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Effects of the hydrogen-bonded network on the molecular polarizability of water[1] DEYU LU, Brookhaven Natl Lab — Electronic polarization plays a crucial role in determining the structural and dynamical properties of water with different boundary conditions. Although it is well known that the molecular polarization in condensed phases behaves substantially differently from that in the vacuum due to the intermolecular interaction, the environmental effects have not been fully understood from first principles methods. As a result, how to rigorously define and calculate the molecular polarizability of a water molecule in different chemical environments remains an open question. A main challenge to this puzzle arises from the intrinsic non-local nature of the electronic susceptibility. Recently we developed an ab initio local dielectric response theory [Phys. Rev. B 92, 241107, 2015] that partitions dielectric response in real space based on a Wannier representation. We apply this method to compute the molecular polarizability of water in the condensed phase, and analyze the effects of the hydrogen-bonded network resulting from the crystal field, spatial confinement, and charge transfer.

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