Dipolar Correlations and Dielectric Permittivity of Water

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The static dielectric properties of liquid and solid water are investigated within linear response theory in the context of ab-initio molecular dynamics. Using maximally localized Wannier functions to treat the macroscopic polarization we formulate a first-principle, parameter-free, generalization of the phenomenological theory due to Kirkwood and Onsager. Our calculated static permittivity is in good agreement with experiment [1]. The same approach based on Wannier functions is also useful to identify the effect of intramolecular and intermolecular dynamic dipolar correlations on the infrared spectrum of water [2].

[1] M. Sharma, R. Resta, and R. Car, Phys. Rev. Lett., in press (2007).

[2] M. Sharma, R. Resta, and R. Car, Phys. Rev. Lett. **95**, 187401 (2005).