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Abstract for an Invited Paper for the MAR12 Meeting of the American Physical Society

Vibrational spectroscopy of interacting water molecules

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I will discuss a new simulation model for water that includes three-body interactions explicitly, and describe our theoretical approach for calculating OH-stretch spectroscopic observables. I will present illustrative examples, involving pump-probe energy-transfer-induced anisotropy decay in liquid water, IR and Raman line shapes in ice Ih, phase-sensitive SFG spectra of the liquid/vapor interface, and energetics and IR spectra for the different conformations of the water hexamer.