

# 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)]

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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.

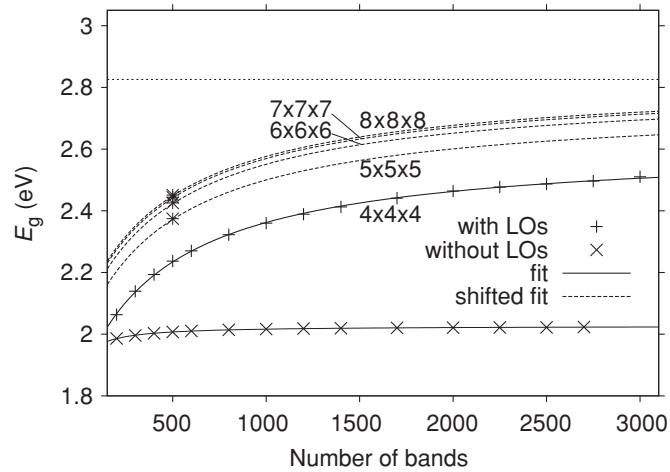


FIG. 1. Band convergence of the quasiparticle band gap of ZnO employing a  $4 \times 4 \times 4$   $\mathbf{k}$ -point set and calculated with (pluses) and without local orbitals (LOs) (crosses) for high-lying states. The solid lines show hyperbolic fits. We also indicate results with finer  $\mathbf{k}$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