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Defect levels of the O vacancy in ZnO in DFT, hybrid-DFT, and GW STEPHAN LANY, National Renewable Energy Laboratory, ALEX ZUNGER — The band gap problem of the LDA and GGA approximations to density-functional theory (DFT) introduce a significant uncertainty in the prediction of the charge transition levels of electrically active defects or impurities. For the case of the O vacancy in ZnO, we here compare the predictions of three methods with an increasing level of computational effort, i.e., (i) GGA+U plus a rigid shift of the conduction band minimum, (ii) hybrid-DFT using the HSE functional, and (iii) GW calculations of the quasi-particle energies of the defect states. In addition to finite-size corrections of DFT (or hybrid-DFT) supercell total energies, which are applied to all methods, we demonstrate here also the need of corrections for the GW quasi-particle energies of charged defect states. Applying the GW quasi-particle energy corrections to the self-consistent GGA+U and HSE calculations, we then obtain the 2+/0 donor level between 1.4 eV (GGA+U) and 1.7 eV (HSE) above the valence band maximum. Without the GW corrections, the transition levels lie at 1.0 eV and 2.3 eV, respectively in GGA+U and HSE, where in the HSE calculation the fraction of the Fock exchange was adjusted so to match the experimental band gap. This work was supported through the Center for Inverse Design, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences.

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