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First Principle Simulations of the Infrared Spectrum of Liquid Water using Hybrid Density Functionals CUI ZHANG, DAVIDE DONADIO, FRANCOIS GYGI, GIULIA GALLI, Univeristy of California, Davis — We report on calculations of the infrared spectrum (IR) of liquid water carried out using first principle molecular dynamics and the hybrid functional PBE0. We find results in much better agreement with experiment than those obtained using semi-local, gradient corrected exchange correlation functionals. In particular the description of the IR stretching band is greatly improved and in good accord with recent measurements. When adopting the PBE0 functional, substantial improvement is also found in the description of the structural properties of the liquid, consistent with a smaller average number of hydrogen bonds, and a reduced molecular dipole moment, as revealed by our analysis of maximally localized Wannier functions. Finally the average electronic gap of the liquid is increased by 60% with respect to PBE, when computed at the PBE0 level of theory, and is in fair agreement with experiment. Work supported by NSF/OCI-0749217.

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