Magnetic properties of Mn-doped $ZnSnAs_2$ chalcopyrite semiconductor

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Mn-doped $ZnSnAs_2$ chalcopyrite structure is one of the most important material to realize semiconductor spintronics because of its high Curie temperature [1-2].

In this work, we study theoretically electronic and magnetic properties of Mn-doped $ZnSnAs_2$ chalcopyrite structure by using first-principles all electron full-potential linearized augmented plane wave (FP-LAPW) method based on density functional theory (DFT). Our calculations were performed for supercells, containing 64 and 128 atoms with the Mn concentrations 3.125% and 6.25%. We studied when Mn magnetic impurity substitutes a single cation (Mn_{Zn} and Mn_{Sn}) or both of the two cation sites ($Mn_{Zn\text{-}Sn}$). From the total energy calculations for 64 atom supercells doped with Mn atoms in Zn-Zn sites were found to be energetically stable in the AFM state. The substitution of Zn-Sn and Sn-Sn positions results in the FM state (Fig.1). In the FM configurations calculated magnetic moment for each Mn is about 4.23μ_B and 3.99 μ_B per unit cell when Zn-Sn and Sn-Sn positions were substituted, respectively. The Curie temperature values are roughly estimated from the mean-field approximation.

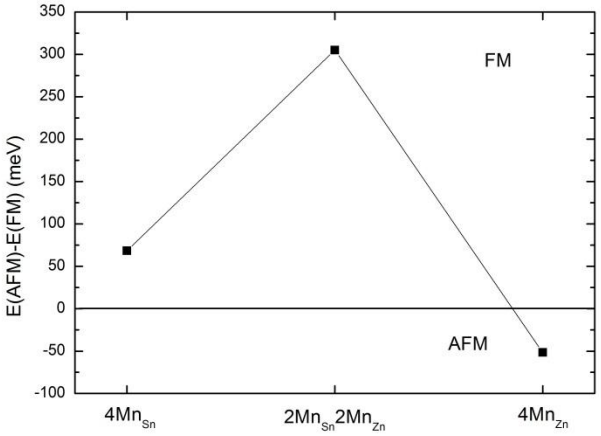

Fig.1. Total energy difference between AFM and FM states in Mn-doped $ZnSnAs_2$ when different cation sites substituted.

References

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