Correlation between the antisite pair and the D_I center in SiC

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The D_I low temperature photoluminescence center is a well-known defect stable up to 1700 °C annealing in SiC, still its structure is not yet known. Combining experimental and theoretical studies, in this paper we will show that the properties of an antisite pair can reproduce the measured one-electron level position and local vibration modes of the D_I center, and are consistent with other experimental findings as well. We give theoretical values of the hyperfine constants of the antisite pair in its paramagnetic state as a means to confirm a model.

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The D_I low temperature photoluminescence (LTPL) center in SiC has been well known for decades.[1] It has been recently shown that room temperature electron irradiation creates sharp PL lines (called alphabet lines) which anneal out at about 750 °C. At a higher annealing temperature only the spectrum of the D_I center appears.[2] The D_I LTPL signal is very efficient, and it can survive annealing above 1700 °C, i.e., the D_I defect is very stable. The D_I center was observed in all polytypes after various kinds of irradiation,[1,3–6] and was also observed in as-grown material after quenching from growth temperature and in epitaxial layers grown by chemical vapor deposition[7–10] or molecular beam epitaxy (MBE).[11] The photon energy of the zero-phonon luminescence is 0.35–0.45 eV below the excitonic gap independent of the polytype. It was shown[12] that the transition of the zero-phonon line can be explained by exciton recombination at an isoelectronic center, which should have at least one doubly occupied defect level in the band gap. Binding of excitons by neutral isoelectronic centers is known from other semiconductors.[13] Since the offset of the valence band maximum is small between polytypes,[14] the transition energy of the zero-phonon line might give the position of the one-electron level of the neutral defect with respect to the conduction band edge (E_c) within 0.1 eV. It was also found by PLE measurements that the hole binds strongly to the D_I defect while the electron only weakly making a hydrogenic series in its excited states.[12] The D_I spectrum consists of three zero-phonon lines at $L_1 = 2.625$ eV, $L_2 = 2.600$ eV, and $L_3 = 2.570$ eV in 6*H*-SiC.[7] In 4*H*-SiC the L_1 line appears at 2.901 eV,[6,8] while the 3*C*-SiC layers show an emission line at $L_1 = 1.972$ eV.[15] These experimental facts indicate that the one-electron level of the neutral defect is about 0.3–0.4 eV above the valence band maximum independently of the polytype. The tight binding of the hole indicates that the defect is a hole trap; in other words, it can be positively ionized. The D_I center appears in *n*-type as well as *p*-type SiC samples.[1,12] Assuming that the exciton is bound to a neutral isoelectronic defect, the D_I center should not give rise to an empty defect level above the doubly occupied defect level because it could then be negatively charged and invisible in *n*-type samples. Another consequence is that the D_I center could originate from an intrinsic defect. The appearance of the D_I defect in irradiated as well as as-grown materials also suggests its native nature. The MBE experiment showed no Si/C ratio dependency of the concentration of the D_I center.[11] However, it was shown that the concentration of the D_I center reduces with higher C/Si ratio during *high speed* CVD growth.[16] It was not shown that this relationship holds at a lower rate of growth.[16] Besides the sharp L_i emission lines phonon assisted sidebands have also been detected[7] and associated with local vibration modes of the D_I defect around 83 meV (669.4 cm^{-1}) in the phonon band gap. Splitting of this vibration mode were reported in 4*H* and 6*H*-SiC, resulting in at least two modes.[7,12]

Several models have been suggested for the D_I center. It was speculated that the L_i lines were coming from the divacancy, or possibly from a carbon divacancy.[17] This has been not supported by a recent theoretical work.[18] It was shown that the divacancy is not stable in the neutral charged state, and the ionization energies of the divacancy is not in the region of the transition energy of the D_I center.[18] An electron paramagnetic resonance (EPR) study assigned the D_I defect to a V_{Si}-N_C complex[19]; however, no correlation of the EPR and the D_I LTPL signal were shown, whatsoever. It has also been suggested that a silicon vacancy might be involved in the D_I defect, based on comparing the calculated (+/0) occupation level with the transition energy of the L_i lines.[11] In a recent theoretical work the alphabet lines in 4*H*-SiC were attributed to various configurations of nearby carbon and silicon antisites.[20] It was speculated that a next neighbor pair (see Fig. 1) might give rise to the D_I center. These calculations (in a 72-atom supercell) predicted a significant total energy difference between different orientations of the pair, and a single Si-related local vibrational mode (LVM) at 624.9 cm^{-1} (77.5 meV) in the phonon gap (which is at variance with our experimental finding).[20] The calculated (+/0) occupation level at E_c-2.66 eV for the close pair at the *h* site was favorably compared to the transition energies of the alphabet lines. It should be noted that the duration of the photon emission due to an electron-hole recombination is much shorter than the relaxation time of the atoms to reach the

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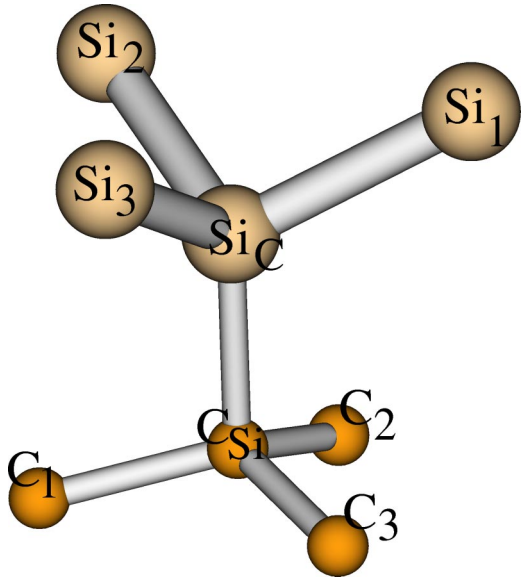

FIG. 1. The geometry of the antisite pair at the *k* site. In the case of C_{1h} symmetry in the single positively charged state Si(1) and C(1) atoms are lying in the mirror plane making the Si(2), Si(3) and C(2), C(3) atoms equivalent.

equilibrium configuration of the charged state; therefore, not the (+/0) occupation level but the one-electron level of the neutral defect, i.e., the *vertical* ionization energy should be compared to the transition energy of the zero phonon-line (the occupation levels are *adiabatic* ionization energies).

In this paper we will report experiments of the D_{I} related local vibrational modes, and we will show by careful *ab initio* 3*C* and 4*H*-SiC supercell calculations that the neutral antisite pair is indeed a good candidate for the D_{I} defect: the calculated local vibration modes can explain the experimental findings, and the calculated one-electron level of the neutral antisite pair is very close to the measured transition energy of the zero-phonon line. We also calculate the hyperfine constants for the antisite pair in the positively charged state in order to facilitate the identification of the D_{I} defect by EPR.

PL measurements were performed in 3*C*-, 4*H*-, and 6*H*-SiC crystals at a temperature of ~ 2 K, with the samples immersed in the liquid helium, using excitation at 334 or 351 nm (Ar-laser with ultraviolet lines) to investigate the phonon replicas of D_{I} center. In the case of the hexagonal polytypes (4*H*- and 6*H*-SiC), the usual near backscattering geometry along the crystal *c* axis was used; thus only light with polarization $\mathbf{E}\perp\mathbf{c}$ was detected. For other details on the material preparation of hexagonal polytypes, see Ref. 12. The 3*C*-SiC sample was a bulk SiC sample. We have found that there are two LVMs close to each other in the phonon gap (see Table I). In 4*H*-and 6*H*-SiC both modes are about equally strong, while for 3*C*-SiC the one at 661.3 cm^{-1} (82.0 meV) is weak and the one at 668.7 cm^{-1} (82.9 meV) is strong. The broadening of the lines may indicate that the lower mode is doubly degenerate or consists of more modes which could not have been resolved experimentally in hexagonal polytypes.

It has been shown earlier that the anti-site pair is more stable than isolated antisites.[21,22] Here we have investigated

TABLE I. The measured phonon gap modes for the D_{I} LTPL center in 4*H* and 6*H*-SiC. The different gap modes corresponding to the different zero-phonon lines are labeled in the first column.

LTPL line	phonon gap modes in meV (cm^{-1})	
3*C*-SiC: L_1	82.0 (661.3)	82.9 (668.7)
4*H*-SiC: L_1	82.7 (667.0)	83.4 (672.7)
6*H*-SiC: L_1	82.8 (667.8)	83.7 (675.1)
L_2	82.3 (663.8)	83.2 (671.1)
L_3	82.1 (662.2)	82.9 (668.7)

the behavior of the antisite pair using three different approaches within the supercell formalism.

(1) *Geometry and occupation levels*. *Ab initio* DFT-LDA (density functional theory in the local density approximation) calculations with the exchange correlation of Ceperley and Alder[23] were carried out in a supercell (SC) model, applying Troullier-Martins pseudopotentials[24] with a plane wave basis using a 36-Ry kinetic energy cutoff in the FHI98MD code.[25] Other details can be found in Ref. 26. For selecting the necessary supercell size we made convergence tests on the well-known V_{C}^{+} defect.[27] We have found that the 72-atom supercell of 4*H*-SiC with the 2^3 *K*-point set does not yield convergent results for the geometry and formation energy of the isolated V_{C}^{+} but the results of a 96-atom supercell calculation agree with those of 4*H*-SiC 128-atom calculations within 0.5%.[28] Therefore, in the SC calculations 3*C*-SiC was modeled by a 128 atom fcc, and 4*H*-SiC by a 96 atom hcp unit cell. A major problem is that the width of the band gap is always severely underestimated in the DFT-LDA. That influences the energy of the electrons on gap levels and, thereby, the total energy as well. For the single positively charged defect the error in the total energy due to the interaction of the charged supercells is partly compensated for by the spin polarization error. We have already demonstrated that using a correction for the one-electron level positions,[42] the occupation levels of known defects in silicon can be reproduced within 0.1 eV.[29]

(2) *Local vibration modes*. There are four inequivalent configurations for the anti-site pair in 4*H*-SiC. The corresponding local vibration modes would be slightly different and difficult to determine whether they can be resolved experimentally. Therefore, the local vibrational modes were calculated only in 3*C*-SiC. Using a plane wave basis for this purpose would be too time consuming; thus we have used the same procedure as Ref. 20 utilizing Gaussian orbitals.[30] This method already provided excellent results for local vibration modes in 3*C*-SiC compared to the experiments.[26,31] Details about this method can be found in Ref. 26, and will be not repeated here.

(3) *Hyperfine constants and one-electron levels*. The calculation of accurate hyperfine constants requires an all electron treatment. We have used the CRYSTAL'98 code[32] for this purpose, on the supercell geometry obtained from the plane wave supercell calculations (with the same *K*-point set). The Kohn-Sham one-particle eigenvalues of the local density approximation (LDA) Hamiltonian are not the vertical ionization energies. As a consequence, the LDA underestimates the

width of the band gap of semiconductors about 50%. In our case the calculated LDA band gaps were 0.5, 1.2, and 2.0 eV for silicon, 3C-SiC, and 4H-SiC, respectively, compared to the experimental values of 1.1, 2,4 and 3.3 eV. The self-consistent solutions for this problem can be the Baraff-Schlüter correction (scissor-operator) in Green-function techniques,[33] the exact-exchange formalism within the density functional theory,[34] or the Hartree-Fock exchange functional mixing in to a LDA correlation functional.[35] We have used the last method in the CRYSTAL'98 code: setting an empirical 20% mixing of the exact exchange into LDA, the calculated band gaps are 1.0, 2.4, and 3.3 eV for Si, 3C-SiC, and 4H-SiC, respectively, which are within 0.1 eV of the experimental values. The defect levels in the band gap also represent a problem in LDA calculations: a defect level in the band gap is a mixture of valence band states and the (excited) conduction band states. The position of that defect level shifts nearly proportional to the overlap with the conduction band states.[33] If electrons occupied that defect level, then this correction influences the formation energy of the corresponding defect as well. This effect is demonstrated here on the well-documented hydrogen interstitial (H_i) in silicon[36] (using the same K-point set in the CRYSTAL'98 calculations for Si as for SiC, details below).[43] The calculated one-electron level of H_i^0 is at $E_v+0.4$ eV with pure LDA Hamiltonian and at $E_v+0.9$ eV with a mixed Hamiltonian compared to the experimental ionization energy of $E_v+0.96$ eV.[36] It is apparent that using a fixed mix (20%) of the exact exchange into the LDA, this method allows us to determine the position of the one-electron levels free of the gap error. We have found that the LDA gap correction for the total energy of the neutral state of the anti-site pair in SiC is 0.4 eV. Using all electrons for all the atoms in the supercell would be computationally prohibitive; therefore, only the antisites and their first neighbor atoms were treated in this manner with an optimized 6-21G* Gaussian-type basis, while for the rest an isomorph ECP-21G* basis[37] was used where the effect of core electrons was treated by an effective core potential. Tests of the hydrogen interstitial in silicon have shown that this method is able to reproduce the measured hyperfine constants typically within 15–25 %.[38] The method has already proven very effective in calculating the hyperfine constants of defects in other materials as well.[39,40]

First, the geometry and the formation energy of the neutral antisite pair were determined in 3C and 4H-SiC. In 3C-SiC the antisite pair has a C_{3v} symmetry and there is one a_1 and one doubly degenerate e level fully occupied above the top of the valence band (E_v) at $E_v+0.19$ eV and at $E_v+0.44$ eV (these are corrected values). The defect levels correspond to the compressed Si-Si bonds of the Si_C. The distance of the Si-Si bonds is about 2.2 Å. The situation is very similar to that of the isolated Si_C, where a triply degenerate t_2 level is lying close to the valence band top.[41] The calculated and corrected formation energy is 6.1 eV, which is between that of the silicon vacancy (8.2 eV) and that of the carbon vacancy (5.3 eV).[44] In 4H-SiC we have calculated the neutral antisite pair parallel to the c axis at the k site and at the h site, as well as the off-axis configurations. We have found that the formation energies of these configurations are within 0.08 eV of each other (the off-axis configuration is slightly more stable than the other ones), and the one-electron defect levels are within 0.02 eV of each other, so they are practically the same within the error bar of our calculational method. The significant energy difference found in Ref. 20 is probably a consequence of the smaller cell size. The corrected formation energy of the antisite pair at the k site is 5.9 eV. In 4H-SiC the symmetry of the neutral antisite pair is C_{3v}, parallel to the c axis, and C_{1h} in the off-axis configuration. The one-electron levels have been determined for the k site by the CRYSTAL'98 code: the a_1 level and the e level are lying at $E_v+0.16$ and $+0.38$ eV, respectively. The calculated and corrected (+/0) level of the k site is at $E_v+0.3$ eV. In the case of the singly positive charge state the antisite pair undergoes Jahn-Teller distortion to a C_{1h} symmetry at the k site. This is a paramagnetic state ($S=1/2$) and the hyperfine constants have been calculated for the antisite pair (see Table II). As can be seen the hyperfine interactions on Si atoms are big enough to be measured by EPR. The localization on carbon atoms is very low. The calculated hyperfine data obviously do not fit those reported in Ref. 19.

TABLE II. The calculated principal values of the hyperfine tensor of the antisite pair at the k site in 4H-SiC. The values are in MHz. See Fig. 1 for atom labels.

atom	principal values of hyperfine tensor in MHz		
	A_x	A_y	A_z
Si_C	−49.6	21.0	−17.4
C_{Si}	−5.0	4.6	−4.0
Si_1	−25.7	9.0	9.0
C_1	5.3	3.1	2.9
$Si_{2,3}$	−12.3	10.0	9.5
$C_{2,3}$	3.7	2.0	2.1

All the calculated LVMs of the antisite pair in 3C-SiC are falling into the phonon continuum except four modes. An a_2 mode at 698 cm^{-1} is due to the twist of the first neighbor C atoms around C_{Si}. The a_2 mode is forbidden for any PL transition, and not expected to appear in the LTPL spectrum. A degenerate e mode at 627 cm^{-1} and an a_1 mode at 641 cm^{-1} correspond to stretching modes of the compressed Si-Si bonds. These values compare to the experimental ones at 661 and 669 cm^{-1} of D_I in 3C-SiC. The intensity difference between the two observed modes can be explained by the selection rules pertinent to C_{3v} symmetry in 3C-SiC, which will make the a_1 mode appear much stronger. However, in hexagonal SiC the off-axis configurations (which may occur three times more frequently as the trigonal ones) posseses a C_{1h} symmetry where the e mode is slightly split and certainly no forbidden states occur. Thus at least two nearly equally strong modes are expected due to the anti-site pair in 4H- and 6H-SiC where the first may consist of two modes very close to each other.[45] The calculated LVMs of the isolated C_{Si} (T_d symmetry) are falling into the phonon continuum, while the isolated Si_C (T_d symmetry) has one triply degenerate t_2 (at 671 cm^{-1}) and one a_1 (at 644 cm^{-1}) LVM in the phonon band gap. (Similar results have been

reported in $4H$-SiC except that only three gap modes were found for Si_C.[20]). This shows that the number of LVMs in the phonon band gap depends on the number of compressed Si-Si bonds: in the case of isolated Si_C four modes appears due to four Si-Si bonds. For the antisite pair there are three compressed Si-Si bonds resulting in three modes. The isotope shift of ^{13}C is also very minor ($0.4\ cm^{-1}$ for a_1 mode) for the antisite pair which also shows that the local vibration modes are related to the compressed Si-Si bonds.

The calculated formation energy of the antisite pair is lower than for the Si-vacancy which indicates that this defect can be created during growth. The calculated highest one-electron defect level at $E_v+0.38\ eV=E_c-2.88\ eV$ in $4H$-SiC is very close to the observed transition energy of the zero-phonon line (2.901 eV). The corresponding calculated and measured values are 1.97 and 1.972 eV in $3C$-SiC, respectively. The antisite pair is an isoelectronic defect: the highest defect level is a fully occupied double degenerate e level (in $4H$-SiC it is a bit split in the off-axis configuration) from where one electron can be excited and then a positively charged defect is left. This is consistent with the PLE experiments.[12] The $(+/0)$ occupation level is at about $E_v+0.3$ eV in $4H$-SiC. This means that the antisite pair is neutral in n-type and moderately p-type materials. Assuming that the exciton binds to a neutral defect this explains why D_I spectra can be seen in n-type and as well as p-type samples. The calculations hint that the D_I defect can be positively charged in heavily Al doped p-type samples where the D_I spectra should disappear. Hyperfine interaction with four silicon atoms should be seen in this case for the positively charged state. The phonon sidebands of the D_I spectra in the phonon gap can appear because of the compressed Si-Si bonds of the antisite pair. The calculated degenerate and single local vibrational modes are in good agreement with the measured PL peaks of D_I in $3C$-SiC. Based on these facts we propose the isolated antisite pair as a promising microscopic model for the D_I center. The experimental justification could be made by EPR in heavily Al doped samples.

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[1] W.J. Choyke and L. Patrick, Phys. Rev. B **4**, 1843 (1971).
[2] T. Egilsson, A. Henry, I.G. Ivanov, J.L. Lindström, and E. Janzén, Phys. Rev. B **59**, 8008 (1999).
[3] J. Schneider and K. Maier, Physica B **185**, 199 (1993).
[4] V.V. Makarov, Sov. Phys. Solid State **13**, 1974 (1972).
[5] L. Patrick and W.J. Choyke, Phys. Rev. B **5**, 3254 (1972).
[6] C. Haberstroh, R. Helbig, and R.A. Stein, J. Appl. Phys. **76**, 509 (1994).
[7] W.J. Choyke, in *The Physics and Chemistry of Carbides, Nitrides and Borides*, Vol. 185 of *NATO Advanced Study Institute*, Series E, edited by R. Freer (Kluwer Academic, Dordrecht, 1990), p. 563.
[8] T.A. Kennedy, J.A. Freitas, and S.G. Bishop, J. Appl. Phys. **68**, 6170 (1990).
[9] K. Nishino, T. Kimoto, and H. Matsunami, Jpn. J. Appl. Phys. **34**, L1110 (1995).
[10] Y.A. Vodakov, G.A. Lomakina, E.N. Mokhov, V.G. Oding, M.G. Ramm, and V.I. Sokolov, Sov. Phys. Semicond. **20**, 900 (1986).
[11] A. Fissel, W. Richter, J. Furthmüller, and F. Bechstedt, Appl. Phys. Lett. **78**, 2512 (2001).
[12] T. Egilsson, J.P. Bergman, I.G. Ivanov, A. Henry, and E. Janzén, Phys. Rev. B **59**, 1956 (1999).
[13] R.K. Watts, *Point Defects in Crystals* (Wiley-Interscience, New York, 1977).
[14] P. Käckell, B. Wenzien, and F. Bechstedt, Phys. Rev. B **50**, 10 761 (1994).
[15] W.J. Choyke, Z.C. Feng, and J.A. Powell, J. Appl. Phys. **64**, 3163 (1988).
[16] K. Fujihira, T. Kimoto, and H. Matsunami, Appl. Phys. Lett. **80**, 1586 (2002).
[17] W.J. Choyke, Inst. Phys. Conf. Ser. **31**, 58 (1977).
[18] L. Torpo, T.E.M. Staab, and R.M. Nieminen, Phys. Rev. B **65**, 085202 (2002).
[19] V.S. Vainer and V.A. Il'in, Sov. Phys. Solid State **23**, 1432 (1981).
[20] T.A.G. Eberlein, C.J. Fall, R. Jones, P.R. Briddon, and S. Öberg, Phys. Rev. B **65**, 184108 (2002).
[21] L. Torpo and R.M. Nieminen, Mater. Sci. Eng., B **61-62**, 593 (1999).
[22] E. Rauls, Z. Hajnal, A. Gali, P. Deák, and T. Frauenheim, Mater. Sci. Forum **353-356**, 435 (2001).
[23] D.M. Ceperley and B.J. Alder, Phys. Rev. Lett. **45**, 566 (1980).
[24] N. Troullier and J.L. Martins, Phys. Rev. B **43**, 1993 (1991).
[25] M. Bockstedte, A. Kley, J. Neugebauer, and M. Scheffler, Comput. Phys. Commun. **107**, 187 (1997).
[26] B. Aradi, A. Gali, P. Deák, J.E. Lowther, N.T. Son, E. Janzén, and W.J. Choyke, Phys. Rev. B **63**, 245202 (2001).
[27] A. Zywietz, J. Furthmüller, and F. Bechstedt, Phys. Rev. B **59**, 15 166 (1999).
[28] A. Gali, P. Deák, N.T. Son, and E. Janzén (unpublished).
[29] A. Gali, D. Heringer, P. Deák, Z. Hajnal, T. Frauenheim, R.P. Devaty, and W.J. Choyke, Phys. Rev. B **66**, 125208 (2002).
[30] R. Jones, Philos. Trans. R. Soc. London, Ser. A **341**, 351 (1992).
[31] A. Gali, B. Aradi, D. Heringer, W.J. Choyke, R.P. Devaty, and S. Bai, Appl. Phys. Lett. **80**, 237 (2002).
[32] V. R. Saunders, R. Dovesi, C. Roetti, M. Caus, N. M. Harrison, R. Orlando, and C. M. Zicovich-Wilson, CRYSTAL98 User's Manual, University of Torino, Torino, 1998.
[33] G.A. Baraff and M. Schlüter, Phys. Rev. B **30**, 1853 (1984).
[34] M. Städele, M. Moukara, J.A. Majewski, P. Vogl, and A. Görling, Phys. Rev. B **59**, 10 031 (1999).
[35] R. Dovesi, R. Orlando, C. Roetti, C. Pisani, and V. R. Saunders, in *Computer Simulation of Materials at Atomic Level*, edited by P. Deák, T. Frauenheim, and M.R. Paderson (VILEY-VCH Verlag, Berlin, 2000), p. 63.
[36] B. Holm, K. Bonde Nielsen, and B. Bech Nielsen, Phys. Rev. Lett. **66**, 2360 (1991).

[37] M. Causá, R. Dovesi, and C. Roetti, Phys. Rev. B **43**, 11 937 (1991).

[38] A. Gali, P. Deák, N.T. Son, E. Janzén, J.-L. Monge, and H.J. von Bardeleben, in *Materials Science Forum* (Trans. Tech. Publication, Uetikon-Zuerich, Switzerland, 2002).

[39] G. Mallia, R. Orlando, C. Roetti, P. Ugliengo, and R. Dovesi, Phys. Rev. B **63**, 235102 (2001).

[40] A. Lichanot, P. Baranek, M. Mérawa, R. Orlando, and R. Dovesi, Phys. Rev. B **62**, 12 812 (2000).

[41] L. Torpo, S. Pöykkö, and R.M. Nieminen, Phys. Rev. B **57**, 6243 (1998).

[42] For correction we have used the level positions obtained from a mixed LDA - exact exchange calculation using the CRYSTAL'98 code as reference.

[43] H_i in Si has very minor relaxation difference between its (+) and (0) states, so the (+/0) occupation level is nearly equal to the position of the singly occupied defect level of H_i^0 in the band gap.

[44] Corrected formation energies were given for stoichiometric conditions.

[45] The *e* mode may be allowed for one of the polarization of the emitted light in hexagonal SiC, which means that the intensity of the lines due to local vibrations in the spectra may vary with the polarization.