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What is the G^0W^0 band gap of ZnO? M. STANKOVSKI, G. ANTONIUS, D. WAROQUIERS, A. MIGLIO, H. DIXIT, P. RINKE, H. JIANG, M. GIANTOMASSI, X. GONZE, M. CÔTÉ, G.-M. RIGNANESE — Recently, there has been considerable attention on ZnO as a candidate material for low-cost transparent conducting oxides. Even in its natural wurtzite bulk phase, it is numerically difficult to evaluate G^0W^0 quasiparticle (QP) corrections for ZnO. Therefore we have a wide range of theoretical QP gaps quoted in the literature (from ∼1.6 eV to ∼3.6 eV to be compared with 3.44 eV experimentally). Typically, many approximations are used *en route*. To find the correct theoretical gap, we have performed calculations of unprecedented accuracy. First, we study the G^0W^0 band gap given different ground-state DFT starting point approximations (LDA and GGA) and the effect of including scalar-relativistic corrections. Second, we present a study of results for norm-conserving pseudopotentials vs. all-electron techniques (both PAW and FP-LAPW). Four different plasmon-pole models are compared with the more accurate contour-deformation approach. Finally, a Hubbard U parameter for the 3d-states of Zn is shown to depend on the exact details of application. This work shows that the band-gap of ZnO is indeed underestimated in the G^0W^0 approach.

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