Revisiting the Mn-doped Ge using the Heyd-Scuseria-Ernzerhof hybrid functional

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We perform a comparative ab-initio study of Mn-doped Germanium semiconductor using the Perdew-Burke-Ernzerhof (PBE) exchange-correlation functional, DFT+U and Heyd-Scuseria-Ernzerhof hybrid functional (HSE). We show that the HSE functional is able to correctly account for the relevant ground state properties of the host matrix as well as of Mn-doped semiconductor. Although the DFT+U and the HSE description are very similar, some differences still remain. In particular, the half-metallicity is lost using DFT+U when a suitable U value, tuned to recover the photoemission spectra, is employed. For comparison, we also discuss the case of Mn in Silicon.

INTRODUCTION

Dilute magnetic semiconductors (DMSs) are still a topic of great current interest.\cite{1, 2, 3} The theoretical description of the interaction of transition metal doped semiconductors is challenging since localized states interact significantly with delocalized states. Density functional theory (DFT) in the local density or generalized gradient approximation (LDA or GGA) for the exchange–correlation energy is not able to properly describe the non-locality of the screened exchange interaction and, furthermore, possesses a sizeable self-interaction error.\cite{4} These limitations are particularly severe in the case of localized orbitals, e.g. Mn-3d states, which are described as too shallow in energy resulting in a large hybridization with anion p-states. As a result, the Mn-3d states are over-delocalized. The situation is particularly serious in the case of small band-gap semiconductors (such as Ge) which are described as metals in LDA/GGA, thus producing an overestimated hybridization among the valence and conduction Ge states and Mn-d states. The physics of localized d states can be partially described using a DFT+U formalism, which introduces a local correction U to recover the proper position of the Mn-d states\cite{5}. However, in Ge, the accurate electronic properties are not completely recovered: e.g. the half-metallicity of the compound is lost within DFT+U scheme.

Very recently, hybrid Hartree-Fock density functionals, which mix a fraction of the exact Fock exchange with the DFT exchange, have been widely applied to extended solid state systems.\cite{6, 7, 8} In this paper, we mainly focus on Mn-doping in bulk Ge by performing hybrid-density functional theory calculations. We will show that the HSE functional gives a satisfactory description of the structural, electronic and magnetic properties of Ge-based DMS, consistent with experimental data. Furthermore, for few selected properties, and, for sake of comparison, we will also include some results of Mn-doped Silicon.

COMPUTATIONAL DETAILS

The calculations were performed within the projector augmented-wave (PAW) method\cite{24} using the Perdew-Burke-Ernzerhof (PBE) exchange-correlation functional (GGA)\cite{25} and Heyd-Scuseria-Ernzerhof (HSE) hybrid functional\cite{26, 27}, recently implemented in the VASP code.\cite{28, 29} We also used the DFT+U method for Mn within Dudarev’s approach\cite{30} fixing U to 6 eV and J to 1 eV (PBE was used for the DFT part). The kinetic energy cutoff used for the orbitals was set to 300 eV. Monkhorst-Pack k-point grids of 10 × 10 × 10 and 6 × 6 × 6 were used to sample the Brillouin zone of the Ge-bulk and of the 64-atom unit cell, respectively. All the atomic internal positions were relaxed. In the following, we will focus on the Ge bulk system, single (substitutional and interstitial) and double substitutional (dimer) Mn impurities in a 64-atom Germanium cell. For Silicon, we will consider the bulk case and the Mn substitutional impurity in a 64-atom unit cell.

BULK GE

For bulk Ge, the calculated equilibrium properties are in good agreement with experiments: the HSE lattice constant is 5.703 (5.792) Å using HSE (PBE) within 0.7 (2.3) % of the experimental value of 5.660 Å.\cite{31} the HSE bulk modulus (731 kbar) improves over the PBE value (571 kbar) when compared to experiment (768 kbar).\cite{32} Furthermore, we remark that within HSE the energy gap is properly described to be indirect (0.63 eV including SOC\cite{33}) compared to the experimental value of 0.74 eV.\cite{31} A similar result was obtained within HSE for Si: the HSE lattice constant is 5.444 Å using HSE\cite{33} compared to the experimental one of 5.430 Å.\cite{32} The cal-
culated indirect energy gap is 1.12 eV\textsuperscript{[33]} while the experimental one is 1.17 eV.\textsuperscript{[32]} It is interesting to note that, for Silicon, self-interaction schemes which are often used to improve the electronic structure description,\textsuperscript{[8] 35} do not open the gap.\textsuperscript{[36]} This is important for our present study, since a faithful description of the equilibrium properties of the host semiconductor is at the basis of an appropriate description of the doped system.

**MN IMPURITIES IN GE**

In Table I we summarize our main results, \textit{i.e.} formation energy $\Delta H$, Mn-Ge bond length ($d_{\text{Mn-Ge}}$) and the Mn magnetic moment ($\mu$) at their respective theoretical lattice constants for the considered Mn-doping cases. The formation energies are evaluated with respect to the calculated Ge and Mn equilibrium bulk phases (diamond Ge and AFM-fcc Mn). Of course, while Ge-rich growth conditions can be safely assumed to fix the Ge chemical potential to its bulk value, the same is not true for Mn so that the formation energy is a function of the Mn chemical potential $\mu_{\text{Mn}}$. In Table I we report the value for Mn-rich conditions fixing $\mu_{\text{Mn}}$ to the corresponding bulk value ($\alpha$-Mn).

We note that the experimental evidence of local Ge-lattice dilation upon Mn-doping is correctly described using HSE yielding a Mn-Ge distance 2 \%'s larger than the ideal Ge-Ge bond-length, while PBE gives a local contraction of $\sim$2\% and DFT+$U$ finds a smaller local dilation of 0.4 (0.8)\% when using the theoretical PBE (HSE or experimental) lattice constant.\textsuperscript{[38] 40} The most recent extended x-ray absorption fine structure results\textsuperscript{[41–43]} yield a Mn-Ge coordination distance of 2.50$\pm$0.03 Å for the samples obtained at low temperature and which are thought to be best candidates for Mn occupation on substitutional sites\textsuperscript{[42]}. Clearly, these results match the HSE result and the DFT+$U$ as well. Similar results for bond-lengths contraction/dilation within different DFT schemes were reported also for III-V based DMS\textsuperscript{[14].}

A simple molecular orbital description, as sketched in Fig. 1, can be useful in order to describe the interaction of Mn in the tetrahedral Ge ligand field, as also done previously for similar compounds.\textsuperscript{[44]} We recall that in diamond like semiconductors, the sp valence states arrange to form $sp^3$ hybrid orbitals, each of them filled with a bonding electron pair. If one Ge atom is removed creating a Ge vacancy, 4 $sp^3$ hybrids point towards the vacant Ge atom, each filled with one electron (dangling bonds). The Ge vacancy is now replaced by a Mn atom. Due to the local tetrahedral symmetry, the Mn d-states are split into 3-fold degenerate $t_{2g}$ and 2-fold degenerate $e_g$-like states, further splitted by the local exchange field (see Fig. 1 right part). From linear combinations of the four $sp^3$ Ge dangling bonds pointing towards the transition-metal impurity, an s-like $a_{1g}$ orbital and three p-like $t_{2g\uparrow\downarrow}$ orbitals are formed. The host $a_{1g}$ orbital and the transition-metal $4s_{\uparrow\downarrow}$ states form a doubly occupied bonding state deep in the semiconductor valence band, and an empty antibonding state high in the conduction band (not included in Fig. 1). For the majority component, the Mn-$t_{2g}$ orbitals are lower in energy than the Ge-$t_{2g}$ $sp^3$ hybrid states. They interact giving rise to 3 bonding states ($3\times\text{Mn}-t_{2g}b$) (see Fig. 1) and 3 anti-bonding states ($3\times\text{Ge}-sp^3b$). The Mn-$e_g$ states do not hybridize because they are non-bonding in a tetrahedral ligand field. For the minority component, the Ge-$t_{2g}$ $sp^3$ orbitals are lower in energy than the Mn-$t_{2g}$ states. Upon interaction, they give rise to 3 bonding orbitals ($3\times\text{Ge}-sp^3b$) and 3 anti-bonding orbitals ($3\times\text{Mn}-t_{2g}ab$). The complex is characterized by a total of 11 electrons (4 from the nearest Ge atoms and 7 from the Mn impurity atom). Disregarding the two electrons occupying the lowest $a_1$ symmetry-like state, one needs to fill the orbitals with nine electrons as shown in Fig. 1. Clearly the Mn impurity is in a high spin state with 5 d-electrons in the majority channel (2 electrons in the $e_g$ and 3 in the $t_{2g}$-like states) and zero d-electrons in the minority channels. However, while the minority valence Ge-$sp^3$ states are fully occupied, the majority states accommodate two holes. This simple molecular picture suggests that: i) the compound is half-metallic, with the Fermi level falling within the Ge majority valence band; ii) the total spin moment of the complex, \textit{i.e.} $n_{\uparrow\downarrow} = n_{\uparrow\downarrow}$, is 3 $\mu_B$; iii) the local Mn $d$ spin moment is 5 $\mu_B$ partially compensated by the
holes in the $sp^3$ states; iv) the induced spin moment on the 4 nearest Ge atoms, i.e. $n_{sp}^{Ge}$−$n_{sp}^{Ge}$ should be sizeable and opposite to the spin on the Mn atom. In line with previous calculations, the calculated results confirm this picture finding a total spin moment of exactly 3 $\mu_B$ in the unit cell, 4.1 $\mu_B$ at the Mn atom, and −0.11 $\mu_B$ at the nearest Ge-atoms. Furthermore the sizeable induced moments on Ge atoms suggest that the holes are rather delocalized.

The local angular momentum decomposed density of states (DOS) shown in Fig. 2 is consistent with this orbital interaction diagram. The top panel shows the HSE results, whereas the bottom panel reports DFT+U results for $U=6$ eV. In the inset, we show the relation between the center of mass of the Mn-$d$ majority states, $\langle e_d \rangle$, and the $U$ value. The horizontal line indicates the $\langle e_d \rangle$ value, which matches the HSE result ($U=6$ eV). Fig. 2 clearly confirms the interpretation discussed above. In particular, integration of the majority total density of states from the Fermi level up to the end of the Ge-valence band exactly sums up to 2 electrons: these are the two holes required to fill the Ge valence band. Mn-substitution into the Ge host matrix does not produce a Jahn-Teller ion, but rather a Mn$^{2+}$ ionic state with a $d^5$ configuration and two spin-polarized holes. Let us now compare the HSE and DFT+U DOS. Due to the choice of the $U$ value, the Mn-$d$ states have the same energy within HSE and DFT+U but the hybridization between Ge-$sp$ and Mn $t_{2g}$ and $e_g$ states (this latter symmetry-allowed away from $\Gamma$) is underestimated within DFT+U compared to HSE. While the on-site $U$ mainly localizes the Mn $d$ states, HSE also acts through the screened exchange on Ge-$p$ states, lowering their energy position and leading to a larger Mn-$d$ Ge-$p$ hybridization. As a matter of fact, the larger hybridization in HSE compared to DFT+U can be recognized just below −4 eV, where a peak in the $e_g$ character (shaded region in Fig. 2) is completely absent in the present DFT+U description. We note that previous LDA+U calculations with $U=4$ eV, although reproducing the peak at −4 eV characteristic of the Mn-Ge bond, gave a quite different density of states for both the $t_{2g}$ and $e_g$ states, which is due to the strong dependence of the localized d-states description on the $U$ parameter. Finally, as found in Ref. 6, the half-metallic character of the compound is destroyed within DFT+U: the energy position of the Mn-$t_{2g}$ Ge-$sp$ bonding minority states, whose energy position is mainly determined by the atomic Ge-$sp$ levels, is raised towards higher energies causing an incomplete filling of the minority valence band.

In a previous study, it was shown that the half-metallicity is favored in Mn doped Ge while in Silicon matrix it is lost. In Fig. 3 we show the HSE DOS for substitutional Mn$_{Si}$ (top panel) and DFT+U, with $U=6$ eV, the same used for Mn$_{Ge}$ (bottom panel). The correction for the self-interaction error has a larger effect on Si-$sp^3$ states, since they are quite localized. Therefore, they are pushed down in energy. According to the orbital energy diagram shown in Fig. 1 also the minority bonding (Si-$sp^3$), is shifted down in energy, favoring the half-metallicity. Obviously, the Mn-$d$ states are also corrected for the self-interaction error, and they are pushed down in energy as well. On the other hand, DFT+U corrects only the Mn-$d$ states, but not the Si-$sp^3$ states. This gives a near-half metallic structure and an underestimation of the hybridization of Mn-Si states compared to the HSE description.

The single interstitial impurity

This defect in a Germanium matrix possesses twice the formation energy as the substitutional impurity (HSE), hence it is unlikely to form. Here we only note that a tendency to a local expansion around Mn is found for all functionals. Interestingly, the local magnetic moment is larger for DFT+U than for HSE, suggesting sizeable differences in the interaction of the impurity with the local environment.

| Mn substitutional site | PBE | DFT+$U$ | HSE |
|------------------------|-----|---------|-----|
| $\Delta H$ (eV/Mn)     | 1.5 | 0.9     |     |
| $d_{Mn-Ge}$ (Å)        | 2.46 (2.51) | 2.53 (2.51) | 2.52 (2.47) |
| $\mu$ ($\mu_B$)        | 3.3 (3.1) | 4.1 (3.4) | 4.1 (3.0) |

| Mn interstitial site    | PBE | DFT+$U$ | HSE |
|-------------------------|-----|---------|-----|
| $\Delta H$ (eV/Mn)      | 2.1 | 1.8     |     |
| $d_{Mn-Ge}$ (Å)         | 2.57 (2.51) | 2.63 (2.51) | 2.58 (2.47) |
| $\mu$ ($\mu_B$)         | 3.4 (4.0) | 4.2 (4.8) | 3.8 (4.1) |

| Mn-Mn dimer             | PBE | DFT+$U$ | HSE |
|-------------------------|-----|---------|-----|
| $\Delta H_{AFM}$ (eV/Mn-pair) | 2.9 | 1.5  |     |
| $\Delta H_{FM} - \Delta H_{AFM}$ | 0.77 | 0.22 | 0.15 |
| $d_{Mn-Mn (FM)}$ (Å)     | 2.55 (2.51) | 2.97 (2.47) | 2.99 (2.47) |
| $d_{Mn-Mn (AFM)}$ (Å)    | 1.95 (2.51) | 2.71 (2.47) | 2.83 (2.47) |

Mn-dimers

Double Mn substitutions on two nearest-neighbouring Ge sites are of particular interest, since they are inferred to occur at experimental growth conditions leading to nucleation of Mn-precipitates. In addition,
they might be also detrimental for the magnetic ordering, since dimers show antiferromagnetic (AFM) coupling with no net spin moment. Unfortunately, GGA-based calculations are not entirely conclusive, since the dimer configuration becomes stable at a too small bond-length (1.95 Å) not compatible with the Mn ionic radius (≃ 1.1-1.3 Å) or bond distances in Mn-Ge compounds. Thus, published results [48, 49] often refer to the ideal unrelaxed structure which, of course, strongly overestimates the heat of formation of the dimer. From the results reported in Tab. I, assuming thermodynamic equilibrium, we can comment on the relative concentration of single substitutional sites and dimers. At thermodynamic equilibrium, the concentration $c$ of a defect with $n_\text{Mn}$ Mn atoms is roughly proportional to $e^{(-\Delta H/v_\text{Mn} \Delta \mu_\text{Mn})/k_B T}$ where $\Delta H$ is the formation energy, $k_B$ the Boltzman constant, and $T$ the temperature. Supposing $\Delta \mu_\text{Mn} \approx 0$ eV (thermodynamic equilibrium with $\alpha$–Mn), the probability of finding a substitutional Mn or dimer is $e^{-0.9/k_BT}$ and $e^{-1.5/k_BT}$, respectively, i.e. monomers are more likely to form than dimers. More generally, for a specific $\Delta \mu_\text{Mn}$ the probabilities for single substitutions and dimers are,

$$e^{(-0.9+\Delta \mu_\text{Mn})/k_BT} \quad \text{and} \quad e^{(-1.5+2\Delta \mu_\text{Mn})/k_BT}.$$ 

Therefore the dimer concentration is larger than the monomer concentration only for $\Delta \mu_\text{Mn} > 0.6$ eV, i.e. at extremely Mn-rich conditions, where $\alpha$–Mn precipitates are anyway already preferred over the formation of monomers (or dimers). Although kinetic effects might well hinder the nucleation of larger precipitates, our calculated thermodynamics suggests a rather low dimer concentration. It is important to note, that the thermodynamic arguments alone, presented here, are not enough to fully discuss the relative probability of occurrence of the monomers with respects to dimers, as these systems are usually grown out of the thermodynamic equilibrium and kinetic effects may have an important role.

Finally, the stabilization energy of AFM over FM coupling of nearby impurities is much lower within HSE than GGA. Furthermore, for HSE (and DFT+U), the calculated Mn-Mn distance for both FM and AFM magnetic alignment, are in line with experiments — always reporting local lattice dilation — as well as in line with the Mn-Mn distances in the FM Mn$_2$Ge$_3$ compound (varying between 2.52 and 3.06 Å) [50, 52].

**CONCLUSIONS**

In summary, we have performed a comparative study of substitutional Mn$_x$Ge$_{1-x}$ by using PBE, PBE+U and HSE functional. The main focus is on the differences arising from three different treatments of the exchange-correlation term, namely the PBE, DFT+U, and HSE. As well known, the PBE treatment can not describe satisfactorily the ground state properties of the Mn in the host semiconductor matrix. Including the $U$ correction at DFT level improves the description. However, some differences still remain when compared to HSE. For example, the HSE Mn-$d$ peak position is found at $\sim -5$ eV with respect to the Fermi energy, i.e. in the same energy region as observed in photoemission experiments. [6] When using the DFT+U method and fixing the $U$ parameter in order to recover the experimental $d$-peak position, the hybridization with $p$ states around $-4$ eV is underestimated compared to HSE and the experimental photo-emission peak. [6] Furthermore for the same $U$, the half-metallic character is not predicted by DFT+U. The fact that HSE accurately describes the host semiconductor and, at the same time, the interaction of localized Mn states with the host valence states makes this functional a valuable approach for studying transition metal defects in semiconductors. It is also true that the HSE calculations are usually quite more computationally demanding with respect to DFT+U. Therefore, whenever
FIG. 3: (Color on line) HSE Density of states projected on the Mn impurity site (top panel) for Mn in Si. Labels as in Fig. 2. DFT+U, U = 6 eV (bottom panel).

a compromise between accuracy and computation effort is required in the calculations, a preliminary HSE study may be useful for choosing an appropriate $U$ value, which is often not accessible from experiments.

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