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First principles study of structural, elastic, electronic and optical properties of triclinic CsAlS2 chalcogenide.

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Abstract
The structural, elastic, electronic and optical properties of triclinic model CsAlS2 are investigated using the plane wave ultrasoft pseudopotentials approximation in the framework of density functional theory as implemented in CASTEP code of Material Studio package. The exchange correlation potential is treated with the generalized gradient approximation within the scheme of Perdew-Burke-Ernzerhof. The ground state properties are determined and the calculated elastic constant show that the CsAlS2 structure obeys the triclinic criterion. The obtained band structure and density of states predict the material to be an insulator with a direct band gap of 3.246 eV at 0 GPa. The optical properties are obtained and discussed, including reflectivity and absorption coefficient, which provide useful information for the future application of CsAlS2 in photovoltaics.

Apply to be considered for a student ; award (Yes / No)?

Yes

Level for award;(Hons, MSc, PhD, N/A)?

MSc

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