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Low frequency modes in iron proteins explored with the 57Fe nuclear probe

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Synchrotron based nuclear resonance scattering techniques are ideal tools to investigate electronic and dynamic properties of iron centers in chemical and biological systems. During the last years Nuclear Inelastic Scattering (NIS) also called Nuclear Resonance Vibrational Spectroscopy (NRVS) has been used to detect iron based vibrational modes of iron proteins and chemical model complexes. We have investigated the vibrational modes of iron-sulphur-proteins [1], both experimentally via NIS and theoretically by density functional theory (DFT) calculations in the spectral region from ~5 to ~800 cm-1. DFT calculations coupled with molecular mechanics allow to investigate not only iron ligand interactions but also solvent effects. The effect of solvent on the low frequency modes as well as on the iron ligand modes of the ligand-binding oxidase from the bacterium Geobacillus kaustophilus (Gklox) [2] will be presented. By means of a novel cryostat especially designed for NIS experiments down to T = 1.9 K installed at beamline P01, PETRA III, it is now possible to explore very low frequency modes down to the range of a few wavenumbers by avoiding multiphonon excitations. First results with this sample environment on Gklox as well as on a chemical spin crossover (SCO) complex will be presented.

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