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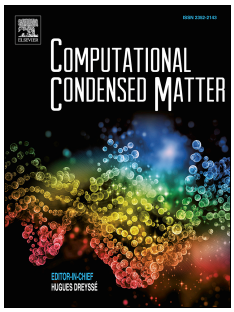

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First Principles study of structural and optoelectronic properties of Li based half Heusler alloys

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Abstract

The study of new semiconducting materials with enhanced structural, electronic, mechanical and optical properties for the advancement of optoelectronic applications has high merits in material science. First- principles calculations are carried out based on density functional theory for the semiconducting Li- based half Heusler compounds (X= Li; Y= Be, Sc; Z= As, Sb, Bi, Ge, Si) for three different atomic configurations namely α, β and γ phases of $C1_b$ crystal structure. It is predicted that α - phase is the lowest energy phase for LiBeAs, LiBeSb, LiBeBi and β - phase for LiScGe and LiScSi. The computed electronic structure profile reveals the semiconducting behavior for these materials. The calculated elastic constants obey the necessary mechanical stability condition suggesting that all the half Heusler alloys are mechanically stable at ambient condition. Also, The study of the optical properties of these Li- based compounds against the incident photon energy radiation illustrates that these materials can be the effective candidates for the optoelectronic devices. These Li- based half Heusler alloys could be promising materials to use in optoelectronic and solar cell applications.

Keywords: First Principles calculations; Metals and alloys; Crystal structure; Structural stability; Optoelectronic properties; Mechanical properties

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