EDITORIAL

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Interfacial water in chemistry and biology

International Discussion Meeting of the Deutsche Bunsen-Gesellschaft für Physikalische Chemie, Velen, September 19th–23rd, 2003

During the last years, widespread and intense activities have led to a deeper understanding of the anomalies of water and directed the focus of many researchers to the properties of metastable, especially supercooled, water. This has led to astonishing new insights, like the possible existence of liquid–liquid phase transitions of one-component fluids or the related phenomenon of polymorphism. In contrast, the function and the properties of water at interfaces are not sufficiently studied and not well understood, although they are of central importance for many biological and technical processes. This is in particular true for biomolecular interfaces as found in cell membranes, proteins or DNA/protein complexes. Interfacial phenomena are also of paramount importance for the design of micro- and nanostructures in bioscience and engineering. Porous systems are considered for reaction selectivity, stability and separation processes and heat storage purposes. Furthermore, a better understanding of the aging process of polymers or the production of water repellent surfaces are demanded.

The meeting discussed intensively the behaviour of water in its central importance for the structure, dynamics and function of hydrated biomolecules, in particular proteins and model biomembranes. Pollak gave an introduction into his view of cells as gel like systems. Garcia reported molecular dynamics simulations to elucidate the protein folding mechanism and the role of water in protein folding scenarios. A new sampling technique allows the determination of the potential energy surfaces of the free energy, entropy and enthalpy for wide ranges of temperature. Berkowitz discussed the structural and dynamical properties of water in the hydration shell of model biomembranes and micelles.

The modified behaviour of water in confined geometries, such as pores and channels, as well as the role of inner surfaces having different chemical and topological characters were also reported. Findenegg and Evans introduced recent experimental and theoretical results in the field. Brovchenko discussed the phase behaviour of water in pores. Gibbs-ensemble Monte Carlo simulations predict that a two-phase-state is the most likely one over wide ranges of pore filling. Morishige reported the influence of pore geometry on the freezing and melting of water.

Several speakers gave new experimental and theoretical results regarding the structure of water at solid and liquid interfaces. Richmond reported spectroscopic studies of hydrogen-bonded water structures at the interface to hydrophobic liquids. The behaviour of water at hydrophilic interfaces based on neutron scattering experiments was discussed by Bellissent-Funel. The current and future possibilities of synchroton radiation for the study of solid-liquid interfaces were summarized by Tolan. Benjamin focussed on dynamical aspects and reported chemical reactions and energy relaxation at such interfaces.

Studies at free surfaces were reported by Saykally and Rignanese. In particular the adsorption of ions at free water surfaces and the hydration of silicon oxide interfaces were discussed. Strey presented empirical functions for the nucleation rate of protonated and deuterated water.

One session addressed the hydration and interaction of dissolved particles. Pratt introduced his 'quasi-chemical theory' for calculating thermodynamic properties of ions in aqueous solution. Paschek discussed electrolyte solutions and reported on interactions between ions and hydrophobic particles.

Proton transfer and proton ordering play an important role in processes at interfaces. Marx reported on proton transfer mechanisms in hydrogen-bonded networks and the application of CPMD methods for a molecular level understanding of the Grotthuss mechanism. Bruni discussed the migration of protons on the surface of globular proteins. Schmitt reported on the dynamics of protons in ion channels.

Unfortunately, no complete list of all the interesting talks and poster contributions can be given here.

The meeting showed impressively that interfacial water in chemistry and biology attains enormous interest. By joint efforts of experiments and simulations, substantial advances can still be expected in the near future.

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Further information about the meeting and the work of the DFG-Forschergruppe "Polymorphism, dynamics and function of water at molecular interfaces" can be found in the internet at http://www.forschergruppe436.de/.

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