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Electronic, elastic and thermoelectric properties of hexagonal CuSe phase

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Density functional theory using full-potential all-electrons linearised augmented plane waves was implemented to study electronic, elastic, and thermoelectric properties of hexagonal CuSe phase. Electronic bands suggest a metallic compound of zero energy gap. Density of states further expose the electron density responsible for this metallic behaviour. Elastic properties reveal mechanical stability and the possibility of being synthesisable. The compound is less compressible with positive calculated Cauchy pressure. High values of the power factor and the Seebeck coefficient allow consideration of the phase for thermoelectric applications.

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

No

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

PHD

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