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Muon Sites in Hexagonal Ice

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Theoretical study using density functional theory (DFT) calculations supports to estimate the stopping site of muon in materials and understand the muon spin rotation and relaxation (μSR) measurements. To understand the temperature dependent zero-field (ZF) μSR measurement in water, we have performed DFT calculations and quantum simulation to estimate the muon sites in hexagonal (Ih) ice. Taking initial lattice parameters from the high-resolution neutron powder diffraction study [1], the muon stopping site was calculated in the Ih supercell containing 2×2×1 conventional cells using Quantum ESPRESSO [2]. The supercell contains 12 water molecules and a muon. The added muon in Ih ice behaves as a defect in a solid which leads to the relaxation of immediate surrounding structure. The water molecules nearby the muon site found reoriented. The stopping site of muon is found at around 2 A distance from three protons (one proton of a water molecule and two of another, total four spin-half (4S) system). It seems like H_2O-Mu-H_2O^+ but the muon site is found neither L-defect nor D-defect but like interstitial. Based on this result and quantum simulation [4], only the slow-oscillating term of ZF spectra at 270 K can reproduce. To satisfy the fast-oscillating term of the ZF spectra, quantum simulation indicates that the muon should be at least 0.99 A distance from one of the protons in the 4S system (indicating two sites of muon). In the program, we will present DFT calculations and quantum simulations to interpret the oscillating ZF spectra at 270 K.

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