

Abstract Submitted
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Quasiparticle properties of ZnO: Effects of semicore states and nonuniform convergence of the Coulomb hole self-energy¹ PEIHONG ZHANG, Department of Physics, University at Buffalo, SUNY, Buffalo, New York 14260, BI-CHING SHIH, YU XUE — Understanding of the quasiparticle properties of ZnO, a supposedly simple *sp* semiconductors, turns out to be rather challenging. The band gap of ZnO calculated within the local density approximation (LDA) is about 0.7 eV if semicore 3*s*, 3 *p*, and 3*d* electrons are considered as valence electrons. Subsequent quasiparticle calculations within the *conventional GW* approximation gives a band gap of about 2.4 eV, which is more than 1 eV smaller than the recent experimental result. We have recently revisited this problem and found that the severe underestimate of the quasiparticle band gap of ZnO can be resolved if (1) The semicore Zn 3*d* states are treated properly, and (2) The evaluation of the Coulomb hole self-energy is adequately converged. We are able to reproduce of the experimental quasiparticle band gap of ZnO without the need of performing self-consistent GW calculations.

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Peihong Zhang
Dept of Physics, University at Buffalo, SUNY, Buffalo, New York 14260

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