

Abstract Submitted
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The protein hydration transition YUNFEN HE, JOSEPH KNAB, JING-YIN CHEN, ANDREA MARKELZ, Physics Department, State University of New York at Buffalo — We previously reported the hydration transition in the THz dielectric response for native state hen egg white lysozyme (HEWL). As hydration increases the response slowly increases until at 0.25h (gm water/gm protein) the absorbance and index sharply increase. The hydration level coincides with the filling of the first solvation shell. The THz dielectric response arises from relaxational and resonant vibrational response, where the vibrational response corresponds to delocalized structural motions sensitive to the conformation and the environment. We examine the contribution of low frequency vibrational modes to the hydration transition by calculating the normal mode density as a function of solvent content using CHARMM. We find that the density of low frequency modes increases with the increasing solvent content, but this increase does not show the transition seen experimentally. We discuss that another source for the hydration transition in the THz response may be the hydration dependence of the activation energy for glass-like beta fluctuations that contribute to the relaxational response.

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