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Accurate band gaps and dielectric properties from one-electron theories

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Abstract

For semiconductor modeling, a major shortcoming of density functional theory is that the predicted band gaps are usually significantly too small. It is generally argued that this shortcoming is related to the fact that density functional theory is a ground state theory, and as a result, one is not allowed to associate the one-electron energies with the energies of quasi-particles. Although this fundamental objection is certainly correct, the modeling of the positioning of donor and acceptor levels in semiconductors faces serious limitations with present density functionals.

Several solutions to this problem have been suggested. A particular attractive and fairly simple one is the inclusion of a small fraction of the non-local exchange in the Hamiltonian (hybrid functionals). This approach leads to sensible band gaps for most semiconductors, but fails for ionic solids. A more reliable approach is via many-electron Green's function techniques, which have made tremendous advances in recent years. Here 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 from conventional density functional theory yield too small band gaps, whereas G_0W_0 calculations following hybrid 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 by showing that the inclusion of the attractive electron-hole interactions (excitonic effects) is required to obtain good static and dynamic dielectric functions using hybrid functionals. The corrections are usually incorporated in GW calculations using 'vertex corrections', and in fact inclusion of these vertex corrections rectifies the predicted band gaps.

Finally, in order to remove the dependence on the initial wavefunctions, self-consistent GW calculations are presented, again including an approximate treatment of vertex corrections. The results are in excellent agreement with experiment, with a few per cent deviation for all materials considered. We conclude that predictive band gap engineering is now possible with the theoretical description approaching experimental accuracy.