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Electronic, elastic, and transport properties of copper sulphide

A full potential all-electron density functional method within generalised gradient approximation is used to investigate the electronic structure of copper sulphide. The electronic structure suggest a semi-metallic material with a zero band gap. Elastic calculations suggest a hard material with the bulk to shear modulus ratio of 0.381. The transport properties were estimated using the Boltzmann transport approach. Electrical conductivity, Seebeck coefficient, and thermal conductivity suggest a potential p-type plasmonic character.

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

yes

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

PHD

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