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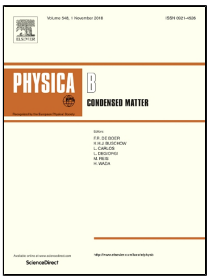

Electronic, magnetic, thermoelectric and lattice dynamical properties of full heusler alloy Mn_2RhSi: DFT study

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Electronic, magnetic, thermoelectric and lattice dynamical properties of full heusler alloy Mn_2RhSi: DFT study

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Abstract

The manganese based heusler compounds are important class of materials having remarkable ferrimagnetic and thermoelectric properties. Among them, Mn_2RhSi which crystallizes in both Hg_2CuTi and Cu_2MnAl type structure have undergone detailed investigation for its electronic, magnetic and mechanical properties in Hg_2CuTi type structure. However, no studies have been performed on Cu_2MnAl type structure of Mn_2RhSi. In this study we have performed a detailed comparative study on electronic, magnetic, mechanical, thermoelectric and lattice dynamical behavior of both types of Mn_2RhSi structures. The higher value of thermal conductivity reduces the thermo electric figure of merit in the material and has large value of Seebeck coefficient making these alloys as a potential candidate for thermoelectric device application. Our results show high value of spin polarization ratio for Mn_2RhSi which can increase the efficiency of spintronics devices which further have direct application in magnetic random access memory device. The heusler compound are least studied for their lattice dynamical behavior. In our work, we perform detail investigation on lattice dynamical behavior of both type structures of Mn_2RhSi. Our