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Bandstructure of Indium and Tin doped $AgAlS_2$

Previous studies of chalcopyrites as absorbers for intermediate band solar cells (IBSC)
mainly focused on Cu-based compounds, whose intermediate band is usually empty
due to its intrinsic p-type conductivity. $AgAlS_2$ chalcopyrite belongs to a group of direct band gap
semiconductors with novel applications in optoelectronic devices. Theoretical studies have hinted the possibility of using $AgAlS_2$ in IBSC due to the fact that its large bandgap can be easily tuned. To this date, this recommendation has not been attempted. It is for this reason that we will carry an *ab initio* study on $AgAlS_2$ to ascertain this prediction.
We will employ the state-of-the-art first principles density functional
theory (DFT) as implemented in the quantum ESPRESSO computer code to calculate the bandstructure of tetragonal $AgAlS_2$. The bandstructre of $AgAlS_2$ will be determined along $\Gamma\ M\ P\ PA\ X$ high symmetry points in the Brillouin zone.
Substitutional doping using tin/indium as dopants will be done using the supercell technique ($2 \times 2 \times 2$) on the trivalent cation site with varying concentrations until a band gap of ≈ 2.4 eV is obtained. This gap is carefully chosen since it is ideal for IBSC. This project is not only for academic purposes but it is also handy in designing solar cells with high efficiency and cost effectiveness.

Keywords

$AgAlS_2$, first-principles, Density functional theory, IBSCs.

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