

Abstract Submitted
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Observation of Protein Structural Vibrational Mode Sensitivity to Ligand Binding¹ KATHERINE NIESSEN, MENG YANG XU, State Univ of NY - Buffalo, EDWARD SNELL, Hauptman-Woodward Medical Research Institute - Buffalo, NY, ANDREA MARKELZ, State Univ of NY - Buffalo — We report the first measurements of the dependence of large-scale protein intramolecular vibrational modes on ligand binding. These collective vibrational modes in the terahertz (THz) frequency range (5-100 cm^{-1}) are of great interest due to their predicted relation to protein function. Our technique, Crystals Anisotropy Terahertz Microscopy (CATM), allows for room temperature, table-top measurements of the optically active intramolecular modes. CATM measurements have revealed surprisingly narrow-band features [1]. CATM measurements are performed on single crystals of chicken egg-white lysozyme (CEWL) as well as CEWL bound to tri-N-acetylglucosamine (CEWL-3NAG) inhibitor. We find narrow band resonances that dramatically shift with binding. Quasiharmonic calculations are performed on CEWL and CEWL-3NAG proteins with CHARMM using normal mode analysis. The expected CATM response of the crystals is then calculated by summing over all protein orientations within the unit cell. We will compare the CATM measurements with the calculated results and discuss the changes which arise with protein-ligand binding.

[1] G. Acbas, K.A. Niessen, E. Snell, and A.G. Markelz, “Optical Measurements of Long-Range Protein Structural Motions,” Nature Communications, In Press.

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