Theoretical Study of Structural, Electronic and Optical Properties of ZnX(X=S,Se,Te) and Mixed Chalcogenids Compounds Using DFT.

By
Iman Ali Laiem
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Supervisor Supervisor
Assist.prof.Dr Hadey Kasim Mohamad Assist.prof.Dr. Ahmed Subhi Jbara

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Abstract

The investigation of semiconductor materials attracted much attention because of their being widely suitable devices fabrication such as solar cells, light emitters, lasers, optical sensors, .etc. In this work, structural, electronic, and optical properties of binary ZnX (X=S, Se, Te) and triple mixed chalcogenides compounds are studied using density functional theory (DFT) within WIEN2k code. The simulation was achieved using highly accurate full-potential linearized augmented plane wave (FP-LAPW) method. The computational approach also combined with different approximations such as generalized gradient approximation (GGA), and modified Becke–Johnson (mBJ) potential. The optimization of all structures studied have been applied to study the effects of doping using supercell calculations, and values of the lattice constant are in good agreement with that obtained earlier experimentally. The electronic investigations confirm that these compounds have a direct bandgap (Γ-Γ), which varied from 3.673 eV to 2.186 eV. Also, different optical parameters of these compounds were calculated, which are represented by real and imaginary parts of the dielectric function, refractive index, reflectivity , and optical absorption coefficient . Variation of bandgap signifies the prospective utilize of considered these compounds that it can high efficiently be seen in multiple optoelectronic applications.