Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

What is the effective molecular polarizability of water in condensed phases?[1] XIAOCHUAN GE, DEYU LU, Brookhaven National Laboratory — 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, these environmental effects have not been fully understood from first principles methods. As a result, how to rigorously define and calculate the effective molecular polarizability of a water molecule in different chemical environments remains an open question. The answer to this question not only improves our fundamental understanding of water, but also has immediate practical impact on computational modeling of water, e.g, through an accurate polarizable force field model. 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 [arxiv 1508.03563] that partitions dielectric response in real space based on a Wannier representation. In this work we apply this method to compute the effective molecular polarizability of water in the condensed phase, and discuss how the effective molecular polarizability evolves from gas phase to the condensed phase.

[1]This research used resources of the Center for Functional Nanomaterials, which is a U.S. DOE Office of Science Facility, at Brookhaven National Laboratory under Contract No. DE-SC0012704.

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Date submitted: 02 Nov 2015 Electronic form version 1.4