Abstract Submitted for the MAR17 Meeting of The American Physical Society

The Dipole Polarizability of a Condensed-Phase Water Molecule KA UN LAO, JACLYN LUNGER, JUNTENG JIA, ROBERT DISTASIO, Cornell University — The dipole polarizability, α , provides a measure of the tendency of a molecule or material to deform (or polarize) in the presence of an electric field and is a critical component of the induction and dispersion interactions. Within the framework of density functional theory (DFT), we present a hierarchy of first principles based approaches for computing the dipole polarizability of a molecule located in the condensed phase. This hierarchy includes a successive treatment of both shortrange (hybridization, Pauli exchange-repulsion, etc.) and long-range (Coulomb) electrodynamical response screening in the computation of α , while simultaneously accounting for the surrounding condensed-phase environment. Utilizing highly accurate liquid water configurations generated from van der Waals inclusive hybrid DFT based ab initio molecular dynamics, we computed α for this ensemble of liquid water molecules as a first application of this approach. In addition, we introduce a practical yet highly accurate scheme for assigning the polarizability of a water molecule on-the-fly during liquid water simulations that is straightforward to use in current polarizable force fields when computing the induction and dispersion interactions in large-scale aqueous environments.

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Date submitted: 11 Nov 2016

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