Quasiparticle band structure of wurtzite ZnO in the GW approximation

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Abstract

We report results of the all-electron GW calculations of ZnO in the wurtzite structure. As for the input of the GW calculation, we use the eigenfunctions given by the full-potential linearized augmented-plane-wave method in the local-density approximation.

In the expansion of the screened Coulomb interaction W, we use the mixed basis which consists of two kinds of basis sets; one is the product-basis in the muffin-tin regions, the other is the plane waves projecting out their parts in the muffin-tin regions. The frequency-dependence of the dielectric function is treated fully without making the plasmon-pole model.

The Zn $3d$ orbitals are treated as valence states and both the core and valence states are included in our calculations. The obtained band gaps are smaller than the experiment by ~ 0.7eV against already reported GW studies for ZnO. We show the exchange and correlation part of the GW self-energy and discuss the role of each part to the quasiparticle energies.