Studies of Water in Hydrophobic Confinement

John Dore
School of Physical Sciences, University of Kent, UK

Abstract:
The last decade has seen a great interest in the study of water in confined geometry. Most of the experimental work has been undertaken with a range of mesoporous silicas in which the surface interaction is essentially hydrophilic. The behaviour of the water [and ice] in these systems shows a strong dependence on a number of factors, such as pore size, pore morphology and fractional filling-factors. Furthermore the nucleation to produce ice is complex, producing a mixture of hexagonal [I_h], cubic [I_c] and disordered states that are temperature-dependent and may also exhibit hysteresis effects; the solid phase has been likened to that occurring in rotationally-disordered crystals and has been referred to as 'plastic ice'.
Consequently, it is of interest to study the behaviour of water in a hydrophobic mesopore environment although this poses a number of technical problems. Two approaches have been adopted that will be reported in this presentation. The first method uses a surface modification technique that introduces a layer structure on to the internal substrate to make the basic interaction hydrophobic. Neutron and NMR techniques have been used to investigate the difference in water/ice characteristics for the modified and non-modified samples; the latest results will be presented. Another approach is to use a different substrate. It is well-known that water is readily adsorbed into carbon nanotubes, despite the fact that the water-graphene interaction is primarily hydrophobic. Experimental measurements have been made for water/ice in carbon nanohorns with a mean pore diameter of 30 Å. In this case, the water features are quite unusual with a lower temperature-dependence, evidence of enhanced connectivity in the H-bond network and a much reduced density. Some recent DINS measurements suggest that there is possibly evidence for de-localisation effects in the H-bond, which will require more detailed investigation.

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[jcd1@kent.ac.uk]