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First principle studies of structural, elastic, electronic and optical properties of chalcogenide LiAlS2 under pressure

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Abstract
In this work, we present the first principles calculations for structural, electronic and optical properties of orthorhombic LiAlS2 under hydrostatic pressure using plane-wave ultrasoft-pseudopotential method within the framework of density functional theory (DFT) as implemented in CASTEP in Material Studio package. The exchange-correlation potential is treated with generalized gradient approximation (GGA).The obtained structural parameters are in good agreement with the available results. The pressure-dependent lattice and elastic constants are obtained using the optimization method. The calculated band structure and density of states predict LiAlS2 to be an insulator with a direct band of 4.21 eV which agrees very well with the theoretical calculation of 4.11 eV. Furthermore, the calculated optical spectra such as absorption, and reflectivity are presented and the results are discussed.

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

Yes

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

Hons

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