The \((e_g \otimes e_u) \otimes E_g\) product Jahn-Teller effect in the neutral group-IV–vacancy quantum bits in diamond

Gergö Thiering\textsuperscript{1,2} and Adam Gali\textsuperscript{1,2,\dagger}

\textsuperscript{1}Wigner Research Centre for Physics, Hungarian Academy of Sciences, PO Box 49, H-1525, Budapest, Hungary
\textsuperscript{2}Department of Atomic Physics, Budapest University of Technology and Economics, Budafoki út 8., H-1111 Budapest, Hungary

Product Jahn-Teller (pJT) effect may occur for such coupled electron-phonon systems in solids where single electrons occupy double degenerate orbitals. We propose that the excited state of the neutral \(XV\) split-vacancy complex in diamond, where \(X\) and \(V\) labels a group-IV impurity atom and the vacancy, respectively, is such a system. We develop and apply \textit{ab initio} theory to quantify the strength of electron-phonon coupling for neutral \(XV\) complexes in diamond for \(X=\text{Si}, \text{Ge}, \text{Sn}, \text{Pb}\) and find an \((e_g \otimes e_u) \otimes E_g\) pJT solution. Our results show good agreement with recent experimental data on the prospective \(\text{SiV}(0)\) quantum bit, and reveals the complex nature of the excited states and the corresponding optical properties.

Fluorescent, paramagnetic point defects in diamond may realize quantum bits for quantum technology. Split-vacancy complexes of group-IV impurity atom (\(X=\text{Si}, \text{Ge}, \text{Sn}, \text{Pb}\)) and vacancy, i.e., \(XV\) defects with \(D_{3d}\) symmetry are in the focus of intense research. The negatively charged \(XV\), i.e., \(XV(−)\) defects have \(S = \frac{1}{2}\) spin state and fluoresce mostly in the visible [1–11]. The inversion symmetry of the centers assumes virtually no Stark-shift in the optical signals that is prerequisite for realization of indistinguishable single photon sources. Among these color centers, \(\text{SiV}(−)\) is the most studied [2, 4, 5, 12–22], and stands out with a large Debye-Waller (DW) factor of 0.7, and the demonstration of quantum communication and sensor applications [12, 13]. On the other hand, the \(\text{SiV}(−)\) exhibits short spin coherence times due to phonon dephasing caused by the dynamic Jahn-Teller effect on the orbital doublet [18], thus cooling to the millikelvin regime is required for quantum bit operations [23, 24]. It is predicted that \(\text{PbV}(−)\) might have much longer spin coherence times because of the enlarged gap of the orbital doublet caused by spin-orbit interaction but with the expense of smaller Debye-Waller factor than that of \(\text{SiV}(−)\) [25].

Alternatively, by removing an electron from \(XV(−)\) centers, an orbital singlet with \(S = 1\) ground state appears [2, 26–29] that should have intrinsically long coherence times. Recently, it has been demonstrated that \(\text{SiV}(0)\) exhibits spin coherence time almost up to a second and relaxation time nearly a minute [30] at 20 K together with a near-infrared fluorescence signal, and proposed for quantum communication applications [30]. This observation naturally shifts the focus towards \(XV(0)\) color centers in diamond. However, the nature of the excited and shelving states and levels are far from being understood for \(\text{SiV}(0)\) [31]. In particular, the 946-nm zero-phonon-line (ZPL) optical transition of \(\text{SiV}(0)\) (see Refs. 30, 32–36) was originally assigned to an \({^3}A_{2g} \leftrightarrow ^3A_{1u}\) electronic excitation from the ground state to the excited state [5, 34], however it has been very recently revealed that the excited state should be a \({^3}E_{g}\) state deduced from stress measurements [36]. Furthermore, a dark \({^3}A_{2u}\) state below the \({^3}E_{u}\) by 6.7 meV was activated in the luminescence spectrum by exerting uniaxial stress on the diamond sample [36]. The optical signals of other \(XV(0)\) centers have not yet been identified at all. First principles methods are major tools to explore the complex physics of point defects that can strongly contribute to understanding \(\text{SiV}(0)\) color center and identifying the other \(XV(0)\) color centers.

In this Letter, we present first principles results on the optical properties of \(XV(0)\) color centers in diamond. We show that the electrons and phonons are strongly coupled in the electronic excited states, and they constitute of a \((e_g \otimes e_u) \otimes E_g\) product Jahn-Teller (pJT) system, where \(e_g\) and \(e_u\) refers to the corresponding electronic orbitals, that are simultaneously coupled to the \(E_g\) symmetry breaking phonons. This pJT effect is responsible for the anomalous optical spectrum of \(\text{SiV}(0)\). We briefly discuss our results in the context of quantum technology applications. We provide the theoretical optical signatures of the other \(XV(0)\) color centers too.

We characterize \(XV(0)\) color centers by plane wave supercell calculations within spin-polarized density functional theory (DFT) as implemented in the \textsc{vasp} 5.4.1 code [37]. We determine the electronic structure within the Born-Oppenheimer approximation where the ions are treated as classical particles where the minimum energy is found by moving the atoms until the quantum mechanical forces acting on the ions fall below \(10^{−3}\) eV/Å. We embed the \(XV(0)\) defects in a 512-atom diamond supercell. The Brillouin-zone is sampled at the Γ-point. We applied an energy cutoff at 370 eV for expressing the plane wave basis set within the applied projector-augmentation-wave-method (PAW) [38, 39]. We calculate the excited states with the constrained-occupation DFT method (CDFT) [40]. We used HSE06 hybrid functional [41, 42] which reproduces the experimental band gap and the charge transition levels in Group-IV semiconductors within 0.1 eV accuracy [43]. For the electron-phonon coupling calculations of \(XV(0)\) defects, we ap-
ply the same machinery that could well reproduce the ZPL energies of XV(−) exhibiting dynamic Jahn-Teller effect [25], thus we expect similar performance for XV(0) too.

Electronic structure XV(0) defect has six carbon dangling bonds and the impurity atoms sits in the inversion center of diamond [see Fig. 1(c)]. These six dangling bonds introduce $a_{1g} \oplus a_{2u} \oplus e_u \oplus e_g$ orbitals [2, 5, 14, 29, 34]. The $a_{1g}$ and $a_{2u}$ levels fall in the valence band (VB) of the diamond [8]. The $e_u$ level is fully occupied with 4 electrons and it either resonant with the valence band or pops up in the gap by increasing $X$ atomic number [25]. The $e_g$ level is occupied two electrons in the band gap of diamond in the ground state. By promoting an electron from the $e_u$ orbital to the $e_g$ orbital (or forming a single hole on both orbitals), the lowest energy optically active and inactive excited states are formed. The 16 electronic configurations from these orbitals are

$$2E_u \otimes 2E_g = 3A_{2u} \oplus 3A_{1u} \oplus 3E_u \oplus 1A_{2u} \oplus 1A_{1u} \oplus 1E_u, \quad (1)$$

where we focus on the 12 dimensional triplet subspace.

The excited triplet two-hole wavefunctions and the $|3A_{2g}\rangle$ ground state can be expressed by the following (2) equations in the hole representation

$$|3A_{1u}\rangle = A \frac{1}{\sqrt{2}} \left( |e_{ux}e_{gy}\rangle - |e_{uy}e_{gx}\rangle \right)$$

$$|3E_{uy}\rangle = A \frac{1}{\sqrt{2}} \left( |e_{ux}e_{gy}\rangle + |e_{uy}e_{gx}\rangle \right)$$

$$|3E_{ux}\rangle = A \frac{1}{\sqrt{2}} \left( |e_{ux}e_{gx}\rangle - |e_{uy}e_{gy}\rangle \right)$$

$$|3A_{2u}\rangle = A \frac{1}{\sqrt{2}} \left( |e_{ux}e_{gx}\rangle - |e_{uy}e_{gy}\rangle \right) \otimes \left| \downarrow \downarrow \right\rangle, \quad (2)$$

$$|3A_{2g}\rangle = A |e_{gx}e_{gy}\rangle$$

where we introduce the anti-symmetrization operator $A(ab) = (ab - |ba\rangle)/\sqrt{2}$ and symmetrization operator $S(ab) = (ab + |ba\rangle)/\sqrt{2}$. It is worth to note that two singlet levels ($|3A_{1g}\rangle, |3E_{eg}\rangle$) from $e^2$ electronic configurations appear between the triplets, and the $(e_u,e_u)$ excited singlet levels of Eq. (1) are expected to lie above the excited triplets due to Coulomb repulsion [31, 36].

Product Jahn-Teller effect Hamiltonian Our DFT calculations indicate a strong Jahn-Teller distortion in the lowest energy triplet excited state of XV(0), going from the high $D_{3d}$ symmetry to the low $C_{2h}$ symmetry. This can be understood by inspection of the $e_g$ and $e_u$ orbitals, that are occupied by a single hole, thus they are both Jahn-Teller unstable. We concluded that the excited state shows a product Jahn-Teller effect. This can be seen by continuously rotating the $|e_u\rangle$ and $|e_g\rangle$ orbitals like a two dimensional vector $|e^2_x\rangle = \cos(\phi)|e_x\rangle + \sin(\phi)|e_y\rangle$ which leads to the expression of

$$|3A_{2u}\rangle = A |e_{ux}e_{gy}\rangle \otimes \{|\uparrow\uparrow\rangle, |\downarrow\downarrow\rangle, |\uparrow\downarrow\rangle\} =$$

$$\frac{1}{\sqrt{2}} |3A_{2u}\rangle + \frac{\cos(\phi)}{\sqrt{2}} |3E_{uy}\rangle + \frac{\sin(\phi)}{\sqrt{2}} |3E_{ux}\rangle, \quad (3)$$

that is like walking on the path of the yellow circle labeled by $|3A_{2u}\rangle$ in Fig. 1(a) which is a valid solution for the strongly coupled electron-phonon limit [44, 45]. The accurate solution can be found by solving the following Hamiltonian,

$$\hat{H} = \hat{H}_{osc} + \hat{H}_{pJT} + \hat{W}, \quad (4)$$

where $\hat{H}_{osc}$ is the two dimensional harmonic oscillator spectrum of the $E_g$ vibration mode, $\hat{H}_{pJT}$ is the the pJT Hamiltonian, and $\hat{W}$ is the electron correlation Hamiltonian between the triplet states in Eq. (2).

The usual $e \otimes E$ linear JT Hamiltonian [44–47] is modified to

$$\hat{H}_{pJT} = F_u \left( X \sigma_z \otimes \sigma_0 + Y \sigma_x \otimes \sigma_0 \right) + F_g \left( X \delta_0 \otimes \sigma_z + Y \delta_0 \otimes \sigma_z \right), \quad (5)$$

where $u/g$ label is responsible for the $e_u/e_g$ orbital. $\sigma_z$ and $\sigma_x$ are the standard Pauli matrices in Eq. (5). $\delta_0$ is the two dimensional unitary matrix which is introduced for the individual electron-phonon coupling strength $F_u$ and $F_g$. $(X,Y) = (a^\dagger_{X,Y} + a_{X,Y})/\sqrt{2}$ defines the two dimensional configuration space spanned by the $E_g$ vibration mode through the harmonic oscillator ladder operators. Finally, the energy splitting $\Lambda$ caused by static
electronic correlation is given by
\[ \hat{W} = \Lambda (|^3A_{1u}\rangle \langle ^3A_{1u}| - |^3A_{2u}\rangle \langle ^3A_{2u}|). \]

where we label the individual single determinant electronic wavefunctions for clarity. The diagonal part of the Jahn-Teller matrix is self-explanatory. If the geometry is distorted towards \(+X\), the \(|e_{ux}e_{gx}\rangle\) wavefunction would lower its energy, by a joint \(F_x + F_y\) coupling strength. In the central part of diagonal Hamiltonian, the two Jahn-Teller effects are destructive, and the joint product Jahn-Teller strength is \(F_x - F_y\). Next, the parameters in Eq. (7) are determined by first principles calculations, and the coupled electron-phonon Hamiltonian will be solved.

Results: We show the \textit{ab initio} parametrization of the full Hamiltonian for SiV(0), and discuss the results in detail. The key results are also summarized for the other XV(0) color centers in Table I as obtained by the same procedure. Our DFT \(\Delta\)SCF method yields the total energy of the four \(\mathcal{A}[e_{uy}e_{gy}], \mathcal{A}[e_{ux}e_{gy}], \mathcal{A}[e_{uy}e_{gx}], \mathcal{A}[e_{ux}e_{gx}]\) electronic configurations. The APES of these states is depicted in Fig. 2(a). In \(D_{3d}\) symmetry, \(E_{tot}[\mathcal{A}[e_{ux}e_{gy}]] = E_{tot}[\mathcal{A}[e_{uy}e_{gx}]]\) and \(E_{tot}[\mathcal{A}[e_{ux}e_{gx}]] = E_{tot}[\mathcal{A}[e_{uy}e_{gy}]]\), where \(E_{tot}\) is the total energy. The former and latter gives \(+0.5\Lambda\) and \(-0.5\Lambda\), respectively, that can be derived from Eq. (2). This yields \(\Lambda = 78.3\) meV for SiV(0).

The effective phonon energy \(\hbar \omega_E\) can be found by fitting to the parabola of the lowest APES curvature in Fig. 2(a) that results in 75.9 meV for SiV(0). The electron-phonon coupling \(F_y\) and \(F_x\) parameters can be derived by reading out the characteristic Jahn-Teller energies \(E_{JT}^{(1)}\) and \(E_{JT}^{(2)}\) in the APES [see Fig. 2(a)] as follows,
\[ E_{JT}^{(1)} = \frac{(F_g + F_u)^2}{2\hbar \omega_E}, \quad E_{JT}^{(2)} = \frac{(F_g - F_u)^2}{2\hbar \omega_E}. \]

In SiV(0), \(E_{JT}^{(1)} = 258\) meV, that is very significant and seriously affect the calculated ZPL energy. On the other hand, \(E_{JT}^{(2)} = 0.47\) meV which is small, and results nearly identical \(F_y\) and \(F_x\). We note here that we neglect the quadratic JT terms in Eq. (5), i.e., the APES in Fig. 2 is axially symmetric. However, the \(\mathcal{A}[e_{uy}e_{gy}]\) has a bit smaller JT energy than that of \(\mathcal{A}[e_{ux}e_{gx}]\) by 43, 46, 46, and 48 meV for SiV, GeV, SnV, and PbV, respectively, that would cause a quadratic JT effect. However, these energies are an order of magnitude smaller than that of \(E_{JT}^{(1)}\), and would only lead to minor correction to the results from linear JT approximation. Therefore, we still apply the linear JT approximation for the sake of simplicity.

Finally, all the parameters could be derived or read out from the calculated APES (see Table I), thus we can setup the full Hamiltonian in Eq. (7). It is intriguing to use \(X\) as a continuous variable at \(Y = 0\) in Eq. (7), and plot the solution in Fig. 2(b). The contribution of the dark \(^3A_{2u}\) state is shown by black balls, while the contribution of the optically active \(^3A_{1u}\) state (\(x\) polarization) and \(^3E_g\) state (\(xy\) polarization) is depicted as red and teal balls, respectively. The lowest energy solution will apparently involves the dark \(^3A_{2u}\) state. For the full quantum mechanical solution (where \(X\) and \(Y\) are operators) we use following wavefunction ansatz [25, 49, 50],
\[ |\Psi\rangle = \sum_{n,m} \left[ c_{n,m} |e_{uy}e_{gy}\rangle + d_{n,m} |e_{ux}e_{gy}\rangle + e_{n,m} |e_{uy}e_{gx}\rangle + f_{n,m} |e_{ux}e_{gx}\rangle \right] \otimes |n,m\rangle, \]
where \(|n,m\rangle\) is the representation of \(E_g\) phonons that we consider up to 15-phonon limit \((n + m \leq 15)\) for the low energy spectrum and up to 50-phonon limit for high energies in Fig. 2(c). The vibronic spectrum shows up two deep levels that are separated by \(\delta = 6.8\) meV, where the deepest level belongs to the vibronic \(^3A_{2u}\) and the second level is associated with the vibronic \(^3E_u\) in SiV(0).

We also show the derived parameters and results for GeV, SnV, and PbV systems in Table I. There is a clear trend that the ZPL energies increase with heavier impurity atom. On the other hand the spin-orbit coupling (SOC) will be significant for heavy impurity atoms, and rapidly increase with the atomic number of the impurity atom. Based on our previous calculations for XV(−) defects [25], the SOC on \(|e_u\rangle\) orbitals, \(\lambda_u\) is 7, 33, 100, and 250 meV for SiV, GeV, SnV, and PbV, respectively. This can be neglected for SiV(0) but can be significant for the other XV(0) defects. As a crude approximation,
FIG. 2. (a) Ab initio APES as obtained from Kohn-Sham DFT for SiV(0) where \( m_c \) refers to reduced mass of the vibration. The \( X = 0 \) point refers to the geometry relaxation in the constraint of \( D_{3d} \) symmetry. The global minimum in APES is obtained upon releasing all symmetry constraints that yields \( E_{JT}^{(1)} \) JT energy. We mapped the APES with linear interpolation between these two geometries. We mirrored the \( X > 0 \) results to \( X < 0 \) regions. We determined the \( E_{JT}^{(2)} \) energy by fitting quadratic polynomials on the data points. (b) Geometry dependence of eigenvalues of Eq. (7) by using \( X \) as continuous variable and \( Y = 0 \). We label the wavefunction character with colored balls. Red (teal) balls correspond to the pure \( |3^1A_{1u}\rangle (|3^1E_{u}\rangle) \) character that are optically active states. Black balls correspond to the pure \( |3^1A_{2u}\rangle \) character that is dark state. (c) The convergent polaronic eigenstates of Eq. (7) with color coded electronic characters and expectation value of the distortion \( \langle R \rangle \) from the \( D_{3d} \) symmetry. We show the lowest energy vibronic solutions and energy gap between them.

the calculated ZPL energies will be lowered by these energies that are shown in the “+ SOC” row in Table I. This can lead to a change in the order of ZPL energies of GeV(0) and SnV(0), that similarly occurs for GeV(−) and SnV(−) [25]. The simultaneous solution for pJT and SOC is out of the scope of this paper but might be required for the ultimately accurate description of the excited states of SnV(0), and PbV(0).

TABLE I. Calculated parameters of Eq. (7) and optical levels of \( XY(0) \) defects. The \( \delta \) is the energy difference between the \( |3^3A_{2u}\rangle \) and \( |3^3E_u\rangle \) states. We note that the data for SnV and PbV may be highly unambiguous, as the SOC and JT effects are on the same energy magnitude. We apply a crude correction for SOC in the ZPL energy (see text), and treated as a notification about our inaccuracy at the SnV(0) and PbV(0). The values inside the parenthesis are experimental data.

| \( h\omega \) (meV) | SiV | GeV | SnV | PbV |
|-----------------|-----|-----|-----|-----|
| \( \Lambda \) (meV) | 75.9 | 78.2 | 81.3 | 81.4 |
| \( E_{JT}^{(1)} \) (meV) | 258 | 242 | 217 | 194 |
| \( E_{JT}^{(2)} \) (meV) | 0.47 | 5.18 | 17.2 | 33.4 |
| \( F_\theta \) (meV) | 95 | 83 | 67 | 52 |
| \( F_\nu \) (meV) | 103 | 112 | 120 | 125 |
| ZPL\(|3^3E_u\rangle + SOC\) (eV) | 1.35 | 1.83 | 1.85 | 2.22 |
| \( \delta \) \(|3^3E_u \leftrightarrow 3^3A_{2u}\rangle \) (meV) | 1.35 (1.31\*) | 1.80 | 1.75 | 1.97 |
| \( \delta \) \(|3^3E_u \leftrightarrow 3^3A_{2u}\rangle \) (meV) | 6.7 (6.8\*) | 7.9 | 9.7 | 11.1 |

\( ^a \) exp. data from Ref. 34
\( ^b \) exp. data from Ref. 36

Discussion of SiV(0) properties Experimental data are only available for SiV(0), thus we can directly compare our results only to them. A recent stress measurement on the photoluminescence (PL) spectrum of SiV(0) revealed a dark state where the corresponding level was below the ZPL energy by 6.8 meV [36]. Our calculations explain this feature by the pJT effect of the three triplet excited states. The lowest energy branch of the excited state triplets yield \( \approx 50\% \) \( |3^3A_{2u}\rangle \) and \( \approx 50\% \) \( |3^3E_u\rangle \) electronic character that can be anticipated from Eq. (3). The lowest energy vibronic state is the dark \( |3^3A_{2u}\rangle \) (951 nm), and the next vibronic level above it by 6.7 meV belongs to the optically allowed \( |3^3E_u\rangle \) (ZPL of 946 nm). We note that in ordinary \( e \otimes E \) JT systems, a degenerate \( E \) level is the lowest vibronic state quickly followed a nondegenerate \( A \) vibronic level by tunneling splitting energy [44, 45, 51–53]. In our present pJT case, the order of these states are reversed, that is a clear signature of the symmetry of the pJT effect.

There are numerous consequences of this finding: (i) The optical polarization of the emitted phonons at the ZPL (946 nm) is perpendicular to the symmetry of the axis. (ii) The emission will be strain dependent as symmetry breaking strain can activate the 951-nm ZPL transition, again with photon polarization perpendicular to the symmetry axis of the defect. (iii) The 946-nm ZPL intensity will be temperature dependent, as it depends on the thermal occupation of the \( |3^3E_u\rangle \) over the lowest energy \( |3^3A_{2u}\rangle \). These properties were indeed observed in previous experiments [34, 36].

Summary We developed a theory for the excited state of
A. Sipahigil, R. E. Evans, D. D. Sukachev, M. J. Burek, J. Borregaard, M. K. Bhaskar, C. T. Nguyen, J. L.
Pacheco, H. A. Atikian, C. Meuwly, R. M. Camacho, F. Jelezko, E. Bielejec, H. Park, M. Lončar, and M. D.
Lukin, Science 354, 847 (2016).
[13] G. Kucsko, P. C. Maurer, N. Y. Yao, M. Kubo, H. J.
Noh, P. K. Lo, H. Park, and M. D. Lukin, Nature 500, 54 (2013).
[14] C. Hepp, T. Müller, V. Waselowski, J. N. Becker, B. Pingualt,
H. Sternschulte, D. Steinmuller-Nethl, A. Gali, J. R. Maze, M. Atature, and C. Becher, Physical Review
Letters 112 (2014), 10.1103/physrevlett.112.036405.
[15] T. Müller, C. Hepp, B. Pingualt, E. Neu, S. Gsell,
M. Schreck, H. Sternschulte, D. Steinmuller-Nethl,
C. Becher, and M. Atature, Nature Communications 5
(2014), 10.1038/ncomms3428.
[16] L. J. Rogers, K. D. Jahnke, M. H. Mutsch, A. Sipahigil,
J. M. Binder, T. Teraji, H. Sumiya, J. Isoya, M. D. Lukin,
P. Hemmer, and F. Jelezko, Physical Review Letters 113, 263602 (2014).
[17] L. J. Rogers, K. D. Jahnke, M. W. Doherty, A. Dietrich,
L. P. McGuinness, C. Müller, T. Teraji, H. Sumiya,
J. Isoya, N. B. Manson, and F. Jelezko, Physical Review
B 89, 235101 (2014).
[18] K. D. Jahnke, A. Sipahigil, J. M. Binder, M. W. Doherty,
M. Mutsch, L. J. Rogers, N. B. Manson, M. D. Lukin,
and F. Jelezko, New Journal of Physics 17, 043011 (2015).
[19] E. Neu, C. Hepp, M. Hauschild, S. Gsell, M. Fischer,
H. Sternschulte, D. Steinmüller-Nethl, M. Schreck,
and C. Becher, New Journal of Physics 15, 043005 (2013).
[20] J. Riedrich-Möller, C. Arend, C. Pauly, F. Mücklich,
M. Fischer, S. Gsell, M. Schreck, and C. Becher,
Nano Letters 14, 5281 (2014).
[21] B. Pingualt, J. N. Becker, C. H. H. Schulte, C. Arend,
C. Hepp, T. Godde, A. I. Tartakovskii, M. Markham,
C. Becher, and M. Atatiure, Phys. Rev. Lett. 113, 263601
(2014).
[22] A. Dietrich, K. D. Jahnke, J. M. Binder, T. Teraji,
J. Isoya, L. J. Rogers, and F. Jelezko, New Journal of
Physics 16, 113019 (2014).
[23] J. N. Becker, B. Pingualt, D. Groß, M. Günidoğan,
N. Kukharchyk, M. Markham, A. Edmonds, M. Atatiure,
P. Bushev, and C. Becher, Physical Review Letters 120
(2018), 10.1103/physrevlett.120.053603.
[24] D. Sukachev, A. Sipahigil, C. Nguyen, M. Bhaskar,
R. Evans, F. Jelezko, and M. Lukin, Physical Review
Letters 119 (2017), 10.1103/physrevlett.119.223602.
[25] G. Thiering and A. Gali, Phys. Rev. X 8, 021063 (2018).
[26] K. Iakoubovskii and A. Stesmans, physica status solidi
(a) 186, 199 (2001).
[27] A. M. Edmonds, M. E. Newton, P. M. Martineau, D. J.
Twitchen, and S. D. Williams, Phys. Rev. B 77, 245205
(2008).
[28] J. P. Goss, P. R. Briddon, M. J. Rayson, S. J. Sque,
and R. Jones, Physical Review B 72, 035214 (2005).
[29] J. P. Goss, P. R. Briddon, and M. J. Shaw, Physical
Review B 76 (2007), 10.1103/physrevb.76.075204.
[30] B. C. Rose, D. Huang, Z.-H. Zhang, P. Stevenson, A. M.
Tyrshikin, S. S. Sangtalesin, S. Srinivasan, L. Loudin,
M. L. Markham, A. M. Edmonds, D. J. Twitchen, S. A.
Lyon, and N. P. de Leon, Science 361, 60 (2018).
[31] B. C. Rose, G. Thiering, A. M. Tyrshikin, A. M. Edmonds,
M. L. Markham, A. Gali, S. A. Lyon, and N. P. de Leon,
arXiv preprint arXiv:1710.03196 (2017).
[32] L. Allers and A. T. Collins, Journal of Applied Physics
[33] C. M. Breeding and W. Wang, Diamond and Related Materials 17, 1335 (2008).
[34] U. F. S. D’Haenens-Johansson, A. M. Edmonds, B. L. Green, M. E. Newton, G. Davies, P. M. Martineau, R. U. A. Khan, and D. J. Twitchen, Phys. Rev. B 84, 245208 (2011).
[35] B. Green, S. Mottishaw, B. Breeze, A. Edmonds, U. D’Haenens-Johansson, M. Doherty, S. Williams, D. Twitchen, and M. Newton, Physical Review Letters 119 (2017), 10.1103/physrevlett.119.096402.
[36] B. Green, M. Doherty, E. Nako, N. Manson, U. D’Haenens-Johansson, S. Williams, D. Twitchen, and M. Newton, arXiv preprint arXiv:1804.09141 (2018).
[37] G. Kresse and J. Furthmüller, Phys. Rev. B 54, 11169 (1996).
[38] P. E. Blöchl, Phys. Rev. B 50, 17953 (1994).
[39] O. Bengone, M. Alouani, P. Blöchl, and J. Hugel, Phys. Rev. B 62, 16392 (2000).
[40] A. Gali, Phys. Rev. B 80, 241204 (2009).
[41] J. Heyd, G. E. Scuseria, and M. Ernzerhof, The Journal of Chemical Physics 118, 8207 (2003).
[42] A. V. Krukau, O. A. Vydrov, A. F. Izmaylov, and G. E. Scuseria, The Journal of Chemical Physics 125, 224106 (2006).
[43] P. Deák, B. Aradi, T. Frauenheim, E. Janzén, and A. Gali, Phys. Rev. B 81, 153203 (2010).
[44] I. Bersuker, The Jahn-Teller effect (Cambridge University Press, 2006).
[45] I. Bersuker and V. Polinger, Vibronic interactions in molecules and crystals, Vol. 49 (Springer Science & Business Media, 2012).
[46] F. S. Ham, Phys. Rev. 166, 307 (1968).
[47] F. S. Ham, Phys. Rev. 138, A1727 (1965).
[48] Q. C. Qiu and A. Ceulemans, in Vibronic Interactions: Jahn-Teller Effect in Crystals and Molecules (Springer Netherlands, 2001) pp. 97–102.
[49] G. Thiering and A. Gali, Phys. Rev. B 96, 081115 (2017).
[50] G. Thiering and A. Gali, arXiv preprint arXiv:1803.02561 (2018).
[51] I. Bersuker, Soviet Physics JETP 16 (1963).
[52] R. W. Reynolds and L. A. Boatner, Physical Review B 12, 4735 (1975).
[53] P. García-Fernández, A. Trueba, M. T. Barriuso, J. A. Aramburu, and M. Moreno, Phys. Rev. Lett. 104, 035901 (2010).