

Electronic Structure and Valence of Mn Impurities in III-V Semiconductors

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Substitutional Mn impurities in III-V semiconductors can acquire either a divalent or a trivalent configuration. For example, it is generally accepted that Mn in GaAs is in a (d^5+h) configuration with five occupied Mn d-orbitals and a delocalized hole in the valence band. In contrast, Mn in GaN is believed to be in a d^4 configuration with a deep impurity state that has d-character. But there have recently been some discussions about the possibility of having some Mn ion in GaN assuming a divalent (d^5+h) type configuration. In order to achieve carrier induced ferromagnetism, the desired state of the Mn ions in III-V semiconductors is the (d^5+h) configuration. We have therefore performed ab-initio calculations of the Mn valence when it substitutes Ga in various III-V semiconductor hosts. We use the self-interaction corrected local spin density (SIC-LSD) method which is able to treat localized impurity orbitals properly. In particular we find that the method is capable of predicting the (d^5+h) state of Mn in GaAs. For Mn in GaP and GaN the calculations predict a trivalent d^4 state in the idealized system. The energy differences between d^4 and (d^5+h) configurations in GaP are, however, very small. Introduction of defects or donors does change the valence of Mn in GaP, favoring the divalent state under certain circumstances.

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