Proton quantum effects in water

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ABSTRACT

Proton quantum effects, for example those associated with the breaking and distortion of hydrogen bonds, are very effectively revealed by measurements of proton momentum distributions, $n(p)$, and mean kinetic energy, $<E_K>$, via Deep Inelastic Neutron Scattering (DINS). DINS investigations complement x-ray and neutron studies on spatial distributions of the proton. Both physical quantities $n(p)$ and $<E_K>$ provide unique information on the "effective potential" that the proton sees as the hydrogen bond network changes, as for instance in presence of proton tunneling, delocalization and breaking of H bonding. Due to the quantum mechanical non commuting property of position and momentum, the shape of proton momentum distribution is directly related to the shape of the effective proton potential. Differences in $n(p)$ between liquid water and ice reflect for example the breaking and distortion of hydrogen bonds that occurs upon melting.

In this talk direct DINS measurements of the proton $n(p)$ and $<E_K>$ in stable and supercooled water are presented. Results show a strong temperature dependence of proton $n(p)$ lineshapes and $<E_K>$ in liquid water around the density maximum and in the metastable phase.