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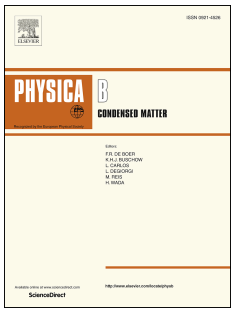

Lattice dynamics of Ru_2FeX (X = Si, Ge) Full Heusler alloys

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Lattice Dynamics of Ru_2FeX (X = Si, Ge) Full Heusler Alloys

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Abstract

In present work, the lattice dynamics of Ru_2FeX (X = Si, Ge) full Heusler alloys are investigated using density functional theory (DFT) within generalized gradient approximation (GGA) in a plane wave basis, with norm-conserving pseudopotentials. Phonon dispersion curves and phonon density of states are obtained using first-principles linear response approach of density functional perturbation theory (DFPT) as implemented in Quantum ESPRESSO code. Phonon dispersion curves indicates for both Heusler alloys that there is no imaginary phonon in whole Brillouin zone, confirming dynamical stability of these alloys in $L2_1$ type structure. There is a considerable overlapping between acoustic and optical phonon modes predicting no phonon band gap exists in dispersion curves of alloys. The same result is shown by phonon density of states curves for both Heusler alloys. Reststrahlen band for Ru_2FeSi is found smaller than Ru_2FeGe.

Keywords: Density functional theory; Full Heusler alloys; vibrational properties; Dispersion relations; Reststrahlen band; Density of states

1. Introduction

Vibrational properties such as phonon density of states and phonon dispersion curves play an important role in explaining the large number of properties

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