ABSTRACT

In this work, the wide band gap semiconductor zinc sulphide is doped with 3d transition metals (TM) such as chromium, manganese, vanadium, scandium and titanium and 4d transition metals like yttrium, zirconium and niobium. The structural properties of these compounds were studied by computing the total energy as a function of the unit cell volume using the Perdew-Burke-Ernzerhof generalized gradient approximation (PBE-GGA). It is found that for each TM concentration, the ferromagnetic (FM) state is lower in energy than the nonmagnetic (NM) state which indicates that the FM state is more stable than the NM state. The electronic and magnetic properties of the compounds Zn$_{0.875}$Cr$_{0.125}$S, Zn$_{0.875}$Mn$_{0.125}$S, Zn$_{0.75}$Cr$_{0.125}$Mn$_{0.125}$S, Zn$_{0.75}$Mn$_{0.125}$Cr$_{0.125}$S, Zn$_{0.875}$V$_{0.125}$S and Zn$_{0.75}$V$_{0.25}$S were studied by both PBE-GGA and modified Becke and Johnson local spin density approximation (mBJ-LSDA). Zn$_{0.875}$Cr$_{0.125}$S exhibits half-metallic ferromagnetic character but Zn$_{0.875}$Mn$_{0.125}$S is not found to be half-metallic. When Cr codoped to ZnMnS (Zn$_{0.75}$Mn$_{0.125}$Cr$_{0.125}$S), it is found to transform into half-metallic ferromagnetism. The density of states and band structure calculations of the compounds Zn$_{0.875}$V$_{0.125}$S and Zn$_{0.75}$V$_{0.25}$S reveal that these compounds exhibit half metallic character with 100 % spin polarization at the Fermi level. The energy gap in the minority spin channel increases with an increase in concentration of doping. The electronic and magnetic properties of Zn$_{0.875}$Sc$_{0.125}$S, Zn$_{0.75}$Sc$_{0.25}$S, Zn$_{0.875}$Ti$_{0.125}$S and Zn$_{0.75}$Ti$_{0.25}$S, Zn$_{0.75}$Y$_{0.125}$S, Zn$_{0.75}$Nb$_{0.25}$S and Zn$_{0.75}$Zr$_{0.125}$S compounds were studied by mBJ-LSDA method. The compounds Zn$_{0.75}$Nb$_{0.25}$S, Zn$_{0.875}$Sc$_{0.125}$S, Zn$_{0.75}$Sc$_{0.25}$S, Zn$_{0.875}$Ti$_{0.125}$S and Zn$_{0.75}$Ti$_{0.25}$S show half metallic nature but their total magnetic moment is low. The compounds Zn$_{0.75}$Y$_{0.25}$S and Zn$_{0.75}$Zr$_{0.25}$S are metallic. The total magnetic moments of all the compounds were mainly arisen from the TM doping. The compounds Zn$_{0.875}$Cr$_{0.125}$S, Zn$_{0.75}$Cr$_{0.125}$Mn$_{0.125}$S, Zn$_{0.75}$Mn$_{0.125}$Cr$_{0.125}$S, Zn$_{0.875}$V$_{0.125}$S and Zn$_{0.75}$V$_{0.25}$S exhibit half metallic ferromagnetism with 100 % spin polarization and their total magnetic moment also high and so they are predicted to be the suitable candidates for the spintronic applications.