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New insights into the picosecond dynamics solvated proteins NGUYEN VINH, Department of Physics, Virginia Tech, JIM ALLEN, Institute for Terahertz Science and Technology, Department of Physics, University of California, Santa Barbara, KEVIN PLAXCO, Department of Chemistry and Biochemistry, University of California, Santa Barbara — According to computer simulations, the slowest, largest-scale harmonic motions of solvated biomolecules and the relaxation times of water occur on the picosecond regime. Experimental methods for the characterization of these collective vibrational modes, however, have been severely lacking. In response, we have developed a unique precision and sensitivity dielectric spectrometer. Operating over the frequency range from 0.5 GHz up to 1.1 THz, this spectrometer provides an unparalleled ability to probe the dynamics of water and aqueous proteins over the 100 fs to 100 ps timescale. Using this spectrometer to characterize the collective dynamics of solvated lysozyme we find that the collective vibrational modes of this protein are characterized by a hitherto unrecognized cutoff at 250 GHz (corresponding to 0.6 ps) arising due to the finite size of the molecule. Employing an effective medium approximation to describe the complex dielectric response of the protein in solution we find that each molecule is surrounded by a tightly held layer of 164 $\pm$ 5 water molecules that behave as if they are an integral part of the protein. The observation sheds new light on the femtosecond to picosecond collective dynamics of water and solvated biomolecules.

Nguyen Vinh
Department of Physics, Virginia Tech

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