Dilute magnetic states and half metal based on chalcopyrite semiconductors

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Electronic states, band structures, dilute magnetic states and magnetic properties of group I-III-VI$_2$ based transition metal (TM) doped chalcopyrite compounds $A(BX)C_2$ and $A(BXY)C_2$ are calculated using the Green’s function method of Korringa-Kohn-Rostoker and full-potential linearized augmented plane wave method, where $A=$Cu, Ag, $B=$Al, In, $C=$S, Se and $X, Y=$Ti, V, Cr, Mn, Fe, Co and Ni are 3$d$ TM. One impurity doped compounds $A(BX)C_2$ exhibit a stable ferromagnetic (FM) states and half metals relative to a disordered spin moment (DSM) state, when $X=$Ti, V, Cr and Mn at low-concentration of each TM ion are doped at host cation $B^{3+}$ site. Some of them exhibit a magnetic transition temperature above room temperature. On the contrary, in Fe, Co and Ni doped alloys instability of FM states to DSM is obtained. The situation is different for a simultaneous doping of a TM pair. The co-doped compounds $A(BXY)C_2$ can exhibit a FM, ferrimagnetic (FiM) and antiferromagnetic (AF) states depending on the orientation of the local spins and net moment. A parallel order of spins determine the FM states, whereas the anti-parallel arrangements give rise to FiM states and specific AF states are obtained for a nullified net moments. Some of the FiM and AF states are stable energetically relative to a DSM state and depicts half metallicity when TM pairs at equal concentrations and with $d$ electrons occupancy less and more than half filled are co-doped at host cation $B^{3+}$ site. In some other co-doped cases instability of FiM states to DSM is obtained. Total energy, electronic charge density, magnetic critical temperatures, net moments, local spin moments, fixed spin moments, spin-orbit interaction properties and hyperfine fields, as well as the enthalpy of formation and Gibbs energy at an entropic states are calculated. Calculated dilute magnetic states, half metals and other magnetic properties imply that chalcopyrite type compounds $A(BX)C_2$ and $A(BXY)C_2$ are promising for respective spintronics applications.

Keywords: Chalcopyrite, Coherent Potential Approximation, Half Metal, KKR-Green’s function, Supercell, FLAPW.

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