MAR05-2004-010095

Abstract for an Invited Paper
for the MAR05 Meeting of
the American Physical Society

X-ray spectroscopy studies of liquid water

ANDERS NILSSON, Stanford Synchrotron Radiation Laboratory, 2575 Sand Hill Road, Menlo Park, CA 94025, USA

We have investigated the electronic structure of water and ice using a combination of experimental and theoretical techniques [1]. Measurements have been performed on the liquid using both X-ray Absorption (XAS) and X-ray Raman Spectroscopy. The spectrum of the liquid is distinctly different from that of the bulk ice, where the liquid shows a distinct pre-edge feature and a strong enhancement of the intensity at the edge. Through spectrum simulations and model experiments (bulk and surface of ice) we show that the specific features in the liquid spectrum are due exclusively to asymmetric configurations with only two strong hydrogen bonds: one donating and one accepting, indicating that the liquid consists of rings or chains embedded in a disordered H-bond network [1]. Current molecular dynamics techniques fail to predict these new experimental data. Recent results on disparities in supercritical water will also be discussed.

[1] Wernet et al, Science 304, 995-999 (2004)