GW quasiparticle energy study of ternary tetradymite Bi2Te2Se and Bi2Te2S thin films

ABSTRACT

In this work, we have evaluated the quasiparticle energies of ternary tetradymite Bi2Te2Se and Bi2Te2S using first-principles calculation within the G 0 W 0 methods. We have also performed a broad convergence tests in order to investigate the quasiparticle corrections to the structural parameters and to the semi core d electrons in both of the compounds. For each case, we have calculated the many-body corrections within a one-shot GW method of the compounds. Our results have shown that for Bi2Te2Se the GW corrections increase the band gap to almost 10%, and for specific atomic positions, the band structure shows a close value to the experimental one. For Bi2Te2S, despite increase in the band gap due to the GW corrections, possibility of bulk resistivity that can be significant for photovoltaic applications was observed.

Keyword: Density functional theory; GW method; Quarsi particle energy; Ternary tetradymite