

Abstract Submitted
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Terahertz Dielectric Response for Cytochrome C YUNFEN HE, Physics Department, University at Buffalo, Buffalo, NY, JING-YIN CHEN, Institute for Shock Physics, Washington State University, Pullman, WA, WENJUN ZHENG, ANDREA MARKELZ, Physics Department, University at Buffalo, Buffalo, NY — Previously we demonstrated a large contrast in the terahertz dielectric response between oxidized and reduced cytochrome c and associated this difference with a change in the collective structural motions associated with protein flexibility (Chen et al. Phys. Rev. E Rapid 72, 040901 (2005).) We present calculations of the terahertz dielectric response of cytochrome c as a function of oxidation state and hydration. Molecular dynamics simulations are performed to equilibrate water content. Quasiharmonic analysis and dipole-dipole correlation analysis is performed after equilibrating the system. We compare the calculated results with the measurements to determine the relative contribution of correlated motions and diffusive motions to the measured dielectric response and how these two different contributions give rise to the observed large oxidation dependence and hydration dependence.

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