

***Ab initio* studies of magnetism in transition-metal-doped silicon carbide**

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Electronic properties of iron-doped 4H silicon carbide (SiC-Fe) are calculated using an *ab initio* full potential linearized augmented plane wave technique. Similar to what is known for iron and its alloys, it is found that volume dependencies of SiC-Fe crystal total energy are multiple valued. The two solutions found correspond to nonmagnetic and ferromagnetic configurations of iron atoms. Calculated densities of states demonstrate close to half-metallic spin polarization of iron bands in the SiC band gap in the latter case. A possibility of obtaining magnetic polarization in a state which is a mix of the magnetic and nonmagnetic configurations in SiC-Fe and other diluted magnetic semiconductor material systems is discussed.

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INTRODUCTION

In the new and fast-growing area of research and development referred to as spin electronics or spintronics, great expectations are placed on diluted magnetic semiconductors (DMSs). There is a hope that semiconductor devices using the spin of free carriers can be integrated into existing technology, giving the possibility of extending the functionality of traditional devices and creating totally new classes of devices.^{1,2} To date, the most extensively studied DMS material system is (Ga,Mn)As. Significant progress has been achieved in increasing the ferromagnetic ordering temperature in this material, and the Curie temperature of 173 K has been reported for thin layers of (Ga,Mn)As.^{3,4} This is, however, still too low for most practical applications. Recent mean-field model calculations of magnetic properties of tetrahedrally coordinated semiconductors by Dietl *et al.*^{5,6} predict above room temperature ferromagnetism in semiconductors consisting of lighter elements and with smaller lattice constants, due to reduced spin-orbit coupling and larger effective densities of states and concentration of magnetic impurities in these materials. The calculation results also demonstrate a tendency for an increase of the DMS Curie temperature as the semiconductor band gap width increases. A number of experimental reports qualitatively confirm the predictions of the Dietl theory.^{7,8}

Silicon carbide is a wide band gap semiconductor aimed at high-frequency and high-power applications, with the material technology matured to commercial device production.⁹ SiC exists in a large number of crystal lattice modifications or polytypes, with the value of the band gap ranging from 2.4 to 3.3 eV and varying material properties.¹⁰ Although the Dietl theory⁵ was not applied to studying magnetic properties of SiC, according to the trends and the underlying physics established by this theory, material properties of silicon carbide make it very promising for demonstrating high ordering temperatures.

Several reports have been published documenting experimental studies of magnetic properties of SiC with transition metal (TM) impurities. Syväjärvi *et al.*¹¹ reported ferromagnetism with the Curie temperatures $T_c \sim 160$ K in

sublimation-grown 4H-SiC doped with Mn in concentrations of up to 5%. Magnetic response was observed in a more heavily doped material, and was attributed to the formation of secondary phases. Theodoropoulou *et al.*¹² observed ferromagnetic ordering in Ni-, Mn-, and Fe-implanted 6H-SiC with T_c of 50, 250, and 270 K, respectively, for the peak concentration of 5% of substitutional TM atoms. Reduction of TM concentration to 3% was reported to result in a paramagnetic response. No secondary phases were found in the ion-implanted samples. Stromberg *et al.*¹³ performed an extensive study of 6H-SiC implanted with various doses of ⁵⁷Fe. The authors found the samples with the peak Fe concentration below 3% to exhibit DMS behavior, with the magnetic ordering disappearing above ~ 20 K. The magnetic response in the samples with Fe concentrations above 3% was determined to originate mostly from superparamagnetic Fe₃Si clusters.

While the Dietl theory establishes the general trends for obtaining magnetic ordering in DMS systems, a necessary condition for obtaining a ferromagnetic material is the existence of nonzero atomic magnetic moments. The electronic structure and magnetic properties of TM atoms depend strongly on their environment and the electronic properties of the host matrix. From studies of magnetism in Fe and other transition metals and their alloys, it is known^{14–18} that changes in lattice atomic configuration affect the magnetic moments of the atoms and can result in a transition from a nonmagnetic to a ferromagnetic state. Similar effects may be expected for TM atoms substituted in a semiconductor host. Optimizing material properties to obtain a large magnetic moment configuration is an important prerequisite for obtaining a high-temperature DMS. The existence of different SiC polytypes provides an additional flexibility in obtaining such an optimized material system.

A number of researchers studied the electronic structure and magnetic properties of SiC-transition-metal DMS material systems theoretically by using *ab initio* calculations. Gubanov *et al.*¹⁹ and Miao and Lambrecht²⁰ utilized the linear muffin-tin orbital (LMTO) technique to calculate substitution energies for a number of transition metal impurities in 3C-SiC. The researchers found that the Si site is more favor-

able compared to the C site for TM substitution. This result holds when lattice relaxation effects are taken into account in the full potential linear muffin-tin orbital (FP-LMTO) calculation. Both research teams found that Fe and Co were non-magnetic, while Cr and Mn possessed nonzero magnetic moments in the 3C-SiC host. Calculation of the magnetic moment in a relaxed supercell containing two TM atoms showed that both Mn and Cr atoms order ferromagnetically. Shaposhnikov and Sobolev²¹ obtained similar results for atomic magnetic moments of TM impurities in 3C-SiC using the full potential linearized augmented plane wave (FLAPW) calculation technique and no lattice relaxation procedure accounting for impurity substitution. The authors additionally studied magnetic properties of TM impurities in 6H-SiC, substituting for 2% or 16% of host atoms. It was found that on the Si site in 6H-SiC, Cr and Mn possessed magnetic moments in both concentrations, while Fe was magnetic only in the concentration of 2%. In a recently reported study,²² Miao and Lambrecht used the FP-LMTO technique with lattice relaxation to compare the electronic and magnetic properties of 3C- and 4H-SiC doped with early first row transition metals. Spin polarization was found to be present in V-, Cr-, and Mn-doped SiC. Ferromagnetic ordering was confirmed for Cr and Mn, while the magnitude and range of the magnetic interaction was very different for the two impurities.

Although significant research efforts have already been devoted to the theoretical and experimental investigation of TM-doped SiC and other DMS materials, the mechanisms responsible for the polarization and ordering in these materials are still far from being clear. In this paper, we present results of *ab initio* calculations of Fe-doped 4H-SiC, which is the most technologically important SiC polytype. In contrast to previous *ab initio* studies of this and similar material systems, we use a highly accurate FLAPW calculation technique and perform a complete, inhomogeneous structural relaxation of the SiC lattice with substitutional iron impurity. This allows us to obtain reliable results for the densities of states and unit cell volume dependencies of the crystal total energy, and also predict different magnetic configurations of transition metal impurity atoms. We analyze the influence of the local lattice environment on the electronic and magnetic properties of substitutional Fe atoms, and speculate on a possibility of obtaining spin polarization in a mixed magnetic configuration, thus attempting to explain the above reviewed discrepancies between experimental and theoretical data for SiC-Fe and suggesting a different approach to the problem of magnetic impurities in a semiconductor host.

METHODOLOGY AND COMPUTATIONAL DETAILS

The crystal lattice of any SiC polytype can be represented by a sequence of hexagonal close-packed silicon-carbon bilayers. Different bilayer stacking sequences correspond to different polytypes. For 4H-SiC, the stacking sequence is ABCB, where A, B, and C denote different hexagonal bilayers.¹⁰ The unit cell consists of four Si-C bilayers or eight atoms. Calculations of lattice parameters and electronic structure were first performed for pure 4H-SiC using a su-

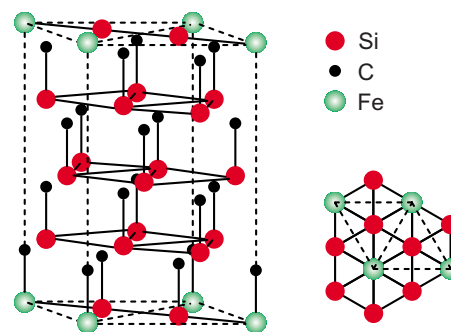


FIG. 1. (Color online) SiC-Fe superlattice used in the calculations (left) and in-plane Fe atom placement (right).

percell consisting of a total of 24 atoms. Then, lattice parameters, electronic structure, and magnetic properties were calculated for 4H-SiC with substitutional Fe atoms. Embedding impurity in the host 4H-SiC lattice was modeled in a supercell similar to the one we used for pure 4H-SiC, with one Si atom per supercell replaced by an Fe atom. The choice of the substitution site preference was made according to the atomic radii of the atoms, which are much closer for Si and Fe than for C and Fe. A much smaller lattice distortion is required in the case of Si site substitution. Results of prior *ab initio* calculations of the TM substitution site preference^{19,20} are in agreement with this intuitive approach.

The $\text{Si}_{11}\text{C}_{12}\text{Fe}$ supercell used in the calculations is presented in Fig. 1. Impurity atoms were placed in the centers of the adjacent close-packed hexagons, so that the distance between them equaled $\sqrt{3}a$. In the *c*-axis direction, the distance between Fe atoms was equal to one 4H-SiC lattice period (four Si-C bilayers). It should be noted that a close-packed cell of 4H-SiC contains inequivalent, the so-called hexagonal and cubic, bilayers differing in their local stacking sequence.¹⁰ The supercell we constructed places impurity atoms in the hexagonal bilayers. The substitution layer typically has a minor influence on the electronic structure (see, e.g., Ref. 22) and should not affect the general trends of atomic magnetic moment creation, which are discussed in this paper. The resultant impurity concentration calculated with respect to the total number of atoms was about 4%. This rather high concentration required for obtaining a diluted magnetic semiconductor behavior is much larger than a typical semiconductor device heavy doping of, say, 10^{19} cm^{-3} . In the present study, we do not consider these lower concentrations of transition metal impurities, which would be the limit of a “very diluted magnetic semiconductor.” In contrast to the latter case where TM impurity charge state could be varied by the position of the Fermi level, at the doping concentrations of several atomic percent, the localized impurity levels smear into impurity bands and by themselves determine the Fermi level position and the impurity charge state.

Another important consideration to note is that since Fe atoms placed in the corners of the supercell are essentially the same atom translated over the supercell vectors, the solution sought will automatically include ferromagnetic ordering, in case a nonzero magnetic moment is obtained on Fe atoms. This is convenient and sufficient to establish the

trends for obtaining spin polarization in the SiC-TM system. The investigation of TM atom magnetic moment ordering, which in a real DMS system can be achieved by different mechanisms such as direct or free-carrier-mediated interactions, is a subject of a separate study.

Electronic structure and magnetic properties of 4H-SiC were calculated using a self-consistent FLAPW technique implemented in the WIEN2K software package.^{23,24} The accuracy of this technique in band structure calculations, including the treatment of the effects of atomic orbital hybridization, structural relaxation, itinerant behavior, and magnetism, exceeds the accuracy of other commonly used *ab initio* techniques. The exchange-correlation potential was calculated using a generalized gradient approximation (GGA) according to the Perdew-Burke-Ernzerhof model.²⁵ Compared to local density approximation, GGA is expected to provide a more accurate description of the systems with abrupt electronic density changes. Atomic sphere radii were chosen such that the spheres had a single common point. It was determined that for the convergence of calculations, the minimum atomic radius for Si and Fe atoms had to be set to 2.0 a.u., which determined the atomic radius of carbon atoms equal to 1.52 a.u. The basis set required 125 plane waves per atom. Within the atomic spheres, lattice harmonics with angular momentum up to $l_{max}=12$ were used for wave function expansion, and with $l_{max}=6$ for the expansion of charge density and potential. In the interstitial volume, these quantities were represented by the Fourier series with a total of 850 harmonics. The calculation was performed for 500 reciprocal lattice points in the Brillouin zone. The parameters chosen provided iteration convergence with the total crystal energy error within 0.1 mRy.

RESULTS AND DISCUSSION

Lattice constants of undoped 4H silicon carbide were obtained by minimizing the crystal total energy as a function of the unit cell volume, which was varied by means of the isotropic expansion of the supercell. Exact values of the optimal lattice parameters and atomic positions were found using a complete, inhomogeneous relaxation procedure minimizing intracell forces. The calculated equilibrium cell volume of 71.31 a.u.³ per atom and positions of the atoms in the SiC cell correlate well with the experimental data.^{10,26} Calculated total and partial densities of states of pure 4H-SiC are presented in Fig. 2. 4H-SiC is an indirect band gap semiconductor, with the experimental value of the gap of approximately 3.2 eV. Our calculations yield a smaller band gap value of about 2.1 eV. A significant underestimation of the band gap values is known to be one of the problems of the density functional theory. Overall, the total and partial densities of states are very similar to the density of states spectra of pure 6H-SiC and 3C-SiC calculated using the FLAPW technique and presented in Ref. 21.

Next, we studied electronic properties of 4H-SiC with 4% of substitutional Fe atoms. Similar to pure SiC, we simulated the isotropic expansion of the lattice and calculated the unit cell volume dependencies of the crystal total energy of the SiC-Fe system. In order to fully account for the effects of

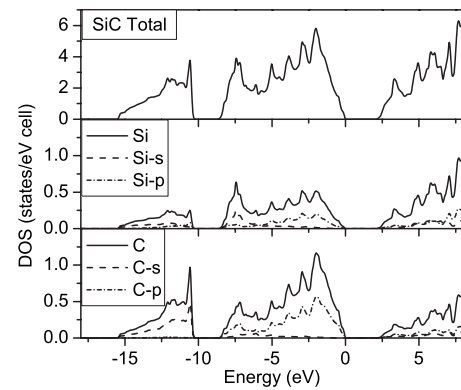


FIG. 2. Total and partial densities of states of undoped 4H-SiC. The energy axis origin is at the Fermi energy.

crystal lattice reconstruction and electronic structure changes caused by the substitution of Si atoms by Fe atoms, we again performed, together with the lattice expansion, a complete relaxation of the internal lattice forces and optimization of the atomic positions. As already mentioned, it is known from studies of the electronic structure of Fe and its alloys that, depending on the crystal lattice configuration and TM atom environment, different electronic and magnetic states may be realized for TM atoms.^{14–18} The unit cell volume or TM “atomic volume” dependencies of the total energy may not be single valued, representing multiple solutions corresponding to different electronic configurations and magnetic states of TM atoms. In these different states, TM atoms can be nonmagnetic or possess a nonzero magnetic moment which can depend on the atomic volume.

Crystal total energy as a function of the atomic volume averaged over all supercell atoms, and also as a function of the distance between Fe atom and C atom above it in the tetrahedron (cf. Fig. 1), is presented in Fig. 3. As can be seen from the plots, the total energy dependencies are multiple valued, similar to what is known for transition metals and alloys. The lower-energy curves in both plots represent a nonmagnetic solution, while the higher-energy curves correspond to the configuration in which Fe atoms possess a magnetic moment, which changes with atomic volume approximately linearly from about $2.95\mu_B$ to $3.1\mu_B$ per atom in the range of the plot. In the two configurations, the positions of

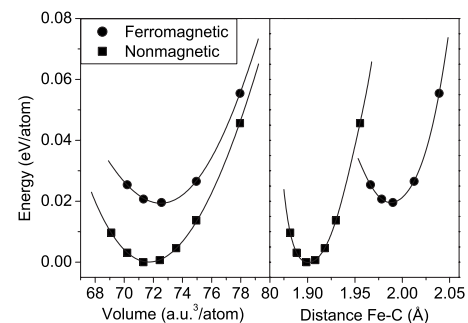


FIG. 3. Dependencies of the crystal total energy on (left) the average atomic volume and (right) the distance between Fe atom and C atom above it in the elemental tetrahedron.

the atoms, their electronic density (and thus, chemical bond structure), and the degree of orbital hybridization are different. It is important to note that the two solutions were not obtained in a constrained magnetic moment calculation. Rather, the calculations converge to the magnetic solution if starting from the sufficiently expanded lattice. The nonmagnetic solution is obtained in the lattice with the unit cell volume approximately corresponding to undoped SiC. Both volume dependency curves are obtained by using the solution at each volume value as the initial approximation for the next one. Thus, we let the calculations naturally follow the underlying physical phenomena.

It could be expected that electronic structure of Fe atoms will be affected strongly by the four C atoms forming the elemental tetrahedra around the Fe atoms. However, the carbon atoms above the Fe atoms were found to have the strongest influence on the electronic and magnetic configurations of Fe atoms. While almost no atomic relaxation was observed in the nonmagnetic case, in the high-spin configuration, the equilibrium distance (defined by the curve minima) between Fe atom and C atom above it in the tetrahedron is significantly increased, with the Fe atom staying practically in plane and the C atom moving about 0.1 Å away from it. On the other hand, the average atomic volume difference between the two cases is relatively small, indicating that only the tetrahedra including Fe atoms are distorted by the impurity substitution, and the atomic plane of C atoms above the impurity plane becomes “corrugated” due to the impurity substitution. The energy separation of the two solutions in equilibrium is about 0.02 eV, comparable to thermal energy at room temperature. It can be suggested that at a high enough temperature, the two configurations may exist concurrently, with a certain distribution of the TM atoms among them. A somewhat similar mixed state is realized in glasses where multiple unstable and easily thermally activated local atomic configurations exist. In these configurations, atoms can occupy with nearly equal probabilities one of the several quasiequilibrium positions, and there is a certain probability of tunneling transitions between these configurations.²⁷ Another analogy to the situation discussed here may be drawn with some transition metals and their alloys, where atomic configurations with different numbers of localized 3d electrons and collective 4s electrons both contribute to the crystal electronic structure, thus creating the overall noninteger magnetic moment system.²⁸

We should recall here that the calculated total crystal energy is a zero temperature ground state quantity. At a non-zero temperature, the free energy entropy term will contain contributions due to both atomic disorder of host and impurity atoms and, in the magnetic case, due to magnetic moment disorder (magnitude and direction). Per atom values of the entropy terms should be of about the same order of magnitude, as similar thermal disordering processes create the corresponding microscopic configuration sets. An estimate of the atomic disorder entropy term using standard molar entropy for hexagonal SiC of 16.5 J/mol K (Ref. 29) yields a room temperature entropy value of about 50 meV/atom. Thus, typical entropy values can be expected to be comparable to or exceed the difference in energy of 20 meV/atom we obtained for nonmagnetic and ferromagnetic configura-

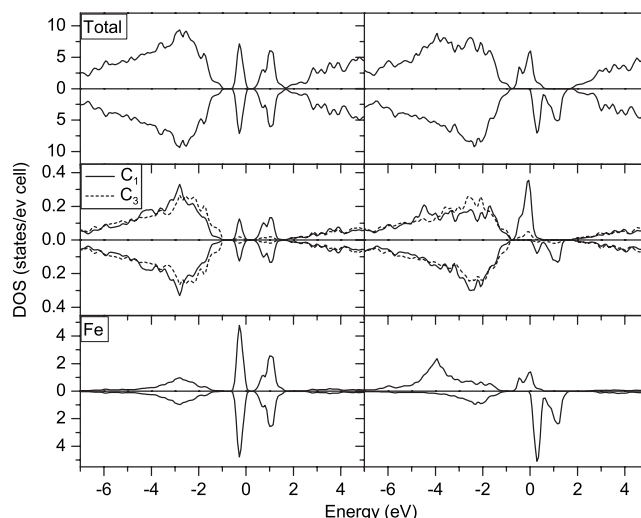


FIG. 4. Total and partial densities of states around the band gap of Fe-doped 4H-SiC for (left) nonmagnetic and (right) ferromagnetic configurations. C_1 denotes the carbon atom, which is above the Fe atom in the c direction, while C_3 denotes the other carbon atoms in the elemental tetrahedron. The energy axis origin is at the Fermi energy.

tions. Consequently, at a nonzero temperature, the relationship between the solutions can change, with the magnetic configuration becoming more energetically favorable.

In the present discussion, we concentrate only on the possibility of creating magnetic moments in SiC-Fe or a similar material system, which is a necessary condition for obtaining a DMS. Although one of the solutions obtained describes ferromagnetically ordered magnetic moments, it is important to keep in mind that, by construction, the SiC-Fe supercell used in the calculations assumes that atomic spins, if they exist, are aligned in parallel. If antiferromagnetic ordering is assumed, the corresponding solution could be lower or higher in energy, although, because a similar exchange energy term defines the density of states splitting in this case, on the energy scale, the antiferromagnetic solution should be close to the ferromagnetic one. In reality, a mixed state including both the antiferromagnetically and ferromagnetically ordered atoms may be realized. For transition metals other than Fe and for other host materials or SiC polytypes, the relationship between the nonmagnetic and magnetic solutions may be different. Further work is needed to investigate various problems related to magnetic moment ordering in SiC-based DMS, including competition between ordered and spin glass states, the exchange mechanisms, TM impurity and free carrier concentration dependencies, the relationships between temperatures at which the magnetic configuration can be realized with a reasonable weight and the corresponding ordering temperatures, etc. The competition between diluted impurity substitution and secondary phase formation also needs to be addressed.

Total and partial densities of states calculated for $\text{Si}_{11}\text{C}_{12}\text{Fe}$ supercell are presented in Fig. 4. Substitution of 4% of Si atoms in the SiC lattice with Fe atoms leads to an emergence of two impurity bands in the gap close to the valence band top (note the above mentioned incorrect den-

sity functional theory calculation of the SiC band gap). A significant degree of coupling is present between Fe $3d$ and C $2p$ orbitals, both in the range of energies corresponding to Fe bands in the gap and in the SiC valence band energy range. The hybridization is strong between Fe atoms and C atoms above them, while it decreases for the other C atoms in the tetrahedra, indicating that the Fe d -orbital electronic density is asymmetric with respect to the Fe–C bonds. In the case of magnetic Fe atoms, hybridization is stronger in the spin-up channel compared to the spin-down channel, further affecting the symmetry of the density of states corresponding to C atoms as well as the overall density of states. In the high-spin configuration, the Fermi level is pinned in the middle of the lower-energy Fe band, which is the spin-up band in this case. This band merges with the SiC valence band, which itself possesses some polarization due to the hybridization between C $2p$ and Fe $3d$ states in this energy range. The spin-down band is nearly empty and, thus, Fe bands in the gap possess close to 100% spin polarization at zero temperature in small electric fields. It should also be noted that in the nonmagnetic configuration, the density of states at the Fermi level is low. In fact, the gap between the Fe bands sets in at the Fermi energy. On the contrary, in the magnetic configuration, the density of states peaks at the Fermi level. These density of states features are consistent with the Stoner criterion for the existence of magnetism in the band magnetism model.

Analyzing the trends established by our calculations, we conclude that finding all solutions for the crystal total energy is very important, as multiple electronic configurations, representing different magnetic states of TM atoms, may exist. Performing a full structural optimization procedure is also a key for obtaining the correct lattice geometry, which has a defining influence on the electronic and magnetic properties of the DMS material (see also Ref. 22). It is not clear how the former consideration was taken into account in the prior *ab initio* calculations of TM-doped SiC and neither of the above reviewed studies of magnetic properties of Fe-doped SiC was performed with an account of the impurity-substitution-caused lattice reconstruction. This may explain the contradictions existing between the results of these calculations and the experimental data as well as the somewhat contradictory character of the results obtained by the authors for different SiC polytypes.^{12,20,21} From a practical standpoint, obtaining magnetic moments in SiC-based DMS may be achieved by doping in the process of crystal growth using, for instance, chemical vapor deposition or sublimation epitaxy. High temperatures involved in the crystal growth using these techniques result in the formation of significantly expanded lattices which can be favorable for the creation of a high-spin configuration of TM atoms. Ion implantation at elevated temperatures and high-temperature annealing can similarly be useful for obtaining the high-spin configuration. Additionally, implantation-induced lattice disorder and ex-

pansion may trigger the formation of the high-spin SiC-TM system. The exact thermal schedule used during the crystal growth or doping may play a key role in obtaining the needed material properties. Although additional work is needed to unambiguously characterize the DMS behavior in TM-doped SiC and exclude the possibility of detecting magnetism due to secondary phases, nevertheless, existing experimental data demonstrating ferromagnetism in Fe-implanted SiC make our expectations promising.

SUMMARY

Using a highly accurate *ab initio* FLAPW technique, we calculated the electronic structure of 4H-SiC with 4% of substitutional Fe atoms. Unit cell volume dependencies of the crystal total energy obtained in an optimized superlattice were found to be multiple valued, similar to what is known for iron and other transition metals and their alloys. The two solutions found correspond to nonmagnetic and ferromagnetic states of iron atoms, with the magnetic moment of $\sim 3\mu_B$ in the latter case. Not surprisingly, the electronic structure of Fe atoms was found to be affected strongly by the neighboring C atoms forming the elemental tetrahedra around the Fe atoms; however, the carbon atoms above the Fe atoms in the c direction were found to have the strongest influence on the electronic and magnetic configurations of Fe atoms. While the difference in the average equilibrium atomic volume between the two solutions is small, there is a noticeable stretching of the c -directed Fe–C bond in the magnetic configuration.

Although the equilibrium energy corresponding to the ferromagnetic configuration was found to be higher, the energy difference between the two configurations is comparable to the thermal energy at room temperature. We speculate on the possibility of creating a mixed state at nonzero temperatures while using standard SiC growth or doping techniques. Additionally, an estimate of free energy entropy terms shows that at temperatures close to room temperature, they become comparable to the difference between total energy values corresponding to the two solutions. The magnetic disorder term, which adds to the entropy in the magnetic configuration, can minimize or even reverse this difference. Further work is, however, needed to investigate the magnetic ordering processes and energy relationships between ordered and disordered states. Our prediction of the existence of the different magnetic configurations in iron-doped SiC (possibly overlooked in prior *ab initio* calculations for SiC-Fe DMS) suggests a different way of approaching the problem of creating a DMS using this material. Similar effects may take place in other TM-doped diluted magnetic semiconductors, and a careful analysis of possibly multiple-valued solutions for crystal total energy as well as accounting for the effects of lattice reconstruction caused by impurity substitution are required to find all electronic and magnetic configurations of a DMS material.

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