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Structural and Electronic properties of NiMnGe half-Heusler compound

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The full potential linear augmented plane wave (FPLAPW) method based on density functional theory (DFT) within the generalized gradient approximation (GGA) is used to investigate the structural and electronic properties of half-heusler NiMnGe compound. The half-Heusler compounds (general formula: XYZ) crystallize in a non-centrosymmetric cubic structure which is a ternary ordered variant of the CaF2 structure and can be derived from the tetrahedral ZnS-type structure by filling the octahedral lattice sites. Half-Heusler phases are known to combine with a wide variety of different elements. Generally, X and Y are alkali metal, transition metal or rare-earth metal, and Z is the main group element. All calculation have been carried out using the Wien2k package. The wave functions in the interstitial region were expanded in plane waves with a cutoff of kmax = 8/RMT (where RMT is the average radius of the MT spheres). (the potential and the charge density Fourier expansion parameter) is taken to be 12. The number of k-points, the irreductible wedge of the Brillouin zone (BZ), which ensures the convergence are 4000 k-points. The structure of half-Heusler compounds consist of three interpenetrating fcc sublattices, each of which are occupied by the X, Y and Z atoms. The equilibrium lattice parameters have been computed by minimizing the total energy with respect to the cell parameters and the atomic positions, to obtain the equilibrium structural properties for three structure type (I, II and III). It is found that ferromagnetic phase have lower energies than the antiferromagnetic and non-magnetic one for this compound.The results show that the half-heusler NiMnGe is metallic ferromagnet in GGA treatment.

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