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Anomalously soft dynamics of water in carbon nanotubes
ALEXANDER KOLESNIKOV, CHUN-KEUNG LOONG, NICOLAS DE SOUZA, Intense Pulsed Neutron Source Division, Argonne National Laboratory, 9700 S. Cass Ave., Argonne, IL 60439, USA, CHRISTIAN BURNHAM, Department of Chemistry, University of Utah, Salt Lake City, UT 84112, USA, ALEXANDER MORAVSKY, RAOUF LOUTFY, MER Corporation, 7960 South Kolb Road, Tucson, AZ 85706, USA — Quasi-one-dimensional water encapsulated inside single-wall carbon nanotubes, here referred to as nanotube-water, was studied by neutron diffraction, inelastic and quasielastic neutron scattering. The study reveals that nanotube-water is a new state of water manifested by weak hydrogen bonds, extended intermolecular water-water distances and very large amplitude of water molecules vibrations. Molecular dynamics simulations well describe the observed spectra and give a possible nanotube- water structure in a form of a square-ice sheet wrapped into a cylinder next to the inner carbon nanotube wall and a water chain in the interior. The soft dynamics of nanotube-water arises mainly from the drastic change in hydrogen-bond connectivity of the central water-chain.

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