Nuclear Resonant Vibrational Spectroscopy (NRVS) of Nitrogenase & Hydrogenase

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Our NRVS work at SPring-8 is focused on two critical enzymes – nitrogenase (N_2ase), which catalyzes the reduction of dinitrogen to ammonia, and hydrogenase (H_2ase), which catalyzes the evolution (or consumption) of dihydrogen. Nature has evolved multiple Fe-based metalloenzymes that accomplish these tasks, both with and without the assistance of a second metal (Mo, V, Ni) at the active site. N_2 fixation is the key step in the nitrogen cycle, and this biological ammonia synthesis is responsible for about half of the protein available for human consumption. H_2 catalysis is crucial for the metabolism of many anaerobic organisms, and knowledge about the mechanism of H_2 evolution may prove critical for a future 'H_2 economy'. I will present NRVS data on small molecule model compounds and the enzymes N_2ase and H_2ase, along with analyses using empirical force fields as well as DFT methods. The interaction between protein diffraction and spectroscopy will be discussed. I will finish with some discussion of what we could do with more spectral brightness.