

Abstract Submitted
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An extended dynamical solvation shell around proteins.¹ SEUNG JOONG KIM, U. of Illinois (UIUC), SIMON EBBINGHAUS, MATTHIAS HEYDEN, Ruhr-Uni. Bochum, Germany, XIN YU, U. of Nevada, UDO HEUGEN, Ruhr-Uni. Bochum, Germany, MARTIN GRUEBELE, U. of Illinois (UIUC), DAVID LEITNER, U. of Nevada, MARTINA HAVENITH, Ruhr-Uni. Bochum, Germany — Water solvating biomolecules in organisms has different properties from the bulk. Such solvation shells can be characterized by a variety of structural and dynamical measures. The fundamental question of biomolecule hydration is: how far out into the solvent does the influence of the biomolecule reach? We use terahertz absorption spectroscopy of the five helix bundle protein Lambda Repressor 6-85, coupled with molecular dynamics simulations, to show that correlated water motion at a sub-psec time scale persists to distances of at least 20 angstrom. We show this by determining that bulk water, water molecules mainly interacting with a single protein molecule, and water molecules interacting with more than one protein molecule have different absorption signatures in the THz frequency range, leading to an experimentally detectable non-monotonic dependence of the absorption coefficient on protein concentration. This trend is supported in the calculations, which further show that long-distance hydration is a dynamical effect correlating many water molecules, not one that noticeably perturbs the structural distribution of one or a few water molecules from the bulk value.

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