Abstract Submitted
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IR and Raman spectroscopy of water and ice by ab initio simulations[1] MANU SHARMA, DAVIDE DONADIO, GIULIA GALLI, UC Davis — We use ab initio molecular dynamics to compute the IR and Raman spectra of a variety of heavy water systems, ranging from pure water and ice, to liquid water confined between graphene foils and D-terminated diamond surfaces. The analysis of the simulated spectra provides the fingerprints of different hydrogen bonding environments, giving access to the complex structural and dynamical properties of water in various conditions. In addition our results provide a detailed, microscopic interpretation of IR and Raman experiments, as they allow us to assign univocaly spectroscopic bands to specific vibrational modes, and to identify electro-dynamic coupling between water molecules and surfaces, in the case of confined water. Our MD simulations also give a quantitative estimate of the anharmonicities and lifetimes of various vibrational modes.

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