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Coherent Oscillations in Hemoglobin and Myoglobin Ligand Complexes and their Dynamical Connection to Global Protein Motion and Gas Discrimination JACOB JANTZI, University of Pittsburgh, KRISTINA WOODS, Carnegie Mellon University

— THz spectroscopy and Molecular Dynamics (MD) simulations are used to investigate the coherent oscillations in the heme group of two heme proteins (hemoglobin and myoglobin) and the affect of the heme dynamics on the collective fluctuations taking place in the proteins. Preliminary experiments have confirmed that the deoxy state (no gas in the active site) of both proteins do not possess a 40 cm^{-1} mode in their THz spectra. The 40 cm^{-1}mode has been observed in both experimental and theoretical investigations of myoglobin dynamics. The low-frequency mode at 40 cm^{-1} has been hypothesized to be connected with energy transport between the active site and the protein-solvent interface. Once a gas is introduced into the ligand, both proteins contain the 40 cm^{-1} mode in their experimental spectra. But both the shape and intensity of the myoglobin peak differs from that of hemoglobin. Additionally, we observe a number of collective protein fluctuations ($\leq$ 100 cm^{-1}) that are altered in the myoglobin spectrum but remain unchanged in the hemoglobin spectrum when a gas is introduced into the protein active site. We will present experimental data of both proteins that have been exposed to a number of different gases. The reaction of the protein collective motions in the gas is linked with the difference in the coupling of the coherent oscillations of the heme group with the protein global modes but also with the mechanism of protein relaxation that controls ligand migration.

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