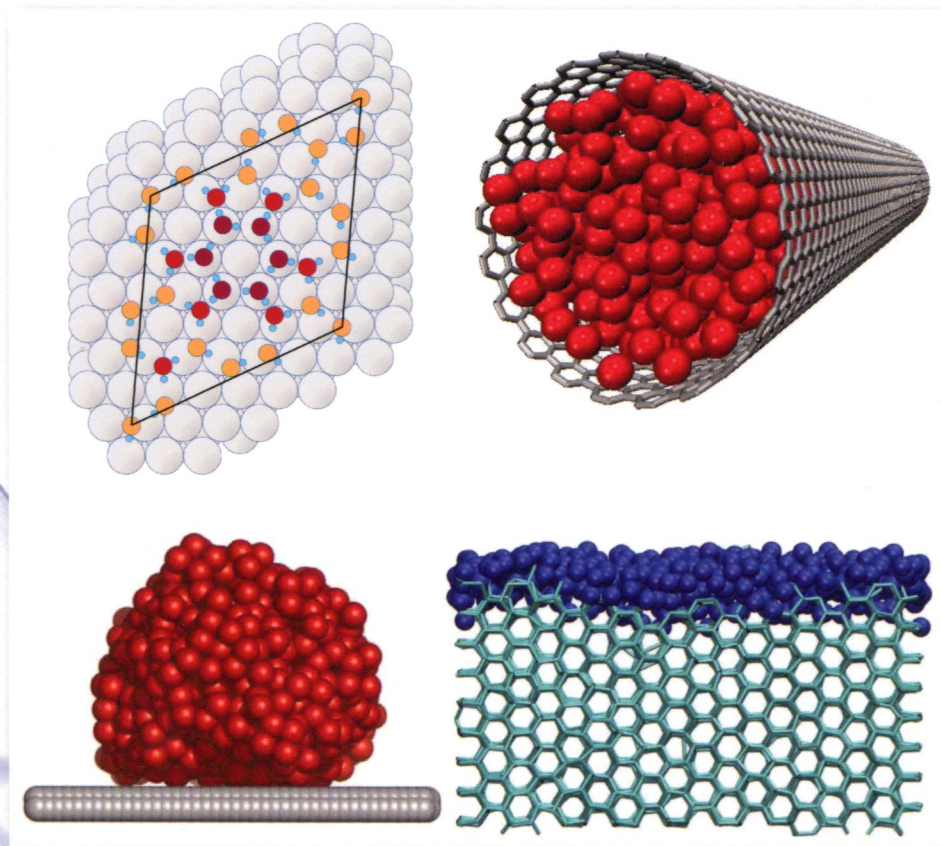


14 November 2014

Volume 141 Number 18

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AIP | The Journal of Chemical Physics



SPECIAL TOPIC:
Interfacial and Confined Water

► Cover image from Valeria Molinero and Bruce D. Kay, *J. Chem. Phys.* **141**, 18C101 (2014).

SPECIAL TOPIC: INTERFACIAL AND CONFINED WATER

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Structure and dynamics of water in nanoscopic spheres and tubes (10 pages)

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Interfacial and confined water are pervasive in nature and in both natural and engineered systems. The physics of interfacial and confined water remains a subject of fundamental importance, and the study of its structure, dynamics, thermodynamics, phase transitions, and reactivity at water and air in water and at fundamental scientific importance, and have far-reaching implications in areas as diverse as atmospheric chemistry, cryopreservation, electrochemistry, and energy storage. The development of new materials, and the operation of nanosystems. This collection of 35 invited papers from leaders in the field represents experimental, theoretical, and computational advances that tackle problems of fundamental importance for interfacial and confined water. These advances define the current state-of-the-art and provide a platform for future study.

Below we provide a brief overview of important topics and outstanding issues that define the field of interfacial and confined water. The choice of topics and issues is biased by our personal research interests and, as such, should be taken as representative rather than comprehensive. In a similar vein, we refrain from providing a list of references to prior work since an list capturing the breadth and depth of this important field would be prohibitive in length. In order to capture the key history and evolution of this rapidly evolving and dynamic area of scientific inquiry we encourage the reader to consult the 37 papers included in this special issue.

The defining characteristic of water is construction of the hydrogen bond network. In bulk water, this network is disrupted at the interface by the presence of a solid surface. The breaking of symmetry at an interface or in confinement can cause the formation of novel structures without counterparts in bulk water. The breaking of symmetry also leads to changes in the reactivity of water at interfaces and confined spaces. The differences can be a pronounced change in the structure of complexity. Interfacial phase is heterogeneous water, and the structure of

water changes and dynamic changes in acidity of the water at the liquid-vapor interface. The effect of the organization of the hydrogen bond network in the dynamics of water, the properties of water as a solvent, the solubility of water and solutes, however, are not fully understood.

Hydrogen bonds remain ubiquitous at the liquid-vapor interface, the best studied of water interfaces. The dialogue between experiments and modeling has resulted in significant advances in this area in the last decades. Several questions, however, are still not fully settled. For example, what drives some water molecules to adsorb on the length scale of the interfacial region, and what are the consequences, whether the interface is rich in hydrogen bonds, and what is the reactivity of these interfacial water? It is not known in which extent water adsorbs at fully or partially solvated at the interface and the impact of this may have on their availability for chemical reactions. The interpretation of the rich vibrational spectroscopy of water at the liquid-vapor interface, the details of the intermolecular hydrogen bonding, is still locally controversial. The elucidation of the order, the number, and strength of hydrogen bonds of liquid water in contact with hydrophobic surfaces, and to which extent they control the behavior of water at the vapor-liquid interface, is an area of active fruitful research.

The properties of the ice-liquid interface are of great relevance in environmental chemistry, cryopreservation, and the prediction of ice crystal nucleation rates. Nevertheless, it was found much less studied than the liquid-vapor interface. Some of the most fundamental properties of the ice-liquid interface are not fully known. The latent heat of phase free energy—key for the prediction of homogeneous ice nucleation rates—has been experimentally determined only at the melting temperature, and with very high uncertainty. Its temperature dependence has not yet been investigated experimentally. Consistent with the fact that superheating, from supercooled whether water is stable and/or ice is metastable at the ice-liquid interface, not only affects the dynamics of this interface, but also the rate of ice crystal growth. The temperature of these properties, and the prediction of the rates of ice nucleation, are of great importance for the study of ice nucleation, and