud II, France</i>
10:30	Morning Coffee
	Session Chair: Andrea Russell, <i>University of Southampton, UK</i>
11:00 Paper 21	Dynamic properties of confined hydration layers Susan Perkin**, Ronit Goldberg, Liraz Chai, Nir Kampf and Jacob Klein* (<i>work being presented by **</i>) <i>Weizmann Institute, Israel</i>
Paper 22	Study of nanoscale water cluster by atomic force microscopy Manhee Lee, Baekman Sung, N Hashemi and Wonho Jhe* <i>Seoul National University, Korea</i>
Paper 23	Water at an electrochemical interface – a simulation study Adam P Willard, Stewart K Reed, Paul A Madden* and David Chandler <i>University of Edinburgh, UK</i>
12:30 Paper 24	Concluding Remarks Peter J Feibelman* <i>Sandia National Laboratories, USA</i>
13:00	Acknowledgements: Martin McCoustra, <i>Heriot-Watt University, UK</i>
13:15	Close of Meeting

* denotes corresponding author to whom affiliation applies