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Full Length Article

A DFT study of the ternary metal chalcogenides ($XAlS_2$) materials for photovoltaic and high-temperature applications

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ABSTRACT

This work employs density functional theory (DFT) to investigate the structural, electronic, and optical properties of $XAlS_2$ (X = Li, Na, K, Rb, and Cs) nanomaterials for potential use in photovoltaic applications. A comprehensive first-principles analysis has been conducted using GGA-PBE, GGA-PBEsol, and LDA functionals to examine $LiAlS_2$, $NaAlS_2$, $KAlS_2$, $RbAlS_2$, and $CsAlS_2$. The findings reveal distinctive band gaps within this set of materials, with $LiAlS_2$ and $NaAlS_2$ exhibiting indirect band gaps and $KAlS_2$, $RbAlS_2$, and $CsAlS_2$ possessing direct band gaps. Analyzing the partial density of states indicates that the valence band predominantly arises from S-3p and Al-3p orbitals, showcasing covalent bonding through hybridization. Furthermore, the examination of the optical properties of $XAlS_2$ materials suggests their notable light absorption in the ultraviolet range, positioning them as promising candidates for photovoltaic applications. Additionally, the lattice thermal conductivity of two dynamically stable systems has been investigated and their thermoelectric properties have been calculated. Notably, a dimensionless figure of merit of 2.78 for $LiAlS_2$ has been identified, marking it as a strong contender for high-temperature thermoelectric applications.