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(Research Article)
Investigation of phononic and thermal properties of the compound FeAl and Fe_3Al using pseudopotentials method

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Abstract

Iron aluminide intermetallic compound, including compounds that have great features is that it's so great properties, due to its increasing use in industry is different. In thiswork, structural and dynamic properties of FeAl compounds including the structure of energybands, density of states, phonon and thermal properties in two-phase structures regularly evaluated and calculated. Calculations using a Pseudoptential, within the framework of density functional theory have been studied PWscf code. The study found that the combination of these features in your base has a metal in ferromagnetic order, the results of the electronicstructure of this compound are indicative of metal and the structure of the electron cloud indicates the ionic bond -covalent for two phases results in good agreement with the experimental results are available.

Keywords: FeAl, Thermal properties, Density functional theory, PWscf.

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