Unified picture for diluted magnetic semiconductors

For more than a decade already and because of their technological potential for incorporation in spintronic devices, diluted magnetic semiconductors (DMS's) have attracted a considerable attention from both experimentalists and theoreticians. A very competitive race started with the discovery that a very small amount of Mn (which introduces a $3d^5$ configuration + itinerant hole) in thin films of the III-V semiconductor GaAs could lead to a relatively high Curie temperature ferromagnet. (Ga,Mn)As rapidly became the most studied prototype, which still exhibits (for a given Mn density and well annealed samples) the highest critical temperature among III-V DMS compounds (190 K). However, even today, from the physical understanding and theoretical point of view, one often finds contradicting theories and results in the literature.

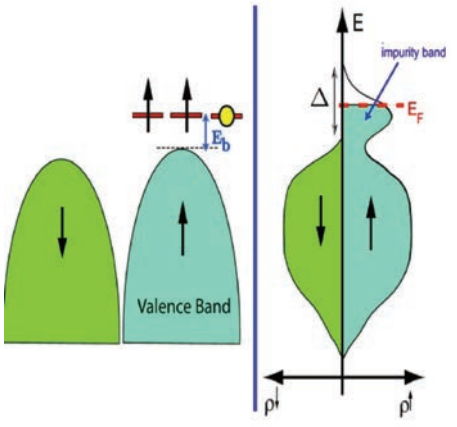

Figure1: (Left) A single Mn in GaAs; the E_b = 113 meV p-d acceptor level is threefold degenerate. (Right) the spin resolved density of states for a finite Mn concentration in the ferromagnetic phase. Δ is the band splitting.

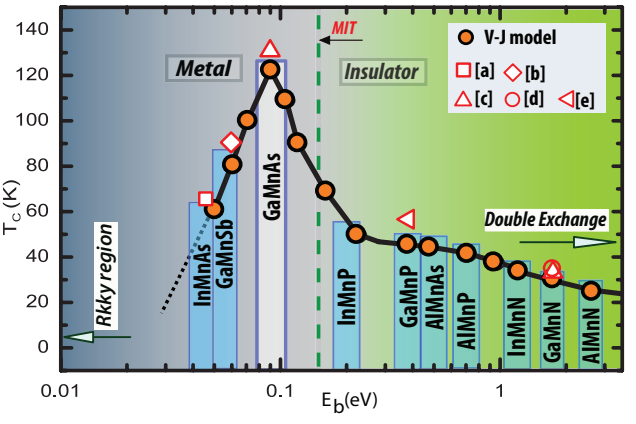

Figure 2: Curie temperature (in K) as a function of the p-d Mn acceptor level position E_b (eV) in various III-V semiconductors. The Mn density is x = 5%. Filled symbols are computed within the V-J model, open symbols (a,b,..e) with ab initio exchange integrals. The agreement between ab initio studies and V-J model calculations is excellent. A metal-insulator transition occurs at E_b=0.15 eV, close to (Ga,Mn)As.

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FURTHER READING

UNIFIED PICTURE FOR DILUTED MAGNETIC SEMICONDUCTORS
R. Bouzerar and G. Bouzerar
Europhys. Lett. 92, 47006 (2010).

FIRST PRINCIPLES THEORY OF DILUTE MAGNETIC SEMICONDUCTORS
K. Sato, G. Bouzerar, et al.
Rev. Mod. Phys. 82, 1633 (2010).

OPTICAL CONDUCTIVITY IN Mn DOPED GaAs
G. Bouzerar and R. Bouzerar
New J.Phys. 13, 023002 (2011).

Several crucial questions are still debated and very controversial. In spite of the great success of ab initio material-specific theory in providing accurate Curie temperatures (TC) in various III-V based materials, the ultimate search for a unifying theory was still an open issue. We have shown recently that a simple one-band model, namely the V-J model (where V is the spin independent scattering of the holes by Mn^{2+} and J is the p-d exchange between Mn d orbitals and host p-holes) is able to provide the missing unified picture and clarify numerous issues. Within this model we can understand and explain magnetic and transport properties simultaneously, not only qualitatively but also quantitatively. It has been shown that the position E_b of the Mn p-d hybridized acceptor level, with respect to the top of the valence band, is the key physical parameter (controlled by V). This term is the source of the crucial differences between II-VI and III-V Mn doped systems. It controls both the magnetic properties (nature of the couplings) and the transport properties. We obtain a very good agreement between the splitting of the valence band density of states as calculated by the model and that obtained from material-specific ab initio calculations. And our calculations agree very well with experimental measurements for optimally prepared samples of various III-V compounds.

The V-J model provides a coherent picture for the drastic change in the nature of the couplings depending on the host: RKKY-like (oscillating long range couplings) in II-VI compounds such as (Zn,Mn)Te, (Cd,Mn)Te and double exchange-like (very short range and ferromagnetic) in wide band gap compounds such as (Ga,Mn)N. It has also been possible to explain why, among all Mn doped materials either II-VI or III-V, the highest critical temperature was measured in (Ga,Mn)As. As seen in Fig.2, (Ga,Mn)As is precisely located on a peak where the Mn-Mn couplings are optimal. The V-J model also explains clearly why it has been observed experimentally that some as grown (Ga,Mn)As samples are insulating and others are metallic at low temperature, or why one can trigger an insulator to metal transition after annealing. Indeed, (Ga,Mn)As appears to be at the boundary of the Metal-Insulator Transition (MIT) as seen in Fig.2. As a further confirmation of the validity of our model, it has also been possible (i) to reproduce quantitatively the measured infrared conductivity and (ii) explain why annealing, which increases the hole density, induces a red shift of the conductivity peak located at about 200 meV.