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GW method in the PAW formalism apply to ZnO and SnO GABRIEL ANTONIUS, Deparement de Physique, Universite de Montreal, MAR-TIN STANKOVSKI, ANNA MIGLIO, GIAN-MARCO RIGNANESE, Unite Physico-Chimie et de Physique des Materiaux, Universite catholique de Louvain, MICHEL COTE, Deparement de Physique, Universite de Montreal — Zinc oxide (ZnO) and tin oxide (SnO, SnO₂) are wide band gap semiconductors of interest for the fabrication of transparent conducting oxides (TCO). We present an initio study of these materials combining the projector augmented wave (PAW) formalism with the GW method to obtain quasiparticles band gaps. The PAW allows an accurate description of the d semi-core states which are important to correctly obtain the quasiparticle energies. The effect of these electrons on the calculated gap will be discussed. We also compare the structural and electronic description of the systems resulting from different exchange-correlation functionals (LDA, GGA and the use of a Hubbard U term). Finally, preliminary results of quasiparticle self-consistent calculations will also be presented.

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