



RESEARCH CONFERENCES

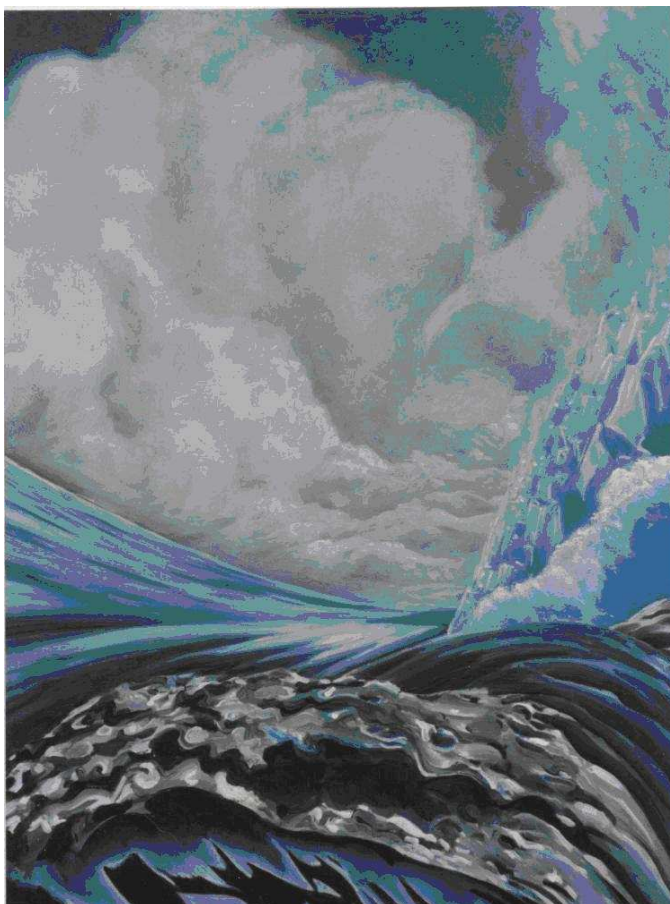
ESF-FWF Conference in Partnership with LFUI

**Water Interfaces in Physics,
Chemistry and Biology:
A Multi-Disciplinary Approach**

Universitätszentrum Obergurgl
(Ötz Valley, near Innsbruck) • Austria
8-13 December 2007

Chair: **Marie-Claire Bellissent-Funel**, LLB CEA-CNRS,
CEA Saclay, FR
Co-Chair: **John Dore**, University of Kent, Canterbury, UK

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Final Programme

Saturday 8 December 2007

Late afternoon / early evening	Registration at the ESF-RC desk
19.00	Welcome Drink
20.00	Dinner

Sunday 9 December 2007

08.45-09.00	Conference Opening
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Session 1: Water/Ice characteristics

Chair: Branka M. Ladanyi, Colorado State University, Fort Collins, US

09.00-09.45	Mark E. Tuckerman New York University, US <i>How accurately can generalized-gradient approximations to density functional theory describe the properties of water and aqueous solutions? Results from ab initio molecular dynamics performed in the complete basis set limit</i>
09.45-10.30	José Teixeira LLB CEA-CNRS, CEA Saclay, FR <i>Study of the dynamics of hydrogen bonds in water and consequences for the unusual behaviour of supercooled water</i>
10.30-11.00	Coffee break
11.00-11.45	Helmut Schober Institut Laue Langevin, Grenoble, FR <i>Characterization of amorphous ice structures via the microscopic dynamics and via the kinetics of the transformation processes</i>
11.45-12.30	Werner Kuhs University of Göttingen, DE <i>Gas - water interactions in crystalline ices and gas hydrates</i>
12.30	Lunch
16.00-16.30	Coffee break

Session 2: Water in confined geometry/ Solid Substrates 1

Chair: Werner Kuhs, University of Göttingen, DE

16.30-17.15	John Dore University of Kent, Canterbury, UK <i>Structural studies of water in a hydrophobic environment</i>
17.15-18.00	Katsumi Kaneko Chiba University, JP <i>Structure of water and hydrated ions confined in carbon nanopores</i>

19.00 Dinner

Poster Session 1

Chair: Helmut Schober, Institut Laue Langevin, Grenoble, FR

20.00-21.00 Very Short Talks

21.00-22.00 Poster session

Monday 10 December 2007

Session 3: Water in confined geometry/ Solid Substrates 2

Chair: José Teixeira, LLB CEA-CNRS, CEA Saclay, FR

09.00-09.45 **Gerhard Findenegg**
Technische Universität Berlin, DE
Limits of freezing and melting of water in MCM-41 type cylindrical nanopores

09.45-10.30 **Sow-Hsin Chen**
MIT, Cambridge, US
Experimental observation of fragile-to-strong dynamic crossover in confined and hydration water and its relation to the liquid-liquid critical point in supercooled water

10.30-11.00 Coffee break

11.00-11.45 **Harald Reichert**
Max-Planck-Institut für Metallforschung, Stuttgart, DE
X-ray investigations of the structure of water and ice at interfaces

11.45-12.00 **Sotiris Xantheas**
Pacific Northwest National Laboratory, Richland, US
Development of a new interaction potential for water from first principles electronic structure calculations and its performance for liquid water and ice

12.00-12.15 **Valeria Molinero**
University of Utah, Salt Lake City, US
Ice nucleation and the liquid-liquid transition in water

12.30 Lunch

15.45-16.15 Coffee break

Session 4: Water in confined geometry/ Soft Systems 1

Chair: Pavel Jungwirth, Academy of Sciences of the Czech Republic, Prague, CZ

16.15-17.00 **Volker Kempter**
Technische Universität Clausthal, DE
Molecules at the interface between vacuum and solid water

17.00-17.45 **Imre Bako**
Hungarian Academy of Sciences, Budapest, HU
Investigation of the structure of aqueous mixtures and electrolyte solutions by different methods

17.45-18.00 **Thomas Loerting**
University of Innsbruck, AT
Multiple first-order like transitions in amorphous ice?

- 18.00-18.15 **Michael Odelius**
Stockholm University, SE
Simulations of x-ray spectroscopies and water adsorption on oxide and metal surfaces
- 18.15-18.30 **Patrick Ayotte**
Université de Sherbrooke, CA
Spectroscopic investigations of acid ionization intermediates trapped in the disordered H-bonded network of amorphous solids
- 18.30-18.45 **Renato Torre**
University of Firenze, IT
Dynamics of supercooled water by ultra-fast optical Kerr effect experiments
- 19.00 Dinner

Poster Session 2

Chair: **John Finney**, University College London, UK

- 20.00-21.15 Very Short Talks
21.15-22.00 Poster Session

Tuesday 11 December 2007

Session 5: Water in confined geometry/ Soft Systems 2

Chair: **John Dore**, University of Kent, Canterbury, UK

- 09.00-09.45 **John Finney**
University College London, UK
Solvent effects in the formation and stabilisation of molecular structures and assemblies: the roles of order and disorder
- 09.45-10.30 **Jan Swenson**
Chalmers University of Technology, Göteborg, SE
Dynamics of hydration water and its implication for biomolecular dynamics
- 10.30-11.00 Coffee break
- 11.00-11.15 **Paola Gallo**
University of Roma Tre, IT
Thermodynamics of supercooled water in solutions
- 11.15-11.30 **Margarita Russina**
Hahn-Meitner-Institut Berlin, DE
Water clathrates: model systems to study hydrogen in confinement
- 11.30-11.45 **Natalie Malikova**
LLB CEA-CNRS, CEA Saclay, FR
Dynamics of water and ions in clays: combining experiment and simulation
- 11.45-12.00 **Bertrand Chazallon**
USTL Lille 1, FR
Organic gas incorporation at the ice surface studied by inelastic Raman scattering
- 12.30 Lunch
- Afternoon Free time

19.00 Dinner
20.00-21.00 Forward Look Plenary Discussion

Wednesday 12 December 2007

Session 6: Water in confined geometry/ Bio-Systems

Chair: Giuseppe Zaccai, Institut Laue Langevin, Grenoble, FR

09.00-09.45 Bertil Halle
Lund University, SE
Exploring biomolecule-water interaction by NMR

09.45-10.30 Joseph Parello
Vanderbilt University, Nashville, US
Hydration in GPCR-mediated signal transduction

10.30-11.00 Coffee break

11.00-11.45 Fabio Bruni
University of Roma III, IT
Proton momentum distribution in a protein hydration shell

11.45-12.00 David Nutt
University of Reading, UK
Towards a greater transferability of water models in biomolecular simulations

12.00-12.15 Arrigo Calzolari
CNR-INFM-S3 National Center on nanoStructures and bioSystems at Surfaces, Modena, IT
Aqueous hydration of cyanin dye molecule: an atomistic insight

12.15-12.30 Stanislas Pommeret
CEA Saclay, Gif-sur-Yvette, FR
Relation between frequency and H bond length in heavy water: towards the understanding of the unusual properties of H bond dynamics in nanoporous media

12.45 Lunch

16.00-16.30 Coffee break

Session 7: Water in confined geometry/ Bio-Systems/Modelling 1

Chair: Volker Kemper, Technische Universität Clausthal, DE

16.30-17.15 Branka M. Ladanyi
Colorado State University, Fort Collins, US
Structural order and dynamics at water/hydrocarbon interfaces and in reverse micelles

17.15-17.30 Ferenc Mezei
SzFKI, Budapest, HU
Glass transition and functionality in hydrated proteins

17.30-17.45 Camille Loupiac
University of Burgundy, Dijon, FR
Hydration effects on beta-lactoglobulin dynamics and stability

- 17.45-18.00 **Maria Grazia Ortore**
Polytecnic of Marche, Ancona, IT
Detailing protein solvation shell in a mixture: a SANS study
- 18.00-18.45 **Giuseppe Zaccai**
Institut Laue Langevin, Grenoble, FR
Water in halophile Dead Sea organisms: neutron scattering studies of adaptation to extreme environments
- 20.00 Get Together & Conference Dinner

Thursday 13 December 2007

Session 8: Water in confined geometry/ Bio-Systems/Modelling 2

Chair: **Marie-Claire Bellissent-Funel**, LLB CEA-CNRS, CEA Saclay, FR

- 09.00-09.45 **Bert de Groot**
MPI for Biophysical Chemistry, Göttingen, DE
Dynamics and energetics of water permeation across biological channels and model peptidic pores
- 09.45-10.30 **Pavel Jungwirth**
Academy of Sciences of the Czech Republic, Prague, CZ
Ions at surfaces of hydrated proteins and other interfaces
- 10.30-11.00 Coffee break
- 11.00-11.15 **Marie-Sousai Appavou**
Forschungszentrum Juelich GmbH, Garching bei München, DE
Effect of high pressure on the global and internal dynamics of a multimeric protein: case of Haemoglobin studied by quasielastic neutron scattering experiment.
- 11.15-11.30 **Stephen Holt**
STFC, Didcot, UK
The assembly of antibody-binding membrane protein arrays
- 11.30-12.00 **Concluding Remarks**
- 12.00 Lunch and Departure

Abstracts, Posters & Short Oral Presentations

Invited lectures are 30+15 minutes discussion, contributed talks are 10+5 minutes discussion.
All abstracts that have not been selected for short talks are accepted for poster presentation.