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Autor(en) des Beitrags: Steinel, Tobias; Asbury, John B.; Corcelli, S. A.; Lawrence, C. P.; Skinner, J. L.; Fayer, M. D.

Titel des Beitrags: Water dynamics: dependence on local structure probed with vibrational echo correlation spectroscopy

Abstract: Ultrafast IR vibrational echo correlation spectroscopy with full phase information of the entire O-D stretching band of HOD in H2O and mol. dynamics simulations are employed to investigate water dynamics. The wavelength dependence of the measured dynamics demonstrates that different hydrogen bonded water species are subject to distinct ultrafast (∼100 fs) local fluctuations and essentially identical slower (0.4 ps to ∼2 ps) structural rearrangements. Simulations provide insights into the nature of the very fast and slower dynamics. The results also show that the theor. methods that are widely used in the description of nonlinear optical expts. need to be advanced to adequately describe water dynamics. [on SciFinder(R)]

Stichworte: Isotope effect (dependence on local structure probed with vibrational echo correlation spectroscopy of deuterated water in water) Simulation and Modeling (mol. dynamics dependence on local structure probed with vibrational echo correlation spectroscopy of deuterated water in water) IR spectra IR spectroscopy (ultrafast, vibrational echo correlation dependence on local structure probed with vibrational echo correlation spectroscopy of deuterated water in water) water deuterated line width vibrational echo correlation spectrum

Kongresstitel: