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Infrared spectra of ice and water from first principles: intra vs. intermolecular dipole correlations[1] WEI CHEN, Department of Physics, Princeton University, Princeton, NJ 08544, USA, MANU SHARMA, Department of Chemistry, University of California, Davis, CA 95616, USA, RAFFAELE RESTA, Dipartimento di Fisica Teorica, Università di Trieste, Strada Costiera 11, 34014 Trieste, Italy, GIULIA GALLI, Department of Chemistry, University of California, Davis, CA 95616, USA, ROBERTO CAR, Department of Chemistry, Princeton University, Princeton, NJ 08544, USA — We report simulated infrared (IR) spectra of deuterated ice and water using Car-Parrinello molecular dynamics with maximally localized Wannier functions. Experimental features of both ice and water are accurately reproduced within the harmonic approximation. Calculated line shapes are further decomposed in terms of intra and intermolecular dipole correlation functions with spatial resolution. This approach proves to be very useful to understand the origin of spectral features and the nature of the underlying hydrogen-bond (H-bond) network. We find that intermolecular dynamic charge fluctuations play a crucial role over the entire frequency range.

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