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Infrared Spectra of Water and Simple Negative Ions from Ab-initio Simulations CUI ZHANG, DAVIDE DONADIO, Department of Chemistry, University of California, Davis, GIULIA GALLI, Department of Chemistry and Department of Physics, University of California, Davis, IVAN DUCHEMIN, Department of Applied Science, University of California, Davis, FRANCOIS GYGI, Department of Applied Science and Department of Computer Science, University of California, Davis — We report an analysis of the much debated infrared spectra (IR) of water, as obtained by ab-initio molecular dynamics simulations with the PBE and PBE0 energy functionals. We compare power spectra of bond-bond correlations, those of Wannier function centers and IR spectra. Such comparison allows us to identify signatures, in IR spectra, arising from ionic vibrations and signatures stemming from the liquid electronic structure. We then analyze the changes the latter undergo in the presence of simple negative ions such as chloride. Finally, we discuss differences between results obtained at the PBE and PBE0 level of theory. Our results contribute a fundamental step toward the understanding of structural and spectroscopic properties of water at interfaces and complex solutions. Work supported by DOE/SciDACDE-FC02-06ER25794 and NSF/OCI-0749217.

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