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Defect Physics without the Band-Gap Problem: Combining DFT and GW[1]

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In computational defect physics and chemistry the local-density and generalized gradient approximations (LDA/GGA) to density functional theory (DFT) are widely applied due to their computational efficiency. However, their predictive power is limited by intrinsic deficiencies like artificial self-interaction and the absence of the derivative discontinuity in the exchange-correlation potential (that give rise to the so called band-gap problem). We present a new formalism that combines DFT with many-body perturbation theory (MBPT) in the G_0W_0 approximation to overcome these deficiencies [1,2]. The formation energy of a defect is expressed as successive charging of a lower charge state, for which the defect level is unoccupied, permitting a decomposition into a lattice (DFT) and an electron addition part (G_0W_0) [2]. For the self-interstitial in silicon the approach increases the LDA formation energy of the neutral state by ∼1.1 eV in good agreement with diffusion Monte Carlo calculations [2,3,4]. For the anion vacancy in bulk MgO (also called F- or color center), which can probably be regarded as *the* classic intrinsic point defect in compound insulators, it proves to be necessary to go one step further in the hierarchy of MBPT. After including the electron-hole and electron-phonon interaction the absorption energies of the neutral and the positively charged F-center become practically identical – a fact that has impeded the F-center's characterization for decades – in good agreement with optical absorption studies [5].

[1] Hedström *et al.* PRL **97**, 226401 (2006)
[2] Rinke *et al.* PRL **102**, 026402 (2009)
[3] Batista *et al.* PRB **74**, 121102(R) (2006)
[4] Leung *et al.* PRL **83**, 2351 (1999)
[5] Kappers *et al.* PRB **1**, 4151(1970)

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