Elastic properties and bonding of the $AgGaSe_2$ chalcopyrite

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Abstract :

Full-potential linearized augmented plane waves (FPLAPW) calculations have been used to determine the equilibrium properties and elastic constants of the chalcopyrite phase of $AgGaSe_2$. The topological analysis of the electron density shows a clear polar bonding, with the integrated basin charges revealing a clear dominance of the covalent over the ionic character. The bonding analysis also provides a partition of the bulk modulus and compressibility into atomic contributions. Se is seen to dominate the global behavior (B=51.2 GPa), with a local bulk modulus intermediate between the values of the other two atoms: 44.8 (Ga), 51.1 (Se), and 56.6 GPa (Ag).

Keywords : FPLAPW calculations; Elastic properties; Quantum theory of atoms in molecules; Chemical bonding in semiconductors.

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