Deep and Inelastic neutron scattering of quantum particles in ice, normal and metastable phases of water

By

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Host: Asst. Prof. Pinaki Sengupta

Abstract

The proton momentum distribution is a very sensitive probe of the potential of mean force experienced by the protons in hydrogen-bonded systems which can be accessed by deep inelastic neutron scattering experiments (DINS). DINS investigations complement x-ray and neutron studies on spatial distributions of the proton.

This talk presents DINS results on H quantum particles in polycrystalline ice [1], preliminary result from DINS on O quantum particles in heavy water and ice, and DINS and INS experiments in metastable (supercooled) and stable (supercritical) phases of water. The experiments are motivated by the need of collecting quantitative and complementary information on both S(Q,E) and n(p) in a wide range of thermodynamic states in stable and metastable phases of water.

The DINS experiment on heavy water and ice is motivated by theoretical prediction of a considerable quantum excess in kinetic energy for oxygen atoms in ice at 269 K, i.e. 21 meV above the classical value of 35 meV.

The INS experiment on supercooled water is motivated by the need to complement DINS experiment in metastable phase of water with vibrational spectra in the same system.

The experiments on supercritical water, part of series of experiments (DINS, INS and Monte Carlo simulation), aim to explore the detail the momentum distribution S(Q,E) and n(p) in a thermodynamic range at~25 MPa in a temperature range 280° - 600°C, where density decreases from over 600 kg/m3 to less than 200 kg/m3 across the pseudo-critical temperature of 385°C.

Reference:


Short Biography

Carla Andreani, experimental physicist, received a Laurea Cum Laude in Physics in 1977 at the Università di Roma “La Sapienza” and is presently full professor in Condensed Matter at Department of Physics – Faculty of Science – at the University of Rome Tor Vergata. From 1981 – 1987 she worked at the A.E.R.E Harwell Laboratory, at the ISIS Spallation neutron Source – Rutherford Appleton Laboratory in UK, and at the IPNS pulsed Neutron source – Argonne National Laboratory, in US.
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