

Abstract Submitted
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Strongly Anisotropic Dielectric Response of Confined Water CUI ZHANG, Department of Chemistry, University of California, Davis, FRANCOIS GYGI, Department of Computer Science, University of California, Davis, GIULIA GALLI, Department of Chemistry, Department of Physics, University of California, Davis — We carried out atomistic simulations of water within hydrophobic surfaces, which revealed remarkable modifications of the dynamics and dielectric relaxation of the liquid under confinement. We found that dipolar fluctuations are modified by the presence of surfaces up to strikingly large distances, i.e., tens of nanometers. Fluctuations are suppressed by approximately an order of magnitude in the z direction, perpendicular to the interface, and are enhanced in the x-y plane, giving rise to strong anisotropies in the components of the dielectric response. Our findings are consistent with recent terahertz and ultrafast infrared pump-probe spectroscopy experiments. Work supported by DOE-CMSN DE-SC0005180.

Cui Zhang
Department of Chemistry, University of California, Davis

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