Emergence of half metallicity in Cr-doped GaP dilute magnetic semiconductor compound within solubility limit

Abstract

The electronic and magnetic properties of $Ga_{1-x}Cr_xP$ dilute magnetic semiconductor (DMS) compound for dopant concentration, x = 0.25, 0.125, 0.06 and 0.03 have been investigated using WIEN2k implementation of full potential linearized augmented plane wave (FPLAPW) method in order to seek out the possibility of new dilute magnetic semiconductor (DMS) compound within generalized gradient approximation (GGA) as exchange-correlation (XC) potential. The calculated results show that the Cr doping in GaP induces the ferromagnetism and originates a half metallic (HM) gap at Fermi level (E_F) in minority spin channel (MIC) for all concentrations. The half metallicity is originated by the hybridization of Cr-d states with P-p states. Moreover, the half metallicity remains intact for all Cr-concentration. We also observed that the HM gap increases with the reduction in doping concentration from 0.25 to 0.03. The total magnetic moment of this compound is mainly due to Cr-d states present at E_F. A small induced magnetic moment on other non magnetic atoms (Ga and P) for all doping concentrations is a consequence of p-d hybridization between Cr-d and P-p states.