

Magnetic and electronic studies of substituted selenospinel

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Abstract

We have studied the magnetism of crystalline $\text{Cd}_{1-x}\text{Zn}_x\text{Cr}_2\text{Se}_4$ spinels with ($0.35 \leq x \leq 0.55$) under magnetic field up to 15 T. The total magnetic moment, Curie temperature, lattice parameter and exchange integrals were found to decrease with Zn substitution. *Ab-initio* calculations carried out using full potential augmented plane wave (FP-LAPW) method were performed to study the magnetic, and electronic structure using generalized gradient approximation (GGA) and the modified Becke-Johnson (mBJ) to correct the gap's energy. The obtained results were in good agreement with the experimental ones. It is shown that there is a competition between ferromagnetic (FM) and antiferromagnetic (AFM) interactions: the superexchange mechanism slightly increases the AFM contribution and keeps the FM the dominant mechanism in this range of substitution. From the density of states, we demonstrate that the system keeps the half-metallic state for the composition range $0.125 \leq x \leq 0.55$ with 100% spin polarization. Our results highlight that it is possible to obtain a half-metallic semiconductor with tunable magnetic state which is promising for applications in spintronics.

Keywords:

Spinels, magnetization, magnetic moment, DOS, mBJ, half-metallic, magnetic competition

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