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Ab Initio Study of Structural, Elastic, Electronic and Thermal Properties of Full Heusler

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Abstract : A theoretical study of structural, elastic, electronic and thermodynamic properties of Fe2VX, (with X = Al and Ga), were studied by means of the full-relativistic version of the full-potential augmented plane wave plus local orbitals method. For exchange and correlation potential we used both generalized-gradient approximation (GGA) and local-density approximation (LDA). Our calculated ground state properties like as lattice constants, bulk modulus and elastic constants appear more accurate when we employed the GGA rather than the LDA approximation, and these results agree very well with the available experimental and theoretical data. Further, prediction of the thermal effects on some macroscopic properties of Fe2VAl and Fe2VGa are given in this paper using the quasi-harmonic Debye model in which the lattice vibrations are taken into account. We have obtained successfully the variations of the primitive cell volume, volume expansion coefficient, heat capacities and Debye temperature with pressure and temperature in the ranges of 0–40 GPa and 0–1500 K.

Keywords : full Heusler, FP-LAPW, electronic properties, thermal properties
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