Water – From Clusters to Nanoconfinement to the Bulk

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The evolution of water from clusters to the bulk provides fundamental insight into the nature of water. One of the most exact methods of understanding small water clusters is with high-resolution far infrared vibration rotation tunneling (VRT) spectroscopy. This method has allowed for a highly detailed study of the structure and dynamics of the water dimer through the octamer.(*1*) While this method cannot provide as detailed information of bulk water, it provides valuable insight into the fundamental interactions of individual water monomers as function of cluster size.

The difficulty of characterizing bulk water can be mitigated by working in a different frequency range, i.e. soft x-rays.(*2*) Square ice is a form of water with a strange square structure as measured by TEM. Despite being initially measured several years ago, this phase remains largely unexplained. By combining soft x-ray spectroscopy with advanced theory, we are able to show that the so-called "square ice" form of water is due to a novel and thermodynamically stable phase of monolayer 2-D water between graphene bilayers that is stabilized by graphene imperfections. We show that this phase is stable at room temperature for up to thousands of water molecules, and we demonstrate how it can be both be made and trapped. We further explain the rest of the observed "square ice" structures based on a few simple guidelines.

Unfortunately, traditional x-ray spectroscopy has limited surface sensitivity to several nanometers. This is far too long for a variety of important topics. With the advent of new free electron lasers, it is possible to perform x-ray nonlinear optics. We recently demonstrated for the first time soft x-ray nonlinear optics, and showed that it is surface and spectrally sensitive based on our studies of graphite.(*3*) The work has been extended to boron thin films and coatings, showing a sensitivity at surfaces not found in traditional x-ray measurements. Finally, we show that while there are challenges in extending soft x-ray nonlinear optics to water and aqueous surfaces, but these challenges should be surmountable.

References

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