Ab initio investigation of the elastic and piezoelectric properties of lithium based Chalcogenides LiMX2 (M = Ga,In; X = S,Se)

Auteur: Lagoun, Brahim; Bentria, Tayeb; Bentria, Bachir

Abstract/Résumé : In this paper we report theoretical ab initio study of the elastic and piezoelectric properties of LiMX2 (M = Ga, In; X = S, Se) by means of density functional theory (DFT)
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