

On the electronic state of Mn impurities in GaAs

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Most phenomenological models of ferromagnetism in Mn doped GaAs assume that the Mn²⁺ impurity substitutes primarily the Ga³⁺ cation with five occupied majority d orbitals that have atomic character and a delocalized acceptor state. While these assumptions are generally thought to be in agreement with experiment, they are presently not supported by ab initio electronic structure calculations. The latter, which are typically based on the Local Spin Density Approximation (LSDA) to Density Functional Theory, find the Mn d orbitals to be strongly hybridized with the As p states. In this picture only four Mn d states are filled with an acceptor states that is localized to the Mn impurity and the first As neighbor shell. It is well known that due to spurious self-interactions LSDA calculations tend to overestimate the hybridization of such impurity states. In the present work we have performed first principles electronic structure calculations of Mn impurities in a GaAs host using the Self Interaction Corrected Local Spin Density Method (SIC-LSD). The method is self interaction free by construction and reproduces the LSDA in the limit of delocalized states. For GaMn-As we find that the self interaction corrections strongly affect the electronic state of Mn. The majority d orbitals are no longer hybridized and are all occupied leaving Mn nominally with $S=5/2$. The nature of the acceptor states changes as well, in that they have mainly p character and are no longer localized to the Mn site and its nearest neighbors.

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