

Density functional study of optical properties of beryllium chalcogenides compounds in nickel arsenide B8 structure

Abstract

The structural, electronic and optical properties of beryllium chalcogenides BeS, BeSe and BeTe using the full-potential linear augmented plane wave (FP-LAPW) method are investigated. The exchange-correlation energy within the local density approximation (LDA) and the generalized gradient approximation (GGA) are described. The Engel-Vosko (EVGGA) formalism is applied for electronic and optical properties. The structural parameters of our model and the transition pressure from zinc-blende (B3) to the NiAs (B8) phase are confirmed. It is found that these compounds have indirect band gaps except for BeTe in NiAs (B8) phase. The results of reflectivity, refractive index and optical dielectric functions of Be compounds are investigated. An agreement is found between our results and those of other theoretical calculations and the experimental data.