

Abstract Submitted
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Dielectric Properties of Ice and Liquid Water from First Principle Calculations¹ DEYU LU, FRANCOIS GYGI, GIULIA GALLI, UC Davis — We present a first-principle study of the dielectric properties of ice and liquid water. The eigenmodes of the dielectric matrix, ϵ^{-1} , are analyzed in terms of maximally localized dielectric functions similar, in their definition, to maximally localized Wannier orbitals obtained from Bloch eigenstates of the electronic Hamiltonian. We show that the lowest eigenmodes of ϵ^{-1} are localized in real space and can be separated into groups related to the screening of lone-pairs, intra-, and inter-molecular bonds, respectively. The local properties of the dielectric matrix can be conveniently exploited to build approximate dielectric matrices for efficient, yet accurate calculations of quasiparticle energies.

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Deyu Lu
UC Davis

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