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Defect Formation Energies without the Band-Gap Problem: Combining DFT and *GW* for the Silicon Self-Interstitial P. RINKE[1], A. JANOTTI, C.G. VAN DE WALLE, M. SCHEFFLER[1], University of California at Santa Barbara — For the self-interstitial in silicon, a defect of high technological relevance, density functional theory (DFT) in the widely applied local-density approximation (LDA) underestimates the formation energies of different configurations in the neutral charge state by ∼1.5 eV compared to diffusion Monte Carlo calculations [1,2]. We attriubte this to artificial self-interaction and the absence of the derivative discontinuity in the LDA exchange-correlation potential that give rise to the band-gap problem. We present a new formalism that combines LDA with quasiparticle energy calculations in the G_0W_0 approximation to overcome these deficiencies. The formation of the neutral defect is expressed as successive charging of its 2+ charge state, for which the defect level is unoccupied, permitting a decomposition into a lattice (LDA) and an electron addition part (G_0W_0) [3]. The G_0W_0 corrections increase the LDA formation energy by ∼1.1 eV. Moreover, the G_0W_0-corrected charge transition levels agree well with recent measurements [4]. [1] Batista *et al.* PRB **74**, 121102(R) (2006), [2] Leung *et al.* PRL **83**, 2351 (1999), [3] Hedström *et al.* PRL **97**, 226401 (2006), [4] Bracht *et al.* PRB **75**, 035211 (2007)

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