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Origin of ferromagnetism in GaMnAs from a new theoretical viewpoint

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Abstract

The prototype dilute magnetic semiconductor GaMnAs has been discovered [1] and investigated during two decades. Previously, ferromagnetism in this material has been known to be induced by the *p-d* exchange interaction of the valence holes and localized *d*-electrons of Mn atoms [2], and the Zener *p-d* exchange interaction model has been widely accepted as the main mechanism inducing ferromagnetism in GaMnAs [3]. Following this model, the *d*-orbitals of Mn atoms hybridize the *p*-orbitals of As atoms and form an Mn-induced impurity band (IB) that merges with the valence band (VB) to expand VB towards the bandgap, and the Fermi level (E_F) lies in the merged VB. Recently, besides many experimental works support this model, several experiments have reported that E_F locates in the separated *d*-band inside the bandgap [4], which suggests that the Zener *p-d* exchange mechanism may not be the dominant mechanism inducing ferromagnetism in GaMnAs. The above-mentioned confliction of the experimental observations is still an open question and needed to be solved. The fact that the previous calculations obtained by using KKR-CPA, or pure DFT show an IB of the *d*-electrons being merged with VB, leads to the conclusion that the ferromagnetism in GaMnAs is originated from the exchange interaction of the valence holes and *d*-electrons. Therefore, it is necessary to employ a more reasonable method to deal with this problem.

In this talk, we show that, in the first time, the long-standing question about the origin of ferromagnetism in GaMnAs can be solved, and the confliction of the experimental observations can be explained by employing the hybrid functional method HSE06. In all of the calculations, the 64-atoms supercells were used. The most preferable configurations of Mn atoms at various concentrations were obtained by a full optimization calculation. Band structure and decomposition band charge density of the most preferable configurations were calculated. In order to explore the dominant mechanism of ferromagnetism in the system, the separation of IB from VB depending on the Mn concentration was emphasized in our talk. In addition, the interaction between the interstitial, anti- and substitution sites, and then the possibility of diffusion of Mn atoms from the interstitial site to the substitution/interstitial sites were also addressed. Our results show an overlap of IB and VB at the dilute concentrations of Mn atoms, which suggests a possibility of ferromagnetism originated from the *p-d* exchange interaction. On the contrary, the separation of IB from VB was found at higher concentrations. This finding implies that the origin of ferromagnetism in GaMnAs would change depending on the Mn concentration.

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