

Abstract Submitted
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Quasiparticle Energies of Liquid Water DEYU LU, GIULIA GALLI,
University of California, Davis — Understanding the electronic structure of liquid water is of great interest for a broad range of physical, chemical and biological processes occurring in solution. In particular, the ability to obtain an accurate description of water electronic states from first principle plays an important role in interpreting experimental observations. We present results of water electronic properties obtained using Many-Body Green's function approaches within the GW approximation. In particular we compare results obtained using the full dielectric matrix and various model dielectric functions. We analyzed the band structure and the absorption spectrum, with focus on the blue shift with respect to density functional theory results, which has been reported in a recent theoretical study [Garbuio *et al.*, PRL: 97, 137402, 2006].

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