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The dilute magnetic semiconductors: A playground for the Zaanen-Sawatzky-Allen phase diagram

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The electronic properties of transition metal compounds have been classified in terms of the Zaanen-Sawatzky-Allen (ZSA) phase diagram and its variants[1,2]. In this talk I will present our results on placing two well studied dilute magnetic semiconductors (DMS) in this phase diagram and try to understand their ensuing magnetic properties depending on where they belong. We find Mn doped GaAs has a negative charge transfer energy which places it in the p-d metal regime of the phase diagram. This explains why Coulomb interactions on the Mn site do not localize the hole associated with Mn doping and drive the system insulating. Unlike in a bulk solid, at the dilute doping limit a good approximation to the levels with which a Mn atom interacts with are the dangling bond states associated with the Ga vacancy that Mn substitutes[3,4]. These follows the valence band maximum of the host semiconductor. Solving for the electronic and magnetic properties within a multiband Hubbard model at the mean field limit, we show that the ferromagnetic stability increases with quantum confinement. This opens up a new route to increase the ferromagnetic transition temperature in Mn doped GaAs. Our results are consistent with recent experimental observations by Kanski et al[5] who find spin polarised bands even at room temperature in Mn doped GaAs where bulk magnetization measurements find a ferromagnetic transition temperature much smaller. Considering the example of Mn doping in GaN we find that the system has a negative charge transfer energy, with the transition metal d bands lying inside the N p bands. Inspite of this the system is insulating and this can be explained by the fact that covalency effects drive the system insulating. The system can be identified as a covalent insulator of the modified ZSA phase diagram[2].

References:

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