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Quantum tunneling and vibrational dynamics of ultra-confined water[1] ALEXANDER I. KOLESNIKOV, LAWRENCE M. ANOVITZ, GEORG EHLERS, EUGENE MAMONTOV, ANDREY PODLESNYAK, TIMOTHY R. PRISK, Oak Ridge National Laboratory, TN, ANDREW SEEL, ISIS Facility, UK, GEORGE F. REITER, University of Houston, TX — Vibrational dynamics of ultra-confined water in single crystals beryl, the structure of which contains ∼ 5 Å diameter channels along the c-axis was studied with inelastic (INS), quasi-elastic (QENS) and deep inelastic (DINS) neutron scattering. The results reveal significantly anisotropic dynamical behavior of confined water, and show that effective potential experienced by water perpendicular to the channels is significantly softer than along them. The observed 7 peaks in the INS spectra (at energies 0.25 to 15 meV), based on their temperature and momentum transfer dependences, are explained by transitions between the split ground states of water in beryl due to water quantum tunneling between the 6-fold equivalent positions across the channels. DINS study of beryl at T=4.3 K shows narrow, anisotropic water proton momentum distribution with corresponding kinetic energy, E_K=95 meV, which is much less than was previously observed in bulk water (∼150 meV). We believe that the exceptionally small E_K in beryl is a result of water quantum tunneling \ delocalization in the nanometer size confinement and weak water-cage interaction.

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