

Variation of half metallicity and magnetism of $\text{Cd}_{1-x}\text{Cr}_x\text{Z}$ (Z=S, Se and Te) DMS compounds on reducing dilute limit

Abstract

The electronic and magnetic properties of Cr-doped Cd-Chalcogenides, $\text{Cd}_{1-x}\text{Cr}_x\text{Z}$ (Z=S, Se and Te) for dopant concentration, $x=0.25$ and 0.125 are presented in order to search new Dilute Magnetic Semiconductor (DMS) compounds suitable for spintronic applications. The calculations have been performed using full potential Linear Augmented Plane Wave (FPLAPW) method within generalized gradient approximation (GGA) as exchange–correlation (XC) potential. The calculated results show that the doping of Cr atom induces ferromagnetism in these compounds. Moreover, all DMS compounds retain half metallicity at both dopant concentrations with 100% spin polarization at Fermi level (E_F). The total magnetic moments of these compounds are mainly due to Cr-d states present at E_F where as there exist small induced magnetic moments on other non-magnetic atoms as well.

Keywords: Band structure, DFT, FPLAPW method, Spintronics, DMS