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Hybrid functional and selfconsistent GWΓ calculations for solids[1]

GEORG KRESSE, University of Vienna, Austria

GW calculations in various flavors are presented for small gap and large gap systems, comprising typical semiconductors (Si, SiC, GaAs, GaN, ZnO, ZnS, CdS and AlP), small gap semiconductors (PbS, PbSe, PbTe), insulators (C, BN, MgO, LiF) and noble gas solids (Ar, Ne). The general finding is that single shot G_0W_0 calculations based on wavefunctions obtained by conventional density functional theory calculations yield too small band gaps, whereas G_0W_0 calculations following hybrid Hartree-Fock density functional calculations tend to overestimate the band gaps by roughly the same amount. This is at first sight astonishing, since the hybrid functionals yield very good band gaps themselves. The contradiction is resolved showing that the inclusion of the attractive electron-hole interactions (excitonic effects) are required to obtain good static and dynamic dielectric functions using hybrid functionals. The corrections are usually incorporated in GW using "vertex corrections", and, in fact, inclusion of vertex corrections rectifies the predicted band gaps. In order to remove the dependency on the initial wavefunctions we furthermore present selfconsistent GW calculations, again including an approximate treatment of vertex corrections. The results are in excellent agreement with experiment, with a few percent deviations for all considered materials. We conclude that predictive band gap engineering is now possible with the theoretical description approaching experimental accuracy. Finally the relationship between the *GW* method and hybrid functionals is use to elaborate on the shortcomings of hybrid functionals for large gap systems and metals.

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