Momentum resolved spin splitting in Mn-doped topologically trivial CdTe and non-trivial HgTe semiconductors

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We have investigated the spin-splitting along the whole Brillouin zone in topologically trivial CdTe and non-trivial HgTe semiconductors doped with magnetic Mn^{+2} impurities by means of relativistic first-principles density functional calculations. The spin splitting of the host significantly varies in the Brillouin zone due to the k-dependence of the host-impurity hybridization. Along almost whole Brillouin zone spin-splitting is strongly antiferromagnetic due to the Kondo-like exchange between the d-states and the host. The notable exception is the vicinity of the Γ point, where the spin-splitting of the conduction band becomes ferromagnetic. The nature of the host quantum state plays a crucial role in the determination of the magnetic spin split. Indeed, the Γ_6 bonding state does not couple to the d-states but it does couple ferromagnetically to Mn-4s. The electronic correlations suppress the antiferromagnetic Kondo-like coupling while do not affect the ferromagnetic direct exchange. In result, we have found a strong suppression of the spin splitting at the L point that explains the anomalous spin splitting found in available experimental works. Moreover, for HgTe we demonstrate that the topologically non-trivial state is also a Γ_6 bonding state. In this case, the spin-orbit coupling increases the magnetic spin-splitting at the Γ point.