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First-principle calculations of structural, electronic, optical, elastic and thermal properties of $MgXAs_2$ (X = Si, Ge) compounds

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Abstract. First-principle calculations on the structural, electronic, optical, elastic and thermal properties of the chalcopyrite $MgXAs_2$ (X = Si, Ge) have been performed within the density functional theory (DFT) using the full-potential linearized augmented plane wave (FP-LAPW) method. The obtained equilibrium structural parameters are in good agreement with the available experimental data and theoretical results. The calculated band structures reveal a direct energy band gap for the interested compounds. The predicted band gaps using the modified Becke–Johnson (mBJ) exchange approximation are in fairly good agreement with the experimental data. The optical constants such as the dielectric function, refractive index, and the extinction coefficient are calculated and analysed. The independent elastic parameters namely, C_{11}, C_{12}, C_{13}, C_{33}, C_{44} and C_{66} are evaluated. The effects of temperature and pressure on some macroscopic properties of $MgSiAs_2$ and $MgGeAs_2$ are predicted using the quasiharmonic Debye model in which the lattice vibrations are taken into account.

Keywords. Chalcopyrites; first-principle calculations; electronic properties; thermal properties; band gap; optical properties.

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1. Introduction

II–IV–V_2 chalcopyrite semiconductors generally crystallize in tetragonal structure with the space group $I\bar{4}2d(D_{2D}^{12})$. These compounds attracted considerable attention due to their photovoltaic characteristics. Chalcopyrites are promising materials for spintronics, electronic and optoelectronic applications such as solar energy converters, infrared detectors, visible and invisible light emitting diodes [1–4]. $MgXAs_2$ (X = Si, Ge) compounds are synthesized in chalcopyrite phase [1,5]. Shaposhnikov *et al* [6] investigated the electronic and the optical properties of $MgSiAs_2$ and $MgGeAs_2$ compounds. Liwei and coworkers [7] performed *ab-initio* band structure calculations for $MgSiAs_2$ compound. The authors [6,7] have found that both $MgSiAs_2$ and $MgGeAs_2$ are direct band-gap semiconductors. Basalaev and Demushin [8] studied the electronic band structure and the chemical bonding properties of the chalcopyrite $MgBX_2$ (B = Si, Ge, Sn; X = As, P, Sb) compounds and the orthorhombic $MgYN_2$ (Si, Ge) compounds. Kocak and Ciftci [9] investigated the elastic and the optical properties of $MgGeAs_2$ whereas Boukabrine *et al* [10] studied the dielectric function of $MgXAs_2$ (X = Si, Ge).

In the present work, we have focussed on the study of the structural, electronic, optical, elastic and thermal properties of $MgXAs_2$ (X = Si, Ge) compounds in their chalcopyrite phase. The computed ground-state structural properties have been compared with the available experimental and theoretical data. The outline of the paper is as follows: In §2 we give a brief description