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 \( \sim 1.6 \) eV to \( \sim 3.6 \) 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.