Erratum: Band convergence and linearization error correction of all-electron *GW* calculations: The extreme case of zinc oxide [Phys. Rev. B 83, 081101(R) (2011)]

Christoph Friedrich, Mathias C. Müller, and Stefan Blügel

(Received 22 June 2011; published 21 July 2011)

DOI: 10.1103/PhysRevB.84.039906 PACS number(s): 71.20.Nr, 71.45.Gm, 71.15.Ap, 99.10.Cd

We correct the extrapolated quasiparticle band gap of ZnO from 2.99 to 2.83 eV after having refined the calculation of the self-consistent effective single-particle potential within the local-density approximation (LDA). Including second-derivative local orbitals into the respective linearized augmented-plane-wave (LAPW) basis improves the description of the electron density and yields a more accurate effective potential. (Third-derivative local orbitals no longer change the result.) Rather unexpectedly, the slight change of the shape of the potential gives rise to a sizable reduction of the LDA band gap from 0.84 to 0.73 eV, which also affects the subsequent *GW* calculations, which we have carried out with the highly converged basis explained in the original paper. The *GW* band-gap values reduce by about 0.15–0.25 eV (see Fig. 1). As the change with respect to our original work is essentially a downward correction of all data points by a small amount, the analysis and interpretation of the data remain valid.

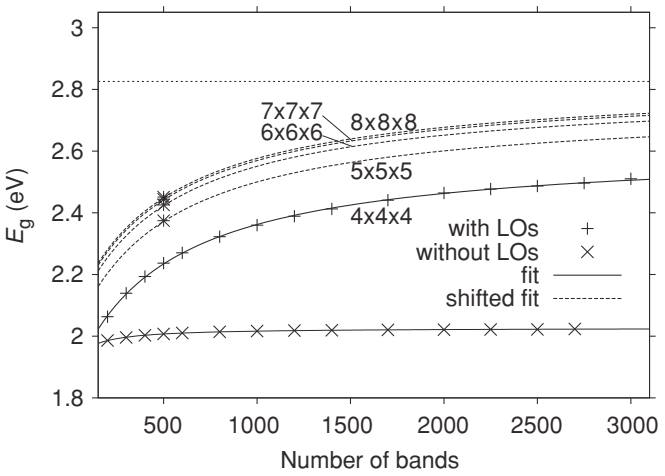

FIG. 1. Band convergence of the quasiparticle band gap of ZnO employing a 4×4×4 **k**-point set and calculated with (pluses) and without local orbitals (LOs) (crosses) for high-lying states. The solid lines show hyperbolical fits. We also indicate results with finer **k**-point samplings (stars) calculated with LOs and 500 bands. The dashed lines show the hyperbolical fit shifted to align with these results. The fit asymptote for the 8×8×8 **k**-point set at 2.83 eV (dotted line) is considered the best estimate for the all-electron one-shot *GW* band gap.

