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

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

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SCIENTIFIC REPORT

Introduction (up to 2 pages)

Introduction on the topic in non-specialist terms (especially for highly technical subjects)

Water is a profoundly unusual liquid, and its peculiarities appear to make it uniquely suited to act as life's 'matrix'. In particular, the characteristics of ***water*** in ***super-cooled state*** are unique and strongly linked to the spatial features of the ***hydrogen-bond networks*** in the ***amorphous ices***. Furthermore, water in ***confined geometry*** has a depressed nucleation temperature, which allows the structural and dynamic characteristics to be studied for the low-temperature liquid phase in well-defined ***mesoporous solids***.

In a biological context, a significant fraction of ***cellular water*** consists of interfacial water, i.e., water that is confined by, or in proximity to macromolecular and other kinds of surfaces. Proximity to interfaces appears to modify the structure and the physical properties of this ***interfacial water***, apparently leading to an enhanced level of ***hydrogen-bonding***. Consequently, the study of simpler 'model' systems using synthetic ***microporous and mesoporous substrates*** can provide a valuable input to the interpretation of biological aspects. However, an understanding of the properties of interfacial water has, to date, escaped a complete and accepted description.
Because interfacial water may govern many or perhaps all aspects of ***cellular***

metabolism and because the physical properties of interfacial water are believed to be different from those of free water, it is of fundamental importance to understand how interfacial water mediates cellular processes. Typical examples are the role of interfacial water in a macromolecular assembly and its function in allosteric regulation of ***proteins and enzymes***, in energy metabolism, in signal transmission, and in the association of macromolecules with one another.

Our purpose was to address a number of highly topical aspects of this emerging research area to progressively emphasise the role of water in biological processes. The subject material was spanning from ***synthetic mesoporous solids*** to biological systems such as ***protein surfaces and membranes*** as well as ***living cells.*** A ***multi-disciplinary presentation*** drawn from areas of physics, chemistry and biosciences and discussion that focuses on the properties of water (and ice) in proximity to different types of interface has been developed successfully.

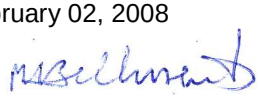
As a result the conference has been an up-to-date account of the latest development on the physics, chemistry and biological aspect of interfacial water.

Various techniques are used to probe the structure of bulk and interfacial water. Among them spectroscopic probes : neutrons, X-rays, (SAXS and SANS, inelastic neutron scattering), NMR, FTIR, Raman are well suited to reveal structural information as well as dynamics of water at solid, soft, vapour, protein, membrane, interfaces, etc, but also IR radiation, electron, and particles beams, metastable atoms of thermal energy. Massive classical force field and ab initio molecular dynamics simulations have been presented as powerful techniques to investigate the hydration properties of a dye molecule.

I hereby authorize ESF - and/or the Fonds zur Förderung der wissenschaftlichen Forschung in Österreich (FWF) and the Leopold-Franzens-Universität Innsbruck (LFUI) - to publish the above two-page Introduction on a special page dedicated to 'Conference Highlights' within the Research Conferences website.

Date & Signature:

February 02, 2008



■ Scientific Content

▪ Summary of the conference sessions focusing on the scientific highlights

The conference programme was based on five different themes and organized into eight sessions, which are given below in the order of presentation. Each invited lecturer reviewed their particular topic and placed it in the general framework of the current research issues; the presentations were followed by an extended discussion period that

was controlled by the session chairperson.

In addition, a number of poster sessions was organized in which the young scientists had the opportunity to present their results of relevance for the conference. These posters were introduced by the young scientists in 5 min short oral contributions.

Session 1: Water/ice characteristics

(i) Structure and dynamics, hydrogen-bonding, water-ice transformations
(ii) Spectroscopic probes: neutrons, X-rays, NMR, FTIR, Raman

Mark E. Tuckerman
New York University, US
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

José Teixeira
LLB CEA-CNRS, CEA Saclay, FR
Study of the dynamics of hydrogen bonds in water and consequences for the unusual behaviour of supercooled water

Helmut Schober
Institut Laue Langevin, Grenoble, FR *via the microscopic dynamics and via the kinetics of the transformation processes*
Characterization of amorphous ice structures

Werner Kuhs
University of Göttingen, DE
Gas - water interactions in crystalline ices and gas hydrates

Sessions 2 and 3 : Water in confined geometry/ Solid Substrates

(i) Interfacial interactions : hydrophobicity/hydrophilicity
(ii) Surface characterisation : Silicas (sol-gel, Vycor, CPG, MCM, SBA……), Zeolites, clays, Activated carbons, carbon nanotubes
(iii) Structure and dynamics (constrained molecular mobility), water-ice transformations

John Dore
University of Kent, Canterbury, UK
Structural studies of water in a hydrophobic environment

Katsumi Kaneko
Chiba University, JP
Structure of water and hydrated ions confined in carbon nanospaces

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

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

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

Sessions 4 and 5: Water in confined geometry/ Soft Systems

(i) Related systems-clathrates, aqueous solutions, amphiphiles, surfactants, lamellar liquid crystals, microemulsions, soluble polymers
(ii) Structure and dynamics (constrained molecular mobility), hydrogen-bonding
(iii) Spectroscopic probes: neutrons, X-rays, NMR, FTIR, Raman

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

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

John Finney
University College London, UK
Solvent effects in the formation and stabilisation of molecular structures and assemblies: the roles of order and disorder

Jan Swenson
Chalmers University of Technology, Göteborg, SE
Dynamics of hydration water and its implication for biomolecular dynamics

Session 6: Water in confined geometry/ Bio-Systems

(i) Biological interfaces, membranes, proteins, biological complexes, cells
(ii) Interfacial water in biological processes, enzymatic catalysis, water channels, ionic channels
(iii) Spectroscopic probes: neutrons, X-rays, NMR, FTIR, Raman

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

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

Giuseppe Zaccai
Institut Laue Langevin, Grenoble, FR
Water in halophile Dead Sea organisms: neutron scattering studies of adaptation to extreme environments

Sessions 7 and 8 : Water in confined geometry/ Bio-Systems/Modelling

(i) Molecular modelling, molecular dynamics, DFT computations, etc
(ii) Interaction potentials, simple and otherwise, ab initio methods
(iii) Hydrogen-bond effects on structure and dynamics in confinement

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

Bert de Groot
MPI for Biophysical Chemistry, Göttingen, DE
Dynamics and energetics of water permeation across biological channels and model peptidic pores
Pavel Jungwirth
Academy of Sciences of the Czech Republic, Prague, CZ
Ions at surfaces of hydrated proteins and other interfaces

Highlights of the contributions:

Super-cooled systems and water/ice in confined geometry certainly featured in the presentations along with amorphous ices and clathrates but it would be difficult to describe the advances shortly and in a non-technical way. At any rate, it can be stated that the similarities and differences between the different forms of ice could be worked out. In particular, the relation between solid amorphous ice and liquid water was discussed at quite some detail.

Not only was the water – water interaction studied on the basis of ab initio potentials. In addition, the water – solute interaction was studied on the basis of ab initio potentials. Presently, their availability allows the detailed study of solvation and segregation processes for species of biological interest in aqueous systems. Both classical MD and ab initio on the flight MD are now employed for this purpose.

High resolution X-ray spectroscopy (new generation of synchrotron source) is very powerful to investigate water and ice structure at interfaces. At ice-SiO2 model interface it has been revealed the presence of a quasi - liquid layer with a density 20 % higher than that of bulk liquid water. At the interface of water to a hydrophobic OTS layer on silicon, it has been revealed a deficit of about half monolayer of water molecules.

Important presentations include the structure of water and hydrated ions confined in carbon nanospaces, in connection with environmentally-friendly technologies The hydrophobic nanospace in water channel should be a role of gate for water penetration. In this context it is important to mention the molecular dynamics study of the dynamics and energetics of permeation events through specialized channels (aquaporins), these channels allow the efficient and selective water and ion release and uptake by biological cells..

There was something on dye cyanin molecules that are photoactive elements in dye-sensitized solar cells. In photosynthesis, due to the uptake of the photon, the structure of photosynthetic biomolecules changes. Massive classical force field and ab initio molecular dynamics simulations were presented to investigate the hydration properties of a cyanin dye molecule.

In bacteriorhodopsin, after excitation by light, water molecules from outside can then penetrate deeper and come into contact with the trapped water molecules. In order to generate energy the photosynthetic biomolecules adsorbs protons in this way transports them to the retinene and discharges them from the cell.

▪ Assessment of the results and their potential impact on future research or applications

One has to focus on the molecular dynamics study of the dynamics and energetics of permeation events through specialized channels (aquaporins), these channels allowing the efficient and selective water and ion release and uptake by biological cells. The understanding of such events could find application into development of medication and design of nanofluidic devices.

■ Forward Look Plenary Discussion

▪ State-of-the-art in the field

The overall research field that is relevant to the 'water interfaces' theme is very wide and the diversity of the presentations has meant that all participants learned new material and gained further insights from topics that they had probably not thought were of direct interest to their own studies.

▪ Emerging topics

There were undoubtedly some emerging topics :

- the study of water surfaces, as well as the study of the water – solute interaction, using not only X-ray/neutron techniques, but also IR radiation, electron, and particles beams, metastable atoms of thermal energy, in particular. The application of metastable He atoms to the study of processes at water surfaces follows the strategy proposed by the physics Nobel price winner of 2007, G. Ertl.

- at molecular level the structure of compounds by coupling simulations and experiments.

- the transient absorption spectroscopy on nanoconfined water that inform about the H-bond network structure and dynamics in nanoconfined water,

- the dynamic properties of water in living cells,

-the attempt to relate the properties of amorphous solid water to those of water in the liquid state. If successful, results obtained for amorphous solid water would also be of relevance for liquid water. This would imply that the interaction of solutes with water, their segregation and solvation properties, could then be studied on a time scale which is orders of magnitude longer than in the liquid. This would also allow for the application of the sophisticated surface - analytical tools to the above - mentioned processes.

▪ Visions for the future of the research field – identification of issues in the 5-10 years & timeframe

The combined effort of experimental physics and chemistry, together with sophisticated ab initio and molecular dynamics studies, will lead to a detailed understanding of the dynamic properties of water under biological conditions, in particular in living cells.

▪ Is there a need for a foresight-type initiative?

The meeting has created a new community of researchers with common interests and it is desirable that the established contacts are maintained into the future. One possibility is to create a Newsletter that can be circulated to the representative groups in order to keep abreast of current developments. This type of action would help to focus relevant new research that, currently, tends to be published in a wide range of different journals.

▪ The reaction of the participants to the location and the organization, including networking, and any other relevant comments

We received much positive comment from the participants. Congratulations about the excellence of the science continue to be sent by e-mail by the participants. Some active participation and lively discussions among a multidisciplinary community took place which demonstrates the needs to organise such a conference. Wishes from participants are to maintain and develop in the future alive interactions between them. Because of that, I consider that the conference was highly successful and fulfilled its objectives.

Date & Signature:

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