Exchange Interactions in Dilute Magnetic Semiconductors

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We discuss the different types of exchange interactions in dilute magnetic semiconductors with impurity d-states in the wide band gaps. Firstly we present density functional–LDA calculations by using the KKR–CPA method for small concentrations of transition metal impurities in GaN and ZnS. The exchange interaction parameters J_{ij} between two TM impurities i and j are calculated by Lichtenstein's formula. We show that the trends of the calculated interactions as a function of the valence of the impurities can be reproduced by rigidly shifting the Fermi level in Lichtenstein's formula. For the considered systems three different behaviours with band filling and with varying concentration c are observed. If the Fermi energy falls in the majority t_{2g} band, as is the case for (Ga,Mn)N or (Zn,Cr)S, double exchange dominates, leading to a $\sqrt{c}$-scaling of the average exchange energy with concentration and to short ranged interactions. If all majority d-states are occupied, as it is the case for (Ga,Fe)N or (Zn,Mn)S, the interaction is dominated by antiferromagnetic super exchange. The exchange interaction parameters are very short ranged and scale linearly with concentration c. Finally if the Fermi level falls between the e_g and t_{2g} states, as it is the case for (Ga,V)N or (Zn,Co)O, the interaction is dominated by ferromagnetic super exchange, which again is very short ranged and scales linearly with concentration. As we will demonstrate, all three types of interactions can be simply understood by the hybridisation between different e_g and t_{2g} states of neighbouring impurity pairs. Due to the short range of all interactions, the Curie and Neel temperatures in these dilute systems are very small due to the percolation effect, so that percolation represents a serious obstacle for high Curie temperatures in dilute magnetic semiconductors.