PHYSICAL REVIEW B **69**, 165212 (2004)

Interstitial Mn in (Ga,Mn)As: Binding energy and exchange coupling

J. Mašek and F. Máca
Institute of Physics ASCR, Na Slovance 2, 182 21 Praha 8, Czech Republic

(Received 27 August 2003; revised manuscript received 22 December 2003; published 28 April 2004)

We present *ab initio* calculations of total energies of Mn atoms in various interstitial positions. The calculations are performed by the full-potential linearized plane-wave method. The minimum energy is found for tetrahedral $T(As_4)$ position, but the energy of the $T(Ga_4)$ site differs by only a few meV. The $T(Ga_4)$ position becomes preferable in the *p*-type materials. In samples with one substitutional and one interstitial Mn, the Mn atoms tend to form a close pair with antiparallel magnetic moments. We also use the spin splitting of the valence band to estimate the exchange coupling J_{pd} for various positions of Mn. The exchange parameter is the same for the substitutional and for the $T(As_4)$ position, and it is somewhat smaller in the case of the $T(Ga_4)$ position.

DOI: 10.1103/PhysRevB.69.165212 PACS number(s): 71.15.Mb, 71.15.Nc, 75.50.Pp

I. INTRODUCTION

Diluted magnetic semiconductors, such as (Ga,Mn)As, are important materials combining ferromagnetic behavior with a sensitivity to doping characteristic for semiconductors. This leads to their interesting physical properties and makes possible their applications, e.g., in spin electronics.[1,2] Although (Ga,Mn)As has been extensively studied in the last years, some aspects of the incorporation of Mn into the crystal lattice still remain unclear. It was assumed that in the well defined samples Mn simply substitutes for the host cation. Only recently it was pointed out[3,4] that the presence of interstitial Mn may explain some peculiar properties of (Ga, Mn)As such as the low doping efficiency of Mn acceptors.[5] The main reason for considering the Mn atoms on the interstitial positions was that they act as double donors and partly compensate the Mn acceptors in the substitutional positions.

At the same time, channeling Rutherford backscattering experiments proved that a large fraction of Mn atoms indeed occupies the interstitial positions (Mn_{int}) in the as-grown samples.[6] A correlation between the removal of Mn interstitials and increase of the conductivity, the Curie temperature, and saturation magnetization has been found.

In addition to the self-compensation effect, the interstitial Mn atoms also reduce the number of local moments that participate in the ferromagnetic state. This was explained by pairing of Mn_{int} with the Mn atoms in the substitutional positions (Mn_{Ga}) due to their Coulomb attraction.[6] At the bonding distance, the antiferromagnetic superexchange within the pair is assumed to outweigh the hole mediated ferromagnetic exchange. As a result, the moments of the paired Mn atoms have opposite directions and the pair as a whole has no magnetic moment.

The *ab initio* studies of the interstitial Mn showed the differences in the electronic structure of the Mn atom in the interstitial and substitutional positions[4,7] and also a possible reaction path for the incorporation of Mn into the GaAs lattice.[8] It was also found that the increase of the lattice constant of $Ga_{1-x}Mn_xAs$ with increasing content of Mn is partly due to the presence of Mn in the interstitial positions.[9]

Recently, Blinowski and Kacman[10,11] investigated the coupling of the local moment on the interstitial Mn to the spin of the carriers in the valence band. Using a simplified tight-binding model they showed that the local moment on Mn atom in the tetrahedral position with four Ga neighbors, $T(Ga_4)$, is effectively decoupled from the spin of the holes in the valence band.

They claimed that the coupling is weak because, in addition to the reduced number of the holes, also the coupling constant J_{pd} is small for the interstitial Mn in the $T(Ga_4)$ position. As a result, the local moment is not subject to the ferromagnetic coupling with the moments around it. This opens the way for the antiferromagnetic exchange to be important in the Mn_{int}-Mn_{Ga} pair, as anticipated in Ref. 6.

There are, however, several open questions concerning the magnetic interactions of Mn in the interstitial positions. First of all, the spin-polarized band structures[4] did not show any indication of different values of J_{pd} for substitutional and interstitial Mn, at least for the $T(As_4)$ positions. In addition, the Mn_{int}-Mn_{Ga} pair as a whole is expected[10,11] to have only a small magnetic moment, but the exchange coupling with Mn_{Ga}—being uncompensated by the contribution of Mn_{int}—should strongly polarize the holes.

That is why we performed a more detailed study of the interstitial Mn and its spin interactions. We use the density-functional, full-potential linearized augmented plane-wave calculations [FPLAPW (Ref. 12)] to obtain the electronic structure of (Ga,Mn)As with Mn atoms in various crystallographic positions. The calculated total energies are used to compare different positions of the interstitial Mn and to estimate the strength of the Mn_{Ga}-Mn_{int} pair interactions. The splitting of the valence band for the majority- and minority-spin electrons is used to compare the corresponding values of the exchange parameters J_{pd}.

II. Mn IN VARIOUS INTERSTITIAL POSITIONS

We compare the total energies for three interstitial positions of Mn in GaAs. There are two inequivalent tetrahedral positions in the zinc-blende structure of GaAs, $T(As_4)$, and $T(Ga_4)$. They are surrounded by four As and Ga atoms, respectively. The (unrelaxed) distances of these nearest neighbors are equal to the length d_1 of the Ga-As bond, i.e., to the Mn-As distance for the substitutional Mn_{Ga}. The local ar-

TABLE I. Total energy E_{tot} and total spin S_{tot} of the unit cell of $Ga_{12}As_{12}Mn$ with various interstitial positions of Mn. $Ga_9Zn_3As_{12}Mn$ samples are used to simulate *p*-type materials.

Sample	Mn position	E_{tot} (eV)	S_{tot}
$Ga_{12}As_{12}Mn$	$T(As_4)$	Ground state	1.665
$Ga_{12}As_{12}Mn$	$T(Ga_4)$	+0.005	1.555
$Ga_{12}As_{12}Mn$	Hexagonal	+0.522	1.519
$Ga_9Zn_3As_{12}Mn$	$T(As_4)$	+0.063	2.331
$Ga_9Zn_3As_{12}Mn$	$T(Ga_4)$	Ground state	2.176
$Ga_9Zn_3As_{12}Mn$	Hexagonal	+1.320	2.136

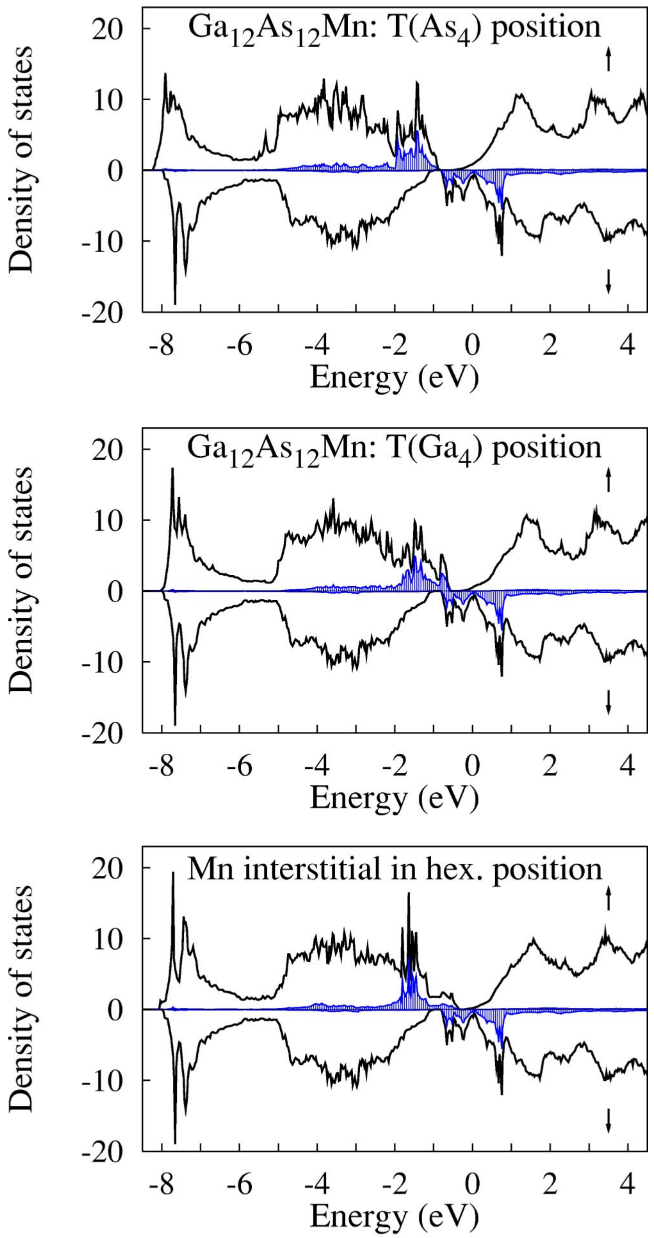

FIG. 1. Spin-polarized densities of states for $Ga_{12}As_{12}Mn$ with an interstitial Mn atom in $T(As_4)$ (upper panel), $T(Ga_4)$ (middle panel), and hexagonal position (lower panel). The contribution of Mn *d* states is indicated by hatched area.

rangement around the interstitial Mn is, in contrast to Mn_{Ga}, characterized by another six close neighbors at the distance $d_2 = \sqrt{9/8}d_1 \approx 1.155d_1$. In the hexagonal position, the interstitial Mn has three Ga and three As atoms at the same distance $d_{hex} = \sqrt{11/12}d_1 \approx 0.957d_1$, and no other close neighbors.

We represent GaAs with Mn_{int} by hexagonal $Ga_{12}As_{12}Mn$ supercells. The *c* axis coincides with the body diagonal of the conventional cubic unit cell. The symmetry of the cell does not change if we shift the Mn interstitial along the *c* axis from $T(As_4)$ to hexagonal and $T(Ga_4)$ positions. This makes possible to perform all calculations under the same conditions.

The results are summarized in Table I. Surprisingly, the binding energy of the interstitial Mn does not depend much on its nearest neighbors. The interstitial Mn has minimum energy in the $T(As_4)$ position. However, the difference of the total energies obtained for Mn in $T(Ga_4)$ and $T(As_4)$ positions is of the order of a few meV and can be neglected in practice. This means that, without intervention of other charged defects, the Mn interstitials can be found with an almost equal probability in either $T(As_4)$ or $T(Ga_4)$ position. The total energy corresponding to the hexagonal interstitial position of Mn is remarkably higher and represents a barrier ≈ 0.5 eV separating the tetrahedral positions. Calculations with similar results have been recently done by Boguslawski.[13]

The weak influence of the nearest neighbors on the interstitial Mn in $T(As_4)$ and $T(Ga_4)$ positions can be observed also in the densities of states in Fig. 1. The total density of states (DOS) and the distribution of the Mn *d* states are almost identical. Also the DOS of $Ga_{12}As_{12}Mn$ with Mn in the hexagonal position is quite similar and differs mainly by the overlap of the valence band for the majority-spin electrons (↑) with the conduction band for the minority-spin (↓) electrons. This tendency to close the gap in the electron spectrum correlates well with the increase of the total energy.

The lattice relaxation around the Mn impurity is not very important for the substitutional Mn as shown by Mirbt *et al.*[14] This is not the case of the interstitial Mn which tends to expand the crystal lattice.[9] The addition of Mn into either $T(As_4)$ or $T(Ga_4)$ positions results in a remarkable repulsion of the nearest and next-nearest neighbors. The positions of the more distant atoms in the supercell are changed much less. The energy gain due to the relaxation is in both cases approximately 20 meV and it does not change the ordering of the total energies for the $T(As_4)$ or $T(Ga_4)$ positions. The lattice relaxation around Mn in the hexagonal position has not been considered because of its minor importance.

In the case of the $T(As_4)$ position, the distance of the four nearest As neighbors was found to increase by $\approx 0.7\%$ from 2.45 Å to 2.47 Å. The distance of the six next-nearest Ga neighbors increases by $\approx 1.5\%$ from 2.835 Å to 2.88 Å.

The relaxation around Mn in the $T(Ga_4)$ position is larger. The nearest Ga neighbors are pushed to the distance 2.515 Å and the relaxed distance of the next-nearest neighbors increases by $\approx 0.5\%$. The enhanced relaxation of the nearest neighbors in this case is due to the Coulomb repulsion be-

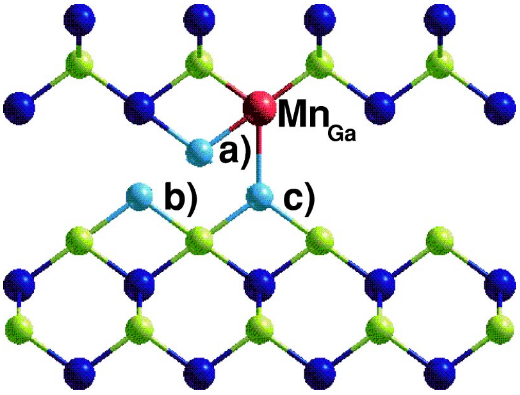

FIG. 2. Configurations of the Mn_{Ga}-Mn_{int} pair in the (110) plane of GaAs crystal (Ref. 15): (a) Mn_{int} in $T(Ga_3Mn)$ position is the nearest neighbor of Mn_{Ga}; (b) Mn_{int} in $T(As_4)$ position representing a partially dissociated pair at a doubled distance; (c) Mn_{int} in the $T(As_4)$ position closest to Mn_{Ga}.

tween Mn and Ga atoms which are both positively charged.

In all cases, there are two electrons in the conduction band, i.e., the Mn_{int} always acts as a double donor. The electrons in the conduction band are almost completely spin polarized. They accumulate in the minority-spin conduction band, so that the total spin of the cell (i.e., the spin per Mn) is reduced to $\approx 3/2$ in accordance with our previous calculations.[4]

For comparison, we performed the same set of calculations also for hypothetical $Ga_9Zn_3As_{12}Mn$ crystals with Zn atoms substituted at the sites most distant from the interstitial Mn. The presence of Zn has only a little effect on the density of states, but the material is converted into the *p* type with one hole in the valence band. In this case, the $T(Ga_4)$ turns to be the stable interstitial position of Mn. The energy difference between the $T(As_4)$ and $T(Ga_4)$ positions, approximately 60 meV, is high enough for a preferential occupation of the $T(Ga_4)$ position at typical growth conditions. The remarkable increase of the energy of the hexagonal position indicates that the mobility of the interstitial Mn may depend on the type and degree of the doping.

III. BINDING ENERGY AND EXCHANGE COUPLING OF A Mn-Mn PAIR

The hexagonal unit cell used in Sec. II is well suited also for the study of the Mn_{int}-Mn_{Ga} pair interactions. We consider a hypothetical $Ga_{11}MnAs_{12}Mn$ crystal with one substitutional and one interstitial Mn in the unit cell. We consider three positions of the interstitial Mn shown in Fig. 2. The positions $T(Ga_3Mn)$ and $T(As_4)$, denoted (a) and (b) in Fig. 2, are located on the *c* axis of our unit cell and correspond to the initial stage of dissociation of the Mn_{Ga}-Mn_{int} pair. On the other hand, the $T(As_4)$ position denoted (c) is very close to Mn_{Ga} and is—together with $T(Ga_3Mn)$—a candidate for the ground state of Mn_{int}.

In the $T(Ga_3Mn)$ position, Mn_{int} and Mn_{Ga} are the nearest neighbors at the distance d_1. We performed the density-functional calculations with two initial conditions, corresponding to parallel and antiparallel alignment of their local moments. In both cases, the self-consistent procedure converges to a locally stable solution without changing the initial alignment of the local moments. The resulting total energies are given in Table II. The antiparallel alignment is energetically more favorable than the parallel alignment, in a good correspondence with the expectations.[6,11] The coupling is strong enough so that the AF state of the Mn_{int}-Mn_{Ga} pair is stable with respect to the thermal fluctuations.

TABLE II. Total energy of $Ga_{11}MnAs_{12}Mn$ unit cell and the spin assigned to Mn_{int} and Mn_{Ga} atoms for various configurations of the Mn_{int}-Mn_{Ga} pair shown in Fig. 2. The configuration (c) is treated separately because of its different symmetry.

Pair configuration	Mn_{Ga}-Mn_{int} distance (Å)	Total energy (eV)	Spin of Mn_{Ga}	Spin of Mn_{int}
(a) ↑↑	2.443	+0.324	1.678	1.617
(a) ↑↓	2.443	Ground state	1.778	−1.531
(b) ↑↑	4.886	+0.502	1.930	1.616
(b) ↑↓	4.886	+0.330	1.899	−1.558
(c) ↑↑	2.835	+0.303	1.774	1.657
(c) ↑↓	2.835	Ground state	1.842	−1.549

Table II shows also the local spins on Mn_{Ga} and Mn_{int} atoms defined as integrals of the spin density over the corresponding atomic spheres. Although these quantities are not directly related to the size of the observable local moments, we can see that the local moments of Mn_{Ga} and Mn_{int} are comparable and that the total magnetic moment of the pair in the ground state is much smaller than the magnetic moment of a single Mn.

Assuming that the exchange coupling between more distant Mn atoms from different unit cells is much smaller than the exchange interaction $J(d_1)$ within the closest pair we can estimate its strength from the difference $\Delta E(d_1) = E_{\uparrow\uparrow}(d_1) - E_{\uparrow\downarrow}(d_1) \approx -2J(d_1)S^2$ of the total energies. Using saturated values $S=5/2$ for both local moments we obtain the lower estimate for $J(d_1)$, namely, $J(d_1) \approx -26$ meV.

The coupling between Mn_{int} and Mn_{Ga} remains antiferromagnetic also if Mn_{int} moves to any of the adjacent $T(As_4)$ positions (b) and (c) in Fig. 2. The energy difference between the parallel and antiparallel alignment of the local moments decreases with the increasing distance of the Mn atoms, as expected for the superexchange. It remains almost the same for the nearest and close next-nearest pairs and it is reduced approximately to one half of $\Delta E(d_1)$ for the doubled distance corresponding to the configuration (b).

It should be pointed out, however, that the density-functional calculations tend to overestimate the strength of the exchange coupling. The reason for this is that the exchange splitting of the Mn *d* states, i.e., the separation of occupied majority-spin and empty minority-spin states on the energy scale levels is systematically underestimated. According to our calculations, the exchange splitting $\varepsilon_d(\downarrow) - \varepsilon_d(\uparrow)$ deduced from the spin-polarized spectral distribution of Mn *d* states ranges from 2 eV to 3 eV. This is roughly one half of the realistic estimate for the exchange splitting in Mn (cf., e.g., Ref. 16). Correspondingly, the above given value of $J(d_1)$ should be divided by 4. In this way, we end with a value close to the result of Ref. 11.

Finally, we estimate the binding energy of the $\mathrm{Mn_{int}}$-$\mathrm{Mn_{Ga}}$ pair. We compare the energies corresponding to the (a) and (b) configurations from Fig. 2, both in the magnetic ground state with the antiparallel alignment of the local moments. The partially dissociated pair has a higher energy and the energy difference $E_{\uparrow\downarrow}(d_2)-E_{\uparrow\downarrow}(d_1)$ is approximately 0.33 eV. It is, however, only the lower estimate for the binding energy of the $\mathrm{Mn_{int}}$-$\mathrm{Mn_{Ga}}$ pair because the dissociation of the pair is far from being complete in our periodic model. Nevertheless, even the value obtained here indicates that the Mn interstitials are strongly attracted by the $\mathrm{Mn_{Ga}}$ atoms. As long as the concentration of $\mathrm{Mn_{int}}$ is lower than the concentration of $\mathrm{Mn_{Ga}}$ we can assume that most of $\mathrm{Mn_{int}}$ atoms are involved in the pairs and that the blocking mechanism proposed in Ref. 6 works.

IV. EXCHANGE INTERACTION OF INTERSTITIAL Mn AND HOLES

Due to the hybridization with the spin-polarized Mn *d* states, also the distribution of the states derived from the GaAs valence band depends on the spin. In particular, the valence-band states for the majority-spin electrons hybridize with the occupied *d* states and are pushed to higher energies. The minority-spin states are, on the other hand, pushed down due to their hybridization with unfilled *d* states.

This effect is formally described by the Kondo exchange interaction between the local spins $\mathbf{S}_i$ at sites R_i occupied by Mn and the spin density $\mathbf{s}(r)$ due to the itinerant holes,[17]

$$H_{\mathrm{int}}=J_{pd}\sum_i \mathbf{S}_i\cdot\mathbf{s}(R_i). \tag{1}$$

The exchange parameter J_{pd} characterizes the strength of the coupling. Within the mean-field theory, the Kondo exchange interaction results in the splitting of the valence-band edge E_v. The splitting ΔE_v is proportional to the size S of the local spins and to the concentration x of magnetic ions,

$$\Delta E_v \equiv E_v(\downarrow)-E_v(\uparrow)=\frac{4x}{a^3}J_{pd}S, \tag{2}$$

assuming spin $\frac{1}{2}$ for the holes, a is the lattice constant. We use Eq. (2) to determine the exchange parameter J_{pd} from our spin-polarized band structures. The results of the calculations for the unrelaxed geometries presented here and in Ref. 4 are summarized in Table III.

The resulting values of J_{pd} are overestimated from the same reasons as discussed above in Sec. III. Being divided by a factor of two (the reduction factor for the energy nominator), they approach the realistic values.[18] In this work, however, we concentrate on the comparison of J_{pd} for different geometries. The overestimate of J_{pd} due to the reduced band gap is expected to be similar in all cases and not very important in this respect.

In Fig. 3, we plot ΔE_v against x to visualize the linear increase of the band splitting with the concentration of Mn. The most noticeable result is that all points in Fig. 3, obtained for substitutional Mn as well for Mn in the interstitial $\mathrm{T(As_4)}$ and $\mathrm{T(Ga_4)}$ positions lie around the same line. This means that the value of J_{pd} does not depend much on the position of the Mn atom in the lattice.

TABLE III. Spin splitting $\Delta E_v = E_v(\uparrow)-E_v(\downarrow)$ for ferromagnetic state of (Ga,Mn)As.

Sample	Mn positions	ΔE_v (eV)	J_{pd} (eV nm^3)
$\mathrm{Ga_{12}MnAs_{12}}$	$\mathrm{T(As_4)}$	0.627	0.14
$\mathrm{Ga_{12}MnAs_{12}}$	$\mathrm{T(Ga_4)}$	0.515	0.11
$\mathrm{Ga_{12}MnAs_{12}}$	hex.	0.653	0.14
$\mathrm{Ga_{16}MnAs_{16}}$	$\mathrm{T(As_4)}$	0.502	0.14
$\mathrm{Ga_{16}MnAs_{16}}$	$\mathrm{T(Ga_4)}$	0.429	0.12
$\mathrm{Ga_{14}Mn_2As_{16}}$	$2\times\mathrm{Mn_{Ga}}$	1.021	0.15
$\mathrm{Ga_{14}Mn_3As_{16}}$	$2\times\mathrm{Mn_{Ga}}+\mathrm{T(As_4)}$	1.328	0.13
$\mathrm{Ga_{30}Mn_3As_{32}}$	$2\times\mathrm{Mn_{Ga}}+\mathrm{T(As_4)}$	0.743	0.14

This result is not very surprising in the case of the substitutional Mn and $\mathrm{T(As_4)}$ position. In either case, Mn is surrounded by four As atoms at the same distance d_1 and the same degree of the hybridization of the valence-band states with Mn *d* states can be expected.

The results for the $\mathrm{T(Ga_4)}$ position are not simple to interpret. The value of J_{pd} for both $\mathrm{Ga_{12}MnAs_{12}}$ and $\mathrm{Ga_{16}MnAs_{16}}$ is smaller than but comparable with the result for the substitutional $\mathrm{Mn_{Ga}}$ site. Assuming for simplicity that only the hybridization of the Mn *d* states with *p* states of the nearest neighbors is relevant for the spin splitting ΔE_v, the values of J_{pd} simply reflect the orbital composition of the valence band. It is well known that the top of the valence band in GaAs, as well as in other III-V semiconductors, is composed of both anion and cation *p* states, in the proportion approximately $c_p^{\mathrm{As}}\approx 3/4$, $c_p^{\mathrm{Ga}}\approx 1/4$.[19] This means that the same proportion (roughly 3:1) should be expected also for the exchange parameters J_{pd} corresponding to Mn atoms in substitutional and $\mathrm{T(Ga_4)}$ positions. The strong deviation of the actual density functional results from this model expectation may indicate that the hybridization of the Mn *d* states with more distant neighbors has a remarkable influence on the magnetic interactions.

The fact that the magnetic behavior of the interstitial Mn is rather insensitive to its position in the crystal has two

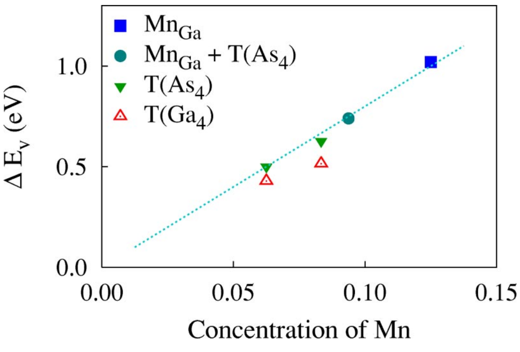

FIG. 3. Spin splitting of the valence band as a function of Mn concentration.

important implications concerning the Mn_{Ga}-Mn_{int} pairs. First of all, the pair as a whole does not interact much with the spin of the holes because the effects due to Mn_{Ga} and Mn_{int} compensate one another. In this respect, our *ab initio* results overcome the troubles of the simplified tight-binding models mentioned in the Introduction.

In addition, the effective ''annihilation'' of Mn_{Ga} due to pairing with Mn_{int} is not restricted to the closest pairs with Mn_{int} in the $T(Ga_3Mn)$ position, but it works as long as the Mn atoms are close one to another and the exchange coupling in the pair remains antiferromagnetic.

V. CONCLUSIONS

We used the FPLAPW method to obtain total energies of supercells simulating various geometric and magnetic configurations of Mn atoms in (Ga,Mn)As. In absence of other defects, the ground state of the Mn interstitials is the tetrahedral $T(As_4)$ position. The energy of the $T(Ga_4)$ position, however, is almost the same. The situation changes in the *p*-type material where the $T(Ga_4)$ position has a lower energy. The hexagonal interstitial position has much higher energy and represents a barrier for diffusion of Mn from one to another interstitial site. The barrier, and consequently also the mobility of the interstitial Mn, depends on the doping.

The exchange coupling J_{pd} of Mn interstitials with the holes in the valence band is, for both $T(As_4)$ and $T(Ga_4)$, close to the value of J_{pd} obtained for the substitutional Mn. This is not consistent with the simplest tight-binding picture of Mn *d* states that hybridize only with the nearest neighbors. In this way, our result indicate that the hybridization with more distant neighbors may be also important for the magnetic interactions.

The Mn interstitials are attracted to the substitutional Mn and form stable and magnetically inactive pairs. The density-functional estimate for both binding energy of the pair and for the energy of the antiferromagnetic coupling is of order of 0.3 eV. This fits well with the present day notion of the interstitial Mn in (Ga,Mn)As.[6,11] In contrary to the general opinion, however, we found that the efficient pairing is not restricted to Mn_{int} in the $T(Ga_3Mn)$ position and we showed the importance of the close next-nearest neighbors for the properties of the interstitial Mn.

ACKNOWLEDGMENTS

This work has been done within the Project No. AVOZ1-010-914 of the ASCR. The financial support provided by the Grant Agency of the ASCR (Grant No. A1010214) and by RTN Project No. HPRN-CT-2000-00143 the EC is acknowledged.

---

[1] T. Dietl, H. Ohno, F. Matsukura, J. Cibert, and D. Ferrand, Science **287**, 1019 (2000).

[2] H. Ohno, J. Cryst. Growth **251**, 285 (2003).

[3] J. Mašek and F. Máca, Acta Phys. Pol. A **100**, 319 (2001).

[4] F. Máca and J. Mašek, Phys. Rev. B **65**, 235209 (2002).

[5] B. Beschoten, P.A. Crowell, I. Malajovich, D.D. Awschalom, F. Matsukura, A. Shen, and H. Ohno, Phys. Rev. Lett. **83**, 3073 (1999).

[6] K.M. Yu, W. Walukiewicz, T. Wojtowicz, I. Kuryliszyn, X. Liu, Y. Sasaki, and J.K. Furdyna, Phys. Rev. B **65**, 201303(R) (2002).

[7] S. Sanvito, G. Theurich, and N. Hill, J. Supercond. **15**, 85 (2002).

[8] S.C. Erwin and A.G. Petukhov, Phys. Rev. Lett. **89**, 227201 (2002).

[9] J. Mašek, J. Kudrnovský, and F. Máca, Phys. Rev. B **67**, 153203 (2003).

[10] J. Blinowski, P. Kacman, K.M. Yu, W. Walukiewicz, T. Wojtowicz, and J.K. Furdyna, *XXXI Int. School Physics of Semicond. Compounds—Jaszowiec 2002* (Ustron-Jaszowiec, Poland, 2002).

[11] J. Blinowski and P. Kacman, Phys. Rev. B **67**, 121204 (2003).

[12] P. Blaha, K. Schwarz, and J. Luitz, *WIEN2k, FPLAPW Package for Calculating Crystal Properties* (unpublished).

[13] K.W. Edmonds, P. Boguslawski, K.Y. Wang, R.P. Campion, N.R.S. Farley, B.L. Gallagher, C.T. Foxon, M. Sawicki, T. Dietl, M.B. Nardelli, and J. Bernholc, cond-mat/0307140 (unpublished).

[14] S. Mirbt, B. Sanyal, and P. Mohn, J. Phys.: Condens. Matter **14**, 30 130 (2002).

[15] A. Kokalj, J. Mol. Graphics Modell. **17**, 176 (1999).

[16] V. Drchal, O. Gunnarsson, and O. Jepsen, Phys. Rev. B **44**, 3518 (1991).

[17] T. Moriya, *Spin Fluctuations in Itinerant Electron Magnetism* (Springer, New York, 1985).

[18] H. Ohno, J. Magn. Magn. Mater. **200**, 110 (1999).

[19] W.A. Harrison, *Electronic Structure and Properties of Solids* (W. H. Freeman and Co., San Francisco, 1980).