Ab initio determination of pseudospin for paramagnetic defects in SiC

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(Dated: September 26, 2019)

Point defects may introduce levels in the fundamental band gap of semiconductors or insulators that radically change the optical and magnetic properties of the host material. In particular, these point defects could be paramagnetic, i.e. the electron spin is greater than zero. The simplest case introducing paramagnetic electronic structure is the Kramers doublet (KD) electron spin state. In particular, neutral vanadium (V) \cite{1, 2} and singly positive charge state of molybdenum (Mo) point defects \cite{4, 5, 6} in hexagonal SiC are identified as KD systems. Recently, highly anisotropic interaction with magnetic field governed by the corresponding $g$-tensors has been observed or tentatively proposed for these KD systems \cite{6, 7}, however the underlying physics has not been understood so far. Here we note that, although parallel component ($g_{∥}$) of $g$-tensor was thoroughly studied for V in 6H SiC by invoking crystal field theory, the emerging strong electron-phonon coupling is not included \cite{2, 8-11} or considered as minor effect \cite{1}. The strong anisotropy in $g$-tensor can be described by an effective Hamiltonian and pseudospins in which parameters cannot be predicted by applying simple models, and rather fitting procedure to known experimental data was applied. In order to identify and understand these spin-related phenomena and correct interpretation of experimental data, there is an urgent need to determine these spin-Hamiltonian parameters from first principles calculations.

In this Letter, we demonstrate that ab initio calculations can reproduce the anisotropy of the observed $g$-tensors for V and Mo defects in hexagonal SiC. We show that both electron-phonon coupling manifested as dynamic Jahn-Teller (DJT) effect \cite{12} and the character of the wavefunction will determine the pseudospin of the system, i.e. its interaction with the external magnetic field. We show that the complex interplay of electronic orbitals, phonons and spins results in reduced parallel ($g_{∥}$) and vanishing transverse ($g_{⊥}$) component. We discuss the relevance of our results in the light of realization of telecom wavelength solid state qubits.

Both transition metal (TM) atoms substitute a Si atom in the SiC lattice as found in earlier studies \cite{5, 13}. However, lattice structures of 4H and 6H polytypes offer inequivalent lattice sites implying $T_{\text{MSi}}$ ($\text{TM} = \{\text{Mo}^+, \text{V}\}$) defects to form two configurations, a hexagonal ($h$) and a quasicubic ($k$) one in 4H, and three configurations a hexagonal ($h$) and two quasicubic ($k_1, k_2$) ones in 6H SiC \cite{cf. Fig. 1(a)} all exhibiting $C_{3v}$ symmetry. However, $\text{Mo}^+_\text{Si}$ favors the $h$ site in hexagonal SiC as implied by earlier theoretical \cite{4} and experimental \cite{6} studies, and hence we consider only $\text{Mo}^+_\text{Si}(h)$ for further discussion. Notwithstanding, all defect configurations of $\text{V}_{\text{Si}}$ have been observed in previous PL studies in both 4H \cite{3} and 6H SiC \cite{1, 2, 8-11}. Recently, we have conclusively identified $\text{V}_{\text{Si}}$ configurations in 4H SiC \cite{3}, thus we restrict our study on $\text{V}_{\text{Si}}$ in this polytype for direct comparison to experimental data.

$T_{\text{MSi}}$ defects were embedded in a 576-atom 4H supercell and a 432-atom 6H supercell. For sampling the Brillouin-zone we used Γ-point which ensures the correct degeneracy of orbitals in $C_{3v}$ symmetry. Plane wave expansion of Kohn-Sham wavefunctions with a cutoff of 420 eV was applied as a natural choice for supercell-method. Relaxed geometries were achieved by minimizing the total energy with respect to the coordinates of the ions where the corresponding quantum mechanical forces are prescribed to fall below 0.01 eV/Å. We treated the core electrons within the framework of Projector Augmented Wave (PAW) method \cite{14} as implemented in the VASP code \cite{15}. In order to compute the spin-orbit (SO) sublevels in the ground state we employed noncollinear approach \cite{16} with fixed spin quantization axis along the crystal axis ($c$-axis), where the geometry was fixed in $C_{3v}$ configurations as obtained from spinpolarized calculations. We employed density functional theory (DFT) to calculate the electronic structure within the hybrid-DFT + $V_w$ scheme introduced by Ivády \textit{et al.} \cite{17, 18}. For the corresponding $w$ values in the ground state we found $w_{\text{Mo}} \approx 0$ eV for $\text{Mo}^+_\text{Si}$ \cite{4} and $w_{\text{V}} = 2.2$ eV for $\text{V}_{\text{Si}}$ \cite{3}.

Both $\text{TM}_{\text{Si}}$ defects introduce spin doublet ($S = \frac{1}{2}$),
i.e. KD ground state is formed by a single electron residing on a degenerate in-gap e level. In addition, higher-energy empty a1 and e levels also occur in the band gap as plotted in Fig. 1(b), however their energy order is site dependent, i.e. a1(0)e(0) for TMSi(h) and e(0)a1(0) for TMSi(k) as already reported in Ref. 3. As a result the all-electron wavefunction transforms as \{E_2, E_2\} representations in the C_3v, double group notation [cf. Fig. 1(c)]. The hybrid-DFT calculations imply that \(E_2^+\) to be the lower and \(E_2^-\) to be the upper SO sublevel in the ground state manifold for each defect as depicted in Fig. 1(c). All in-gap one-electron levels exhibit closely atomic-like d-orbital character, thus the symmetry of the KD wavefunction may be determined by the atomic KD states for each TMSi as constructed from d-orbitals (see Table I) [6]. For instance, the lower SO sublevel is established by the linear combination of \(\Psi_2\) and \(\Psi_3\) as \(E_2^\pm = \frac{1}{\sqrt{2}} (\alpha \cdot \Psi_2 + \beta \cdot \Psi_3)\).

In this work, we aim to reveal the pivotal role of shape defects in both 4H and 6H SiC. In the Electronic structure introduced by the TM defects and the corresponding single and double group irreducible representations under C_3v symmetry. We give widespread notations for double group irreducible representations (irreps).

| labels | orbitals | single | double |
|--------|----------|--------|--------|
| \(\Psi_1\) | \([d_{+2}, +\frac{1}{2}]; [d_{-2}, -\frac{1}{2}]\) | \(^2E\) | \(E_2^+ (\Gamma_4)\) |
| \(\Psi_2\) | \([d_{+2}, -\frac{1}{2}]; [d_{-2}, +\frac{1}{2}]\) | \(^2E\) | \(E_2^- (\Gamma_5, 6)\) |
| \(\Psi_3\) | \([d_{+1}, +\frac{1}{2}]; [d_{-1}, -\frac{1}{2}]\) | \(^2E\) | \(E_2^- (\Gamma_5, 6)\) |
| \(\Psi_4\) | \([d_{+1}, -\frac{1}{2}]; [d_{-1}, +\frac{1}{2}]\) | \(^2E\) | \(E_2^+ (\Gamma_4)\) |
| \(\Psi_5\) | \([d_{0}, +\frac{1}{2}]; [d_{0}, -\frac{1}{2}]\) | \(^2E\) | \(E_2^- (\Gamma_4)\) |

In the expression of \(\hat{H}_{SO}\) (Eq. 1) \(\hat{L}_z\) and \(\hat{S}_z\) are the z-components of the spin and angular momentum operators, \(\hat{S}\) and \(\hat{L}\), respectively, \(\lambda_0\) is the SO constant and \(p\) stands for the so-called Ham reduction factor [12, 19] arising from the electron-phonon coupling. HF interaction is definitely active because of the presence of the impurity atom with non-zero nuclear spin. In the HF Hamiltonian \(\hat{I}\) is the nuclear spin operator and \(\hat{A}\) is the HF tensor which can be separated into a Fermi-contact and a dipolar spin-spin interaction where the latter can rotate the electron spin because of the spin ladder operators \((\hat{S}^+\hat{S}^- + \hat{S}^\dagger\hat{S})\). The formula of \(\hat{H}_{Zee}\) (Eq. 1) \(\hat{B}\) represents the external magnetic field and the dipole moment operator \(\hat{\mu}\) can be expressed as

\[
\hat{\mu} = -\left(\mu_B \rho \hat{\mathbf{L}} B + \mu_B g_0 \hat{\mathbf{S}} \mathbf{B}\right) = -\mu_B \hat{\mathbf{g}} \hat{\mathbf{S}},
\]

where the contributions of \(\hat{\mathbf{L}}\) and \(\hat{\mathbf{S}}\) are separated [20] and \(\hat{\mathbf{g}}\) is also expressed in the phenomenological pseudospin (\(\hat{\mathbf{S}}\)) formalism [21], where \(\hat{\mathbf{S}} = \frac{1}{2} \hat{\mathbf{S}}\) for KD systems [22]. In Eq. 2 \(\mu_B\) is the Bohr magneton, \(g_0\) is the free electron spin \(g\)-factor and \(r\) represents the Stevens orbital reduction factor [23]. From Eq. 2 parallel \((g_\parallel)\) and transverse \((g_\perp)\) components of the g-tensor \((\hat{\mathbf{g}})\) can be expressed as

\[
g_\parallel = 2(g_0 S_z + L_{eff}^z) = \frac{2\mu_z}{\mu_B},
\]

\[
g_\perp = \frac{\mu_+ + \mu_- + i(\mu_- - \mu_+)}{\mu_B},
\]

where we use expectation values of the ladder dipole moment operators \((\mu_{\pm})\) to express \(g_\perp\) (Eq. 4) [6]. In Eq. 3 \(S_z\) and \(L_{eff}^z\) are expectation values of \(S_z\) and the effective angular momentum operator, \(L_{eff}^z = p\hat{L}_z\), respectively.

 foremost, we calculate \(g_\parallel\) based on Eq. 3 via obtaining \(L_{eff}^z\) arising from the double reduction of the atomic angular moment, \(L_z\). To this end, first we consider the emerging strong electron-phonon coupling for calculating \(p\), then we derive the orbital reduction factor \((r)\) from \textit{ab initio} parameters of the wavefunction. Finally, we determine \(g_\parallel\) according to Eq. 4.

Electronic structure introduced by the TMSi defects

\[\text{Figure 1. (a) Employed 4H (left) and 6H (right) SiC supercells in orthographic view embedding a TM atom at a Si(h) site. Crystal axis (c-axis), bilayer structures and labeling of atoms are indicated. (b) One-electron structure and (c) splittings in d-orbitals of TMSi(h) defects in both 4H and 6H SiC. In the level structure of TMSi(k) defects order of \(a^*_1\) and \(e^*\) levels are reversed and hence \(^2A_1\) and the upper \(^2E\) levels are also swapped. Energy of SO splittings in the ground and excited states are denoted by \(E_{SO}^G\) and \(E_{SO}^E\), respectively.}\]
by the Hamiltonian \( H_{\text{JT}} \) and Ham reduction factor \( (p) \). Intrinsic (reduced) SO splitting energies \( (E_{\text{SOC}}^{\text{red}}) \) are also presented. Coefficients of \( \Psi_2 \) and \( \Psi_3 \) along with orbitally reduced (effective) angular momenta \( (L_{\text{eff}}^z) \) are also provided for ground state of Mo\( _6^\text{Si}(h) \) and V\( _\text{Si} \) in 4H and 6H SiC.

Table II. Parameters of the corresponding quadratic DJT APES \( (E_{\text{JT}}, \delta_{\text{JT}}) \) allowing the calculation of the effective phonon energy \( (\hbar \omega) \) and Ham reduction factor \( (p) \). Intrinsic (reduced) SO splitting energies \( (E_{\text{SOC}}^{\text{red}}) \) are also presented. Coefficients of \( \Psi_2 \) and \( \Psi_3 \) along with orbitally reduced (effective) angular momenta \( (L_{\text{eff}}^z) \) are also provided for ground state of Mo\( _6^\text{Si}(h) \) and V\( _\text{Si} \) in 4H and 6H SiC.

| Defect | Polytype | Site | \( E_{\text{JT}} \) (meV) | \( \delta_{\text{JT}} \) (meV) | \( \hbar \omega \) (meV) | \( p \) | \( E_{\text{SOC}} \) (GHz) | \( E_{\text{SOC}}^{\text{red}} \) (GHz) | \( \alpha \) | \( \beta \) | \( L_z \) | \( L_{\text{eff}} \) |
|--------|----------|------|-----------------|-----------------|-----------------|-------|-----------------|-----------------|-----|-----|------|------|
| Mo\( _6^\text{Si} \) | 4H | \( h \) | 17.1 | 4.5 | 56.27 | 0.46 | 198.28 | 91.88 | 0.572 | 0.820 | -0.324 | -0.15 |
| | 6H | \( h \) | 19.2 | 6.6 | 46.86 | 0.55 | 522.29 | 287.74 | 0.578 | 0.816 | -0.340 | -0.19 |
| V\( _\text{Si} \) | 4H | \( h \) | 9.4 | 5.6 | 60.19 | 0.63 | 9.91 | 6.29 | 0.571 | 0.821 | -0.321 | -0.203 |
| | 6H | \( k \) | 13.1 | 7.1 | 49.81 | 0.55 | 819.21 | 490.37 | 0.525 | 0.851 | -0.199 | -0.109 |

Figure 2. Schematic illustration of a general quadratic DJT APES, where \( Q_{x/y} \) denote the configurational coordinates. Trivial points and energy separations between them are indicated. \( C_{1h}(\text{min}) \) represents the three global minima separated by three barriers denoted by \( C_{1h}(\text{barrier}) \).

(cf. Fig. 1(b)), i.e. the half-filled orbitally degenerate \( e \) level may split by coupling with \( e \) phonon modes as manifestation of \( E \otimes e \) JT effect \([12, 19]\). Experimental results imply no symmetry reduction thus dynamic JT (DJT) is expected for these systems \([3, 6]\). To estimate the magnitude of DJT effect originating from the electron-phonon coupling we calculated the trivial points of the quadratic DJT adiabatic potential energy surface (APES) \([12]\), i.e. the three minima \( (C_{1h}) \), the three barrier \( (C_{1h}) \) and the high symmetry \( (C_{3v}) \) points. Energy separation between the \( C_{3v} \) and the three minima is the JT energy \( (E_{\text{JT}}) \), while barrier points are separated by the barrier energy \( (\delta_{\text{JT}}) \). A general quadratic DJT APES is shown in Fig. 2. As a result angular momentum might be severely reduced by the persisting DJT effect known as Ham effect \([12, 19]\) resulting in the reduction of the spin-orbit coupling (SOC) and the \( g \)-tensor elements. Reduction can be expressed as \( pL \), where \( p \) is the already introduced Ham reduction factor. For calculation of \( p \) corresponding APES have to be determined as described by the Hamiltonian \([12]\) of

\[
\hat{H}_{\text{DJT}} = \frac{\hbar}{2}\sum_{nm}(\hbar a_{x}^\dagger a_{x}^\gamma + \hbar a_{y}^\dagger a_{y}^\gamma + 1) + F(x\sigma_{z} + y\sigma_{x}) + G[(x^2 - y^2)\sigma_{z} + 2xy\sigma_{x}],
\]

where \( a_{x}^\dagger \) represent annihilation (creation) operators of two-dimensional \( e \) modes in the \( xy \) plane and electrons are represented by the Pauli matrices \( \sigma_{x} \) and \( \sigma_{z} \).

In Eq. 5, \( \hbar \omega \) stands for the effective energy of the \( e \) modes, while \( F = \sqrt{E_{\text{JT}}^2 - 2\hbar \omega} \) and \( G = \delta_{\text{JT}}\hbar \omega/2E_{\text{JT}} \) govern the linear and quadratic nature of the APES, respectively. In this way all parameters in DJT Hamiltonian can be directly readout from the corresponding APES enabling the numerical solution of Eq. 5 and yet the determination of the polaronic wavefunctions that can be obtained in the form of

\[
|\Psi_\pm\rangle = \sum_{nm}(c_{nm}|E_{\pm}^z\rangle \otimes |n,m\rangle + d_{nm}|E_{\mp}^z\rangle \otimes |n,m\rangle).
\]

In Eq. 6 \( E_{\pm}^z \) represents the complex components of the \( ^2E \) ground state mixed by the vibronic wavefunctions of \( |n,m\rangle \), where \( n + m \leq 10 \) basis set provides convergent \( |\Psi_\pm\rangle \). In this way mixing coefficients of \( c_{nm} \) and \( d_{nm} \) can be calculated that enables us to determine \( p \) via the formula of

\[
p = \sum_{nm}(c_{nm}^2 - d_{nm}^2)
\]

as derived and implemented by Thiering et al. \([20]\). The corresponding calculated values of \( E_{\text{JT}}, \delta_{\text{JT}} \) and \( p \) are listed in Table II.

We also report the corresponding ground state intrinsic and reduced SO splittings \( (E_{\text{SOC}}) \) in Table II as obtained by our calculations. Reduced SOC can be calculated as

\[
E_{\text{SOC}}^{\text{red}} = pE_{\text{SOC}} = p\lambda_0\langle\hat{L}_z\hat{S}_z\rangle,
\]

where \( E_{\text{SOC}}^{\text{red}} \) stands for the intrinsic (reduced) SOC energy, \( \lambda_0 \) is the intrinsic SOC constant and \( \langle\hat{L}_z\hat{S}_z\rangle \) represents the expectation value of the \( \hat{L}_z\hat{S}_z \) product where \( \hat{L}_z, \hat{S}_z \) is the \( z \)-components of angular momentum \( (L) \) and spin operator \( (S) \), respectively. Here we note that SOC energies provided in Table II are highly sensitive for the cell size and hence values of \( E_{\text{SOC}}^{\text{red}} \) should be treated with caution. In this way, the larger \( E_{\text{SOC}} \) for Mo\( _6^\text{Si}(h) \)
in 6H SiC than that in 4H SiC might be attributed to the relatively small supercell size. Notwithstanding, in case of VSi calculated values of $E_{\text{SOC}}$ are in good agreement with the previously reported experimental ground state values as $\sim 540$ GHz for VSi(k) and $< 40$ GHz for VSi(h) [3]. Nevertheless, these results implied that character of the SO sublevels is well-described by our method which is pivotal for determining g-tensors.

In order to account for the orbital reduction, the factor of $r$ was introduced by Stevens et al. [23] and hence the orbitally reduced angular momentum takes the form of $L'_z = rL_z$. Similar quenching effect appears for the investigated TM$_{\text{Si}}$ defects in 4H and 6H SiC arising from mixing of certain atomic KD states constituting the SO sublevels under $C_{3v}$ symmetry. In this way, orbitally reduced part of $L_z$ ($L_z^o = rL_z$) can be directly determined (cf. Eq. 9) from SO calculations by analyzing the mixing coefficients of $d$-orbitals participating in the SO sublevels. Expectation values of effective angular momentum can be calculated using these coefficients as

$$L_z^o = \alpha L_z^{\Psi_2} + \beta L_z^{\Psi_3},$$

where $L_z^{\Psi_2} = -2$ and $L_z^{\Psi_3} = +1$. Calculated values of $L_z^o$ are provided in Table II. Values of $\alpha$ and $\beta = \sqrt{1 - \alpha^2}$ were determined based on hybrid-DFT calculations (see Table II).

At this point we are ready to calculate $g_{\parallel}$ according to Eq. 3: values are included in Table III. We find good agreement between the trends of the calculated and that of the experimental $g_{\parallel}$ values for TM$_{\text{Si}}(h)$ defects in 4H SiC.

For the calculation of $g_{\perp}$ (Eq. 4), we determined the corresponding matrix elements of the ladder magnetic dipole operator as

$$\mu_{\pm} = \frac{1}{2} (\alpha \cdot \Psi_2 + \beta \cdot \Psi_3) | \mu_{\perp} | \alpha \cdot \Psi_2 + \beta \cdot \Psi_3 \rangle.$$ (10)

$\mu_{\perp}$ can couple state $|m_j\rangle$ to state $|m_j \pm 1\rangle$, where $m_j = m_l + m_s$, however $m_j^{\Psi_2} = -\frac{3}{2}$ and $m_j^{\Psi_3} = +\frac{3}{2}$ and hence cannot be coupled to each other and therefore $g_{\perp} = 0$ (cf. Table III) in each case. Here we note that second order contributions to $g_{\perp}$ might occur by mixing $\Psi_2$ or $\Psi_3$ with $\Psi_5$, since $\langle \Psi_5 | \mu_{\perp} | \Psi_5 \rangle \neq 0$. Coupling of states $\{\Psi_2, \Psi_3\}$ and $\Psi_5$ may occur vibronically or by the hyperfine interaction. Experimental ground state HF parameters are available in the literature which are around 15-70 MHz for Mo$_{\text{Si}}^+$ in 6H SiC [7]; 160-230 MHz for VSi(h) and 100-190 MHz for VSi(k) [24] in 4H SiC. HF will mix the corresponding wavefunctions only in the second order, thus it is expected that the final $g_{\perp}$ factor will be at least two orders of magnitude smaller than that of $g_{\parallel}$.

Our results have implications on quantum information processing based on solid state defect qubits. It has been proposed [3, 6] that Mo and V dopants in SiC with optical transitions near or inside telecom wavelength bands make possible to integrate these solid state qubits to telecommunication technology. Indeed, all-optical identification and coherent control of ensemble Mo center have been realized [6]. Parallel to our study, vanadium defects have been isolated and coherent control of single spins have been demonstrated with showing all the ingredients required for a highly efficient spin-photon interface [24]. Our study shows the nature of the ground state spin of these systems, namely, the order of spin levels and the origin of zero-field-splitting. This knowledge is crucial in optimizing the quantum optics protocols. Our results reveal the microscopic mechanism behind the phenomena of giant anisotropy in the interaction of the electron spin with the external stray magnetic fields which is only observable in the parallel component but minor in the transverse components.

In summary, we carried out hybrid-DFT calculations in order to reveal microscopic origin behind the highly anisotropic magnetic properties of KD systems as observed in experiments [6]. To this end, we shed light on the ground state electronic structure and we addressed the ground state SO sublevels as superposition of KDs by hybrid DFT calculations. From the spin Hamiltonian we derived $g_{\perp}$ and $g_{\parallel}$ (Eqs. 3 and 4) and found good agreement between the known experimental and calculated values for Mo$_{\text{Si}}^+$ supporting the significant role of electron-phonon coupling and character of the wavefunction in evolving the interaction of the electron spin with the magnetic field. We also note that calculated values for VSi(h) and (k) defects in 4H SiC exhibit a slightly different trend than was reported in experiments [1, 24]. However, the data at (h) and (k) configurations were taken at very different experimental conditions, methods and samples. The exact values might be reexamined in future focused experimental studies.

The support from ÚNKP-18-3-I New National Excellence Program of the Ministry of Human Capacities of Hungary is acknowledged by A. Cs. A. G. acknowledges the Hungarian NKFIH grants No. KKP129866 of the National Excellence Program of Quantum-coherent

| Defect Polyt. Site | Experiment | Theory |
|-------------------|------------|--------|
| Mo$_{\text{Si}}^+$ |            |        |
| 4H                | $g_{\parallel}$ | 1.87±0.2$^a$ | 1.70 |
|                   | $g_{\perp}$  | 0.04±0.04$^a$ | 1.63 |
| V$_{\text{Si}}$   | $g_{\parallel}$ | 1.870$^b$ | 1.595 |
|                   | $g_{\perp}$  | 1.748$^c$ | 1.781 |

$^a$ Ref. [6]  
$^b$ Ref. [24]  
$^c$ Ref. [1]
materials project, No. 127902 of the EU QuantERA Nanospin project, EU H2020 Quantum Technology Flagship project ASTERIQS (Grant No. 820394), the NVKP project (Grant No. NVKP_16-1-2016-0043) as well as the National Quantum Technology Program (Grant No. 2017-1.2.1-NKP-2017-00001).

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