

Abstract Submitted  
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**Water in Carbon Nanotubes: A New Quantum Phase of Water<sup>1</sup>**

GEORGE REITER, University of Houston, CHRISTIAN BURNHAM, DIRAR HOMOZ, University of Houston, PHILIP PLATZMAN, JEREMY MAYERS, TYNO ABDUL-REDAH, ISIS, Rutherford-Appleton Laboratory, ALEXANDER MORAVSKY, MER Corporation, JICHEN LI, University of Manchester, C.-K. LOONG, ALEXANDER KOLESNIKOV, Argonne National Laboratory — The momentum distribution of the protons in ice Ih, ice VI, high density amorphous ice and water in carbon nanotubes has been measured using deep inelastic neutron scattering. We find that, at low temperatures, the momentum distribution for the water in the nanotubes is qualitatively unlike that in any other phase of water or ice. The kinetic energy of the protons is 35meV less than that in ice Ih at the same temperature, and the high momentum tail of the distribution, characteristic of the molecular covalent bond and the stretch mode of the proton in the molecule, is not present. We observe a phase transition between 230K and 268K in the nanotube data. The high momentum tail is present in the higher temperature measurement, which resembles that of ice Ih at the same temperature. Molecular dynamics simulations show the phase transition to be associated with the reordering of the hydrogen bonds of the 2-D ice layer, coating the interior of the nanotube at low temperatures, into a 3-D structure at 268K. Although there is yet no model for water that explains the low temperature momentum distribution, our data reveals that the protons in the hydrogen bonds in the 2-D ice layer are coherently delocalized, and that the 2-D ice layer is a qualitatively new phase of ice.

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