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PREFACE

Water at interfaces

Guest Editors

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This special issue is devoted to illustrating important aspects and significant results in the field of modeling and simulation of water at interfaces with solutes or with confining substrates, focusing on a range of temperatures from ambient to supercooled.

Understanding the behavior of water, in contact with different substrates and/or in solutions, is of pivotal importance for a wide range of applications in physics, chemistry and biochemistry.

Simulations of confined and/or interfacial water are also relevant for testing how different its behavior is with respect to bulk water. Simulations and modeling in this field are of particular importance when studying supercooled regions where water shows anomalous properties.

These considerations motivated the organization of a workshop at CECAM in the summer of 2009 which aimed to bring together scientists working with computer simulations on the properties of water in various environments with different methodologies.

In this special issue, we collected a variety of interesting contributions from some of the speakers of the workshop. We have roughly classified the contributions into four groups.

The papers of the first group address the properties of interfacial and confined water upon supercooling in an effort to understand the relation with anomalous behavior of supercooled bulk water. The second group deals with the specific problem of solvation. The next group deals with water in different environments by considering problems of great importance in technological and biological applications. Finally, the last group deals with quantum mechanical calculations related to the role of water in chemical processes.

The first group of papers is introduced by the general paper of Stanley *et al*. The authors discuss recent progress in understanding the anomalies of water in bulk, nanoconfined, and biological environments. They present evidence that liquid water may display 'polymorphism', a property that can be present in other liquids also. Recent evidence of a close relation between thermodynamical properties and dynamical behaviour of water are also discussed.

Gallo *et al* present the results of a computer simulation of water confined in a cylindrical pore of MCM-41 silica material. The mobile portion of the confined water shows a fragile to strong dynamic transition similar to the bulk. In the bound water, an anomalous diffusion connected to the residence time distribution is found.

Franzese *et al* report calculations on lattice models adapted to describe general properties of water in contact with protein surfaces. The results of Monte Carlo and mean field calculations show the presence of two-dynamical crossovers.

Corradini *et al* investigate the supercooled region of ionic aqueous solutions in order to study the effect of ions on the limit of mechanical stability, the lines of maximum density and the liquid–liquid critical point for different ionic concentrations.

The paper by Vallauri *et al* deals with the dynamical behavior of water close to the liquid–liquid transition by considering the velocity correlation functions calculated in three supercooled states.

Suffritti *et al* study water adsorbed in zeolites with a new empirical potential, structural and dynamical properties are studied in the supercooled region.

The second group starts with a paper on the problem of solvation by Lynden-Bell. The author shows how the properties of water and, in particular, solvation properties are modified by changes in the site–site interaction potential of water.

Henchman *et al* derive equations for different thermodynamical quantities like partial enthalpy and partial entropy for dilute solutions of noble gases.

The third group starts with Buldyrev *et al* who study the swelling of bead-on-a-string polymers in Jagla water-like particles, finding similarities with respect to cold denaturation of protein in water.

Pellenq *et al* consider water confined in pores of different materials with different size scales. Silicalite and tobermorite, a layered calcio-silicate model of cement and Vycor are analyzed.

Gordillo and Martí consider structural and dynamical properties of water confined or close to carbon nanotubes or inside a slit pore of a single graphene sheet.

Jedlovszky *et al* introduce a new method to determine the molecules located right at the boundary of two phases in a computer simulation. The new method is applied to the analysis of the interface of water with different apolar phases.

Melchionna *et al* consider phenomena related to water in contact with thermophilic protein interfaces. In particular, they discuss the role of water in stabilizing these proteins.

Rotenberg *et al* report results on the structure and dynamics of water at a clay surface. They analyze, in particular, the influence on the H-bond network of the surface oxygens and ions and investigate the surface H-bond formation and dissociation dynamics.

Smirnov and Bougeard present examples of the spatial organization of molecules and of the short- and long-time dynamical behaviour of water confined in the pores of crystalline aluminosilicates, such as zeolites and clays, and in nanostructured materials.

The last group opens with Sulpizi and Sprik who present density functional calculations of the dissociation constant of liquid water, implemented with a proton insertion/removal method.

Jung and Marcus consider, more specifically, the properties of water in organic catalysis and discuss theoretical models and results obtained with quantum mechanical calculations.

As organizers of the CECAM workshop ‘Modeling and Simulation of Water at Interfaces from Ambient to Supercooled Conditions’ we would like to thank CECAM, ESF-Simbioma, Wanda Andreoni, Emilie Bernard and Jordi Brusa. As guest editors of this special issue we would like to thank Gerhard Kahl and Philip Semple.