Abstract

The majority of commercial photovoltaic products are based on silicon-based technologies. The design of economical solar cell materials that offer high efficiency is a challenging field of modern day research. Due to the large scale demand for optoelectronics and photovoltaics devices, the study of chalcopyrite-type semiconducting materials has emerged as one of the significant domains for research.

In the present work, the structural, elastic, electronic, optical, and thermoelectric properties of $XCrS_2$ (X = Zn, Cd, and Hg) compounds with chalcopyrite structure were studied within the WIEN2k code using density functional theory combined with Boltzmann transport theory for thermoelectric properties. Stability along with the parameters of the crystal structures of the compounds were evaluated on the basis of generalized gradient approximation (GGA). Mechanical properties reveal that $ZnCrS_2$ and $CdCrS_2$ are mechanically stable and their elastic constants, linear and volume compressibility, as well as bulk modulus, shear modulus, Young's modulus, and Poisson ratio exhibit that $ZnCrS_2$ is brittle while $CdCrS_2$ is ductile. Furthermore, in order to investigate electronic, optical, and thermoelectric features, Tran-Blaha modified Becke-Johnson (TB-mBJ) was adopted for the solution of exchange and correlation potential. The XCrS2 compounds have 1.30, 1.27, and 1.33 eV band gaps, respectively, with a direct bandgap semiconductor. All compounds have strong absorption and photoconductivity in the visible region. In particular, $HgCrS_2$ has the greatest absorption and optical conductivity with energy loss, indicating the strongest absorption and the best photovoltaic activity. Electrical and thermal conductivity increase with an increase in temperature, especially for $HgCrS_2$ has greater electrical and thermal conductivity. The results also reveal that Seebeck coefficients for all the compounds increase from 50 to 350 K and then decrease. Also, $ZnCrS_2$ has the highest figure of merit as compared to other compounds. According to direct photovoltaic functionality screening, we find the studied compounds would be good photovoltaic absorbers.