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The Dipole Polarizability of a Water Molecule *in* Liquid Water
ROBERT DISTASIO, RAHUL MAITRA, 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. Within the framework of density functional theory (DFT), we present a hierarchy of first principles based approaches for computing α of a molecule located in the condensed phase. This hierarchy includes a successive treatment of both short-range (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 a given water molecule *in* liquid water as a first application of this approach. Our findings will be compared and contrasted with α computed for an isolated gas-phase water molecule.

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