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Probing the conformational changes of proteins in liquid water by dielectric terahertz spectroscopy ALI CHARKHESHT, DEEPU GEORGE, NGUYEN VINH, Virginia Tech — Proteins solvated in their biological milieu are expected to exhibit strong absorption in the terahertz range that contain information on their global and sub-global collective vibrational modes (conformational dynamics) and global dynamical correlations among solvent water molecules and proteins. Measurements in this region, however, are challenging due to the strong absorption of water and often severe interference artifacts. In response, we have developed a highly sensitive dielectric terahertz frequency-domain system and a terahertz-time domain system for probing the collective dynamics in aqueous solution. Using these techniques we explore the complex dielectric response from 5 GHz up to 3 THz that directly probes such questions as the hydration level around proteins and the large scale vibrational modes of biological polymers. We make a direct comparison to the existing molecular dynamic simulations and normal mode calculations and investigate the dependence of the terahertz frequency dynamics on protein concentration. Our measurements shed light on the macromolecular motions in a biologically relevant water environment.

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