Nanocomposites and Nanomaterials

Theoretical Study on ZnHgSSe Alloys for Wide Range Optoelectronic Applications

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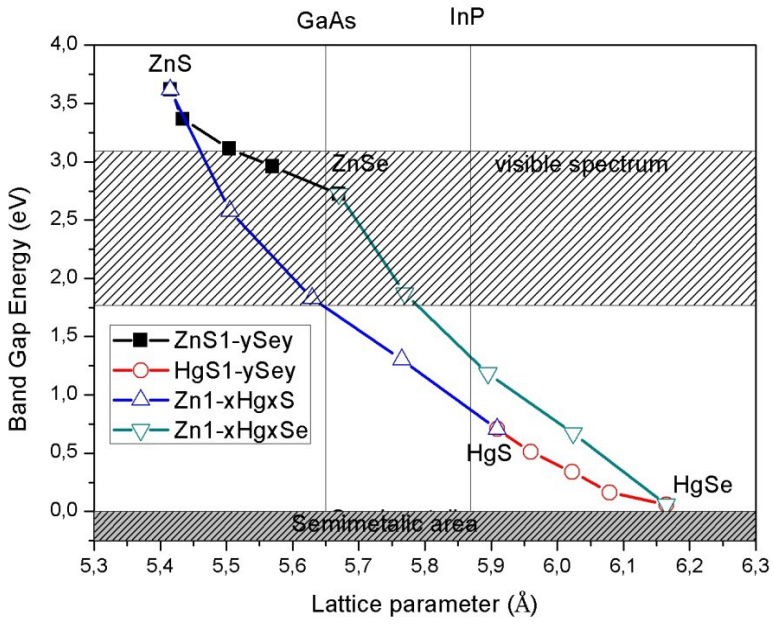
Abstract:

We present a calculation of the structural, electronic and optical properties of the four binary members of ZnHgSSe quaternary system by means of wien2k software package [1]. The exchange-correlation potential is treated by generalized gradient approximation (GGA) within the schema of Wu and Cohen [2]. Also, we have used modified Becke-Johnson (mBJ) formalism [3] to improve the band gap results. All the calculations have been performed after geometry optimization. We have determined that the direct band gap of the system can vary from 0.06 eV (HgSe) to 3.6 eV (ZnS) as shown in Figure. Because of the band gab range cover near UV, visible and IR spectrum regions ZnHgSSe alloys are candidate for many optoelectronic applications. The system is also offer the possibility of grown on lattice matched to the common substrates of GaAs and InP.

Keywords: II-VI alloys, physical properties, Wien2k



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