New findings on Zintl phased $K_3Ag_3As_2$ ternary semiconductor compound for photovoltaic applications by first-principles methods

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ABSTRACT

A Zintl-phased K3Ag3As2 ternary compound previously unstudied by ab initio techniques was analysed for structural, electronic, mechanical, elastic, and optical properties using LDA-PZ, GGA-EV, GGA-PBE, GGA-PBESol, GGA-revPBE, and SO-GGA as the exchange correlation functionals. The structural properties showed that the material adopts a rhombohedral crystal structure with a mean lattice parameter of 15.1808 a.u. The material has been found to have a direct bandgap where the lowest value has been found to be 1.07 eV while the highest value was 1.74 eV when using PZ-LDA and EVGGA, respectively. The density of states has shown that the valence band formation is dominated by orbitals As 2p and Ag 3d, whereas the conduction band is mainly through the hybridisation of Ag 2p and As 2p, orbitals. This material has been found to be mechanically stable, ductile and has ionic bonding. The optical properties have shown that it is suitable for optoelectronic applications. The obtained values have been found to be consistent with the experimental values observed previously.