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Equilibrium and electronic properties of cubic copper sulphide

Thursday, 11 July 2019 15:00 (2 hours)

The equilibrium and electronic properties of the cubic copper sulphide are investigated using the full-potential all electrons first principle density functional theory. Convincing equilibrium and electronic properties are obtained using the GGA-PBEsol type exchange-correlation functional. Equilibrium properties suggest the mechanical stability with elastic anisotropy. The electronic band structure and the density of states suggest the material to be semi-metallic with no energy bap.

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

no

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

n/a

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