Magnetic properties of AII–BIV–C2V chalcopyrite semiconductors doped with 3d-elements

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Abstract

The ab initio calculations of electronic and magnetic properties of inline image chalcopyrites (II = Be, Zn, Cd; IV = Si, Ge; V = P, As) doped with 3d metals are presented within the scope of interest for semiconductor spintronics. Different concentrations of V, Cr, Mn, Fe, and Co atoms replacing II–II, II–IV, and IV–IV group sites are checked and the most stable configurations for each case are determined. The appearance of magnetic moments and the ferromagnetic state upon doping is analyzed. It is revealed that for all materials incorporation of Cr or Mn atoms leads to the appearance of magnetic moments, but only substitution of II group atoms yields a stable configuration with a ferromagnetic state. High spin polarization is obtained for Zn–IV–P2 and Zn–IV–As2 compounds whose lattice parameters are close to that of silicon and germanium (or GaAs), respectively. Moreover, the substitution of Be by Cr atoms in Be–IV–As2 semiconductors (having a lattice parameter close to silicon) transforms them into half-metals stable in the ferromagnetic state. Recommendations upon the further applicability of investigated materials for spintronics are proposed.