First-principle study of Zincblende $Fe_xGa_{1-x}N$ alloys

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Abstract:

We present first-principle calculations of the structural, electronic, and magnetic properties of zincblende of ternary alloy $Fe_xGa_{1-x}N$ for different concentrations x(0, 0.25, 0.50 0,75, 1.0). The computational method is based on the full-potential linearized augmented plane wave method (FP-LAPW). The exchange and correlation energy is described in the generalized gradient approximation (GGA) and the local spin density approximation (LSDA). We have investigated the lattice parameters, bulk modulus, pressure derivative, band gap, and total magnetic moment of the zincblende FeN, GaN, and $Fe_xGa_{1-x}N$ alloys. The results obtained are in a good agreement with theoretical and experimental values. A reasonable agreement is found from the comparison of our results with other theoretical calculations or experimental results.