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Theory of the Novel Mn-doped II-II-V Dilute Magnetic Semiconductors

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A recently discovered magnetic semiconductor $Ba_{1-x}K_x(Zn_{1-y}Mn_y)_2As_2$, with its decoupled spin and charge doping, provides a unique opportunity to elucidate the microscopic origin of the magnetic interaction and ordering in dilute magnetic semiconductors (DMS). We show that (i) the conventional density functional theory (DFT) accurately describes this material, and (ii) the magnetic interaction emerges from the competition of the short-range superexchange and a longer-range interaction mediated by the itinerant As holes, coupled to Mn *via* the Schrieffer-Wolff $p-d$ interaction representing an effective Hund's rule coupling, $J_H^{\rm eff}$. The key difference between the classical double exchange and the actual interaction in DMS is that an effective $J_H^{\rm eff}$, as opposed to the standard Hund's coupling J_H, depends on the Mn $d-$band position with respect to the Fermi level, and thus allows tuning of the magnetic interactions. The physical picture revealed for this transparent system may also be applicable to more complicated DMS systems.