

# Carbon dangling-bond center (carbon $P_b$ center) at 4H-SiC(0001)/SiO<sub>2</sub> interface

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## ABSTRACT

We identify a carbon dangling-bond center intrinsically formed at thermally oxidized 4H-SiC(0001)/SiO<sub>2</sub> interfaces. Our electrically detected-magnetic-resonance spectroscopy and first-principles calculations demonstrate that this center, which we name “the  $P_{bc}$  center,” is formed at a carbon adatom on the 4H-SiC(0001) honeycomb-like structure. The  $P_{bc}$  center ( $\text{Si}_3\equiv\text{C}\cdot$ , where “ $\cdot$ ” represents an unpaired electron) is determined to be a just carbon version of the famous  $P_b$  center (Si dangling-bond center,  $\text{Si}_3\equiv\text{Si}\cdot$ ) at Si(111)/SiO<sub>2</sub> interfaces because we found close similarities between their wave functions. The  $P_{bc}$  center acts as one of the major interfacial traps in 4H-SiC(0001) metal-oxide-semiconductor field-effect transistors (MOSFETs), which decreases the free-carrier density and the field-effect mobility of 4H-SiC(0001) MOSFETs. The formation of the  $P_{bc}$  centers has the role of reducing the oxidation-induced strain, similar to the case of the formation of the  $P_b$  centers.

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Metal-oxide-semiconductor (MOS) interfaces are crucial for various modern electronic devices.<sup>1</sup> They are the heart of Si MOS field-effect transistors (Si MOSFETs) in state-of-the-art complementary-MOS integrated circuits.<sup>1</sup> The MOS structures are also indispensable to various power devices such as power MOSFETs for power electronics.<sup>2–6</sup> The development of power MOSFETs is expanding over widebandgap semiconductors such as 4H-SiC (bandgap,  $E_g = 3.26$  eV),<sup>2,3</sup> GaN ( $E_g = 3.4$  eV),<sup>4</sup> Ga<sub>2</sub>O<sub>3</sub> ( $E_g = 4.8$  eV),<sup>5</sup> and even diamond ( $E_g = 5.4$  eV)<sup>6</sup> to meet the demand of continuously growing electric-power consumption. However, the performance of their MOSFETs is generally limited due to the poorer quality of their MOS interfaces, which suffer from many more MOS interface defects than Si-MOS systems.<sup>2–6</sup> In Si, major interface defects are identified as so-called “ $P_b$  centers,”<sup>7,8</sup> which are found at every Si(111),<sup>9–11</sup> Si(100),<sup>12,13</sup> and Si(110) surface.<sup>14</sup> Essentially,  $P_b$  centers are a family of Si dangling bonds (DBs) intrinsically formed at Si/SiO<sub>2</sub> interfaces.<sup>7,8</sup> Similar to Si-MOS systems, Ge-MOS interfaces also generate the same type of interface defect, i.e., “Ge  $P_b$  centers.”<sup>15,16</sup> In contrast, wideband-gap semiconductors seem to have no such benchmark model for their MOS interface defects. For instance, 4H-SiC/SiO<sub>2</sub> interfaces have been widely studied over two decades; however, the search for benchmark models of their interface defects is still ongoing.<sup>17–24</sup>

In this Letter, we present a spectroscopic and theoretical identification of a  $P_b$ -like interface defect in 4H-SiC MOS systems, which we call the “ $P_{bc}$  center.” The  $P_{bc}$  center is intrinsically formed after thermal oxidation of the 4H-SiC(0001) surface (the Si-face), which is the standard surface of 4H-SiC wafers. This center is just a carbon version of the famous  $P_b$  center, i.e., an ideal carbon DB at the interface. We believe that the  $P_{bc}$  center is identical to a previous “interface carbon defect” with a typical density of  $3\text{--}4 \times 10^{12} \text{ cm}^{-2}$  observed by electron-spin-resonance (ESR) spectroscopy on thermally oxidized 4H-SiC(0001)/SiO<sub>2</sub> substrates.<sup>17,18</sup> Instead of ESR, we here used electrically detected-magnetic-resonance (EDMR) spectroscopy,<sup>19–23</sup> which enabled us to complete a full analysis of <sup>13</sup>C and <sup>29</sup>Si hyperfine (HF) interactions of this center. Like the  $P_b$  center in Si/SiO<sub>2</sub> systems, the formation of the  $P_{bc}$  center is closely correlated with relaxation of the oxidation-induced strain at 4H-SiC/SiO<sub>2</sub> interfaces, which was quantitatively confirmed from first-principles calculations. The calculations also demonstrated that the  $P_{bc}$  center is formed at a carbon adatom (C adatom) on the 4H-SiC(0001) surface. We also discuss significant influences of the  $P_{bc}$  center on the performance of 4H-SiC MOSFETs.

For highly sensitive EDMR measurements, we prepared  $n$ -channel lateral 4H-SiC MOSFETs with a special dimension (gate length/

width =  $5/2000 \mu\text{m}$ ) on a  $4^\circ$ -off  $p$ -type 4H-SiC(0001) epitaxial layer (Al doping of  $5 \times 10^{15} \text{cm}^{-3}$ ). The 30-nm thick gate oxide was formed by a standard thermal oxidation at  $1200^\circ\text{C}$  using dry  $\text{O}_2$ . Further details of the fabrication processes are published in previous papers.<sup>25</sup> The MOSFETs exhibited a maximum field-effect mobility ( $\mu_{\text{FE}}$ ) of  $7 \text{cm}^2 \text{V}^{-1} \text{s}^{-1}$ , which is slightly higher than conventional values of Si-face 4H-SiC MOSFETs,<sup>2,3,25</sup> because of optimal dry oxidation and epitaxial layer. However, this value is still far from an ideal electron mobility of 4H-SiC ( $1000 \text{cm}^2 \text{V}^{-1} \text{s}^{-1}$ ),<sup>12,3</sup> indicating a great influence of interface defects. We then conducted bipolar-amplification-effect (BAE) EDMR measurements<sup>19</sup> to amplify EDMR signals of the interface defects. We used a standard lock-in amplification technique synchronized to a magnetic-field modulation at  $1.56 \text{kHz}$ .<sup>18,23</sup> ESR transitions were excited by a microwave at  $9.45 \text{GHz}$  and  $200 \text{mW}$  at room temperature.

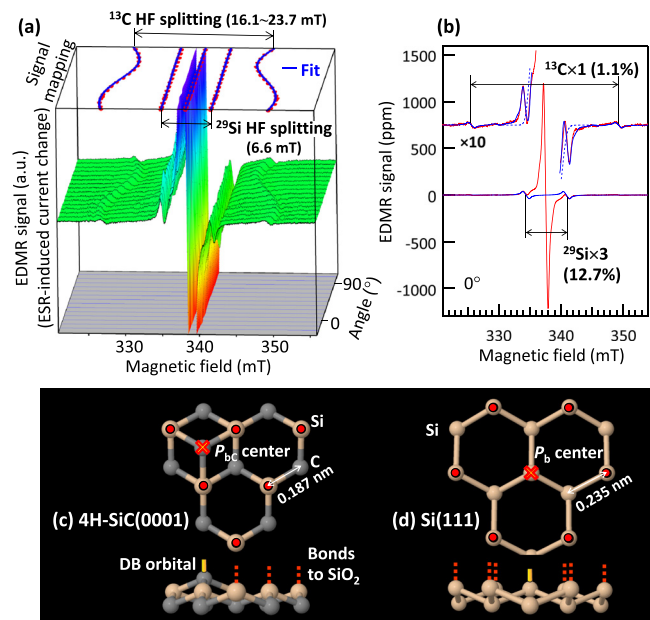
Figure 1(a) shows room-temperature EDMR spectra of the Si-face 4H-SiC MOSFET as a function of magnetic-field angles. Only one strong EDMR signal was observed, which is the  $P_{\text{bC}}$ -center signal (an electron spin =  $1/2$ ), showing slightly  $c$ -axial gyromagnetic factors ( $g$ ) of  $g_{\parallel} = 2.0029$  and  $g_{\perp} = 2.0032$ . We believe that this EDMR signal is

identical to an ESR signal with a spin density of  $3\text{--}4 \times 10^{12} \text{cm}^{-2}$  observed in the as-oxidized 4H-SiC(0001) epitaxial layers.<sup>17,18</sup> An extremely higher signal-to-noise ratio of EDMR spectra can reveal a full angular dependence of HF interactions of this center.

As shown in Fig. 1(a), this center clearly exhibits two sets of HF doublet structures (splitting widths of  $16.1\text{--}23.7 \text{mT}$  and  $6.6 \text{mT}$ ), which we assign to HF satellite signals due to a  $^{13}\text{C}$  nuclear spin (nuclear spin  $I = 1/2$ , natural abundance  $p = 1.1\%$ ) and  $^{29}\text{Si}$  nuclear spins ( $I = 1/2$ ,  $p = 4.7\%$ ), respectively. These HF signals can be excellently fitted by HF interactions due to one C site and three equivalent Si sites, as demonstrated in Fig. 1(b). The former C site generates HF doublet signals with a relative intensity of  $1.1\%$  as shown in the figure. The latter Si sites cause a doublet splitting with a relative intensity of  $6[(p/2)^3 + (p/2)(1-p)^2] = 12.7\%$ , supposing one to three  $^{29}\text{Si}$  nuclear spins at three equivalent Si sites. The  $^{13}\text{C}$  HF splitting reveals a  $c$ -axial ( $C_{3v}$ ) symmetry, as seen in the angular map of Fig. 1(a), indicating that the C site has a  $c$ -axial  $2p$ -orbital. The  $c$ -axial  $^{13}\text{C}$  HF tensor was determined to have  $A_{\parallel} = 23.70 \text{mT}$  and  $A_{\perp} = 16.09 \text{mT}$ .

The above  $^{13}\text{C}$  and  $^{29}\text{Si}$  HF interactions are in good agreement with a carbon-DB model such as a  $\text{Si}_3\equiv\text{C}$ - structure (“ $\equiv$ ” means a DB) at the 4H-SiC(0001)/ $\text{SiO}_2$  interface, which is just analogous to the  $P_{\text{b}}$  center (a  $\text{Si}_3\equiv\text{Si}$ - structure) at the Si(111)/ $\text{SiO}_2$  interface.<sup>7,10,11</sup> The largest HF splitting of  $^{13}\text{C}$  with a  $c$ -axial symmetry is generated from a surface-normal ( $c$ -axial) carbon DB. The second largest HF interaction due to  $^{29}\text{Si}$  is caused by three equivalent Si atoms adjacent to the C DB site. In Fig. 1(c), we draw the atomic structure of the  $P_{\text{bC}}$  center at the 4H-SiC(0001) surface, in addition to that of the  $P_{\text{b}}$  center at the Si(111) surface [Fig. 1(d)]. Obviously, both surfaces have similar honeycomb-like structures, except their lattice constants. They commonly have surface-normal Si bonds, as indicated by “ $\bullet$ ” in the figure. The  $P_{\text{b}}$  center is formed by breaking one of such Si bonds, as denoted with “ $\times$ ” in Fig. 1(d). In contrast, at the 4H-SiC(0001) surface, there are *no* surface-normal C bonds. Thus, we must consider an additional atomic configuration where a carbon DB stands up. Our conclusion is shown in Fig. 1(c) on the basis of the first-principles calculations. A carbon DB can be formed at a C adatom bonded to three Si atoms on the 4H-SiC(0001) surface. The advantages of such a configuration are obvious, though quantitative arguments will be given later. When connecting to a top  $\text{SiO}_2$  layer, the Si(111) surface shown in Fig. 1(d) must be affected by a tensile strain due to a larger unit cell of  $\text{SiO}_2$ .<sup>7,8,11,26</sup> Eventually, some Si bonds must be disconnected, resulting in the formation of the  $P_{\text{b}}$  center.<sup>7,8,11</sup> On the other hand, since a unit cell of 4H-SiC(0001) is smaller than that of Si(111), we must disconnect more Si bonds at the 4H-SiC(0001)/ $\text{SiO}_2$  interface. A C-adatom structure consumes three Si bonds at the interface, reducing the above constraint. Simultaneously, it can also fix residual C atoms that are unavoidably emitted during the thermal oxidation of 4H-SiC. Further discussions are shown in Ref. 27.

From the obtained  $^{13}\text{C}$  HF tensor, we can experimentally determine the wave function<sup>7,10,13,28,29</sup> of the  $P_{\text{bC}}$  center, as summarized in Table I. One of the notable features is a very strong spin localization on a DB site for the  $P_{\text{bC}}$  center.  $\eta^2$  reaches  $80\%$ , which is the largest value obtained in SiC.<sup>29</sup> Such strongest spin localization is also characteristic of the original  $P_{\text{b}}$  center in Si.<sup>7,10</sup> Table I also shows the  $s/p$  hybridization ratio ( $\alpha^2/\beta^2$ ), which is significantly higher for  $P_{\text{bC}}$  ( $21\%$ ) than for  $P_{\text{b}}$  ( $13\%$ ). This indicates a more  $sp^3$ -like tetrahedral structure for  $P_{\text{bC}}$ , which is naturally understandable by the C-adatom structure.



**FIG. 1.** (a) EDMR spectroscopy on the  $P_{\text{bC}}$  center at the 4H-SiC(0001)/ $\text{SiO}_2$  interface as a function of magnetic-field angles. For  $0^\circ$  and  $90^\circ$ , the magnetic field was parallel and perpendicular to the [0001] axis, respectively. Solid blue lines in the angular map (upper plane of this graph) were simulated using the  $g$  and HF tensors shown in the text. EDMR spectra were measured using a source current of  $180 \text{nA}$  with a negative gate bias of  $-7.5 \text{V}$  and a constant drain current of  $-10 \mu\text{A}$  in BAE EDMR mode. (b) Spectral simulation of  $^{13}\text{C}$  and  $^{29}\text{Si}$  HF doublet signals (solid blue lines). The  $^{29}\text{Si}$  HF structure was fitted to the experimental spectrum by adding smooth tail curves (dashed blue lines in the upper spectrum). Each HF signal consists of replica made from the experimental spectrum with relative intensities shown in figure. (c) Atomic structures of the  $P_{\text{bC}}$  center at the 4H-SiC(0001) surface and (d)  $P_{\text{b}}$  center at the Si(111) surface. In top views, solid circles on Si atoms indicate surface-normal Si bonds. These structures were unrelaxed, and their optimized structures are seen in Fig. 2.

**TABLE I.** Wave-function parameters of  $P_{bc}$  and  $P_b$  centers. Fractions of  $s$ - and  $p$ -orbitals,  $\eta^2\alpha^2$  and  $\eta^2\beta^2$  ( $\alpha^2 + \beta^2 = 1$ ), are directly calculated from isotropic and anisotropic HF constants  $A_{iso}$  and  $A_{aniso}$ , via  $\eta^2\alpha^2 = |A_{iso}/A_0|$  and  $\eta^2\beta^2 = |b_0/b_0|$ , respectively.<sup>7,10,11,24,28,29</sup> Note that  $A_{iso} = (A_{||} + 2A_{\perp})/3$  and  $A_{aniso} = (A_{||} - A_{\perp})/3$ .<sup>28,29</sup> We used known HF constants of  $A_0 = 134.77$  mT and  $b_0 = 3.83$  mT for  $^{13}\text{C}$  and  $A_0 = -163.93$  mT and  $b_0 = -4.075$  mT for  $^{29}\text{Si}$ .<sup>28</sup> The calculated  $^{13}\text{C}$  HF constants of a C adatom were  $A_{||} = 10.9$  mT and  $A_{\perp} = 4.0$  mT. In lower part, we estimated  $\eta^2\alpha^2$  and  $\eta^2\beta^2$  in the same manner from the calculated  $^{13}\text{C}$  and  $^{29}\text{Si}$  HF tensors for  $P_{bc}$  and  $P_b$ , respectively.

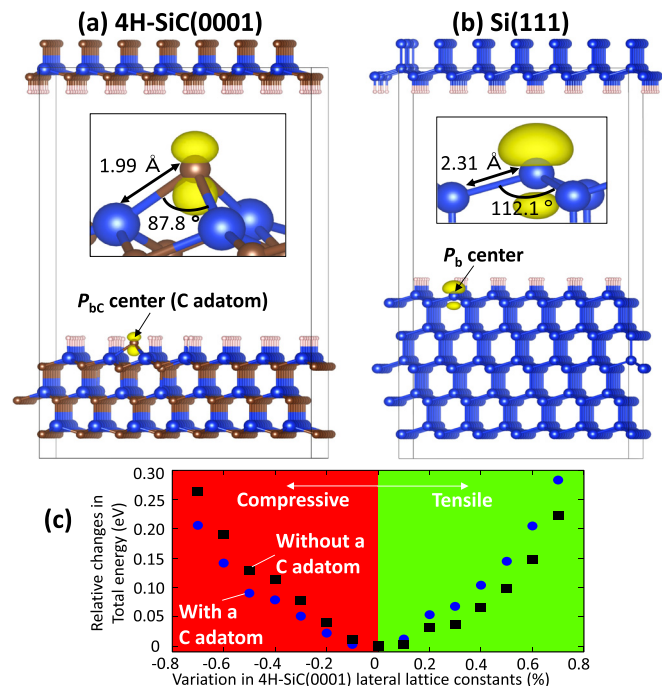
Center	$s$ -orbital ( $\eta^2\alpha^2$ )	$p$ -orbital ( $\eta^2\beta^2$ )	Spin localization ( $\eta^2$ )	$s/p$ ratio ( $\alpha^2/\beta^2$ )	References
Experiment					
$P_{bc}$ at 4H-SiC(0001)/SiO <sub>2</sub>	14%	66%	80%	21%	This work
$P_b$ at Si(111)/SiO <sub>2</sub>	7%	53%	60%	13%	10
<i>porous</i> - $P_{bc}$ at <i>porous</i> -SiC/SiO <sub>2</sub>	4%	35%	39%	11%	24
Theory					
C adatom ( $P_{bc}$ ) at 4H-SiC(0001)	5%	60%	65%	8%	This work
Si DB ( $P_b$ ) at Si(111)	6%	60%	66%	9%	This work

In contrast, the original  $P_b$  center bound on the Si(111) surface is stabilized in an  $sp^2$ -like planar structure.<sup>7,8</sup>

As tabulated in Table I, in *porous*-SiC/SiO<sub>2</sub> structures, different  $P_{bc}$  centers (we here call “*porous*- $P_{bc}$ ”) were observed,<sup>24</sup> showing a quite different nature, e.g., their  $\eta^2$  is only 39% and their  $\alpha^2/\beta^2$  (11%) is close to that of  $P_b$ . Since such  $\eta^2$  is widely seen for bulk defects in SiC,<sup>29</sup> the *porous*- $P_{bc}$  centers may be formed in the bulk side of the interfaces. Note that for other previous interface defects such as the “Si-vacancy center”<sup>20,21</sup> and “dual- $P_{bc}$  centers,”<sup>22</sup> complete analyses on their HF interactions and their wave functions have not yet been reported.

To examine the  $P_{bc}$  center more quantitatively, we carried out first-principles calculations on both the  $P_{bc}$  and  $P_b$  centers. All calculations were carried out on the basis of density functional theory by using the Vienna *ab initio* simulation package (VASP). The projector augmented-wave method, as implemented in the VASP code, was applied in the calculations. Figures 2(a) and 2(b) show our H-terminated 4H-SiC(0001) and Si(111) slab units for optimizing the calculations on semiconductor surfaces. They include either a  $P_{bc}$  center (a DB on a C adatom) or a  $P_b$  center (a Si DB formed at the surface). The lattice parameters of SiC were fixed to the values obtained in our previous calculations,<sup>30,31</sup> and the defect structures were relaxed using the Perdew–Burke–Ernzerhof functional<sup>32</sup> until the remaining forces were less than 40 meV/Å. Note that, by calculating the formation energies of 114 types of mono- and di-carbon defects in 4H-SiC(0001)/SiO<sub>2</sub> systems, we found that the C adatom shown in Fig. 2(a) appears as one of the metastable forms of carbon-related defects.<sup>30,31</sup>

Next, we check the HF constants of the  $P_{bc}$  center, which was performed using the Heyd–Scuseria–Ernzerhof (HSE06) hybrid functional.<sup>34–36</sup> The contribution of core states ( $A_{1c}$ )<sup>36</sup> is included in the calculation of HF constants. A single  $k$ -point (the  $\Gamma$  point) was sampled during the calculations, and spin-polarization was taken into account. As summarized in Table I, the experimental and theoretical values are basically in good agreement with each other for both the  $P_{bc}$  and  $P_b$  centers, ensuring the validity of the C-adatom model as well as the validity of our calculation strategy. Only an exception was a smaller calculated value for the  $2s$ -orbital ( $\eta^2\alpha^2$ ) of the  $P_{bc}$  center. This larger deviation may be related to the fact that the isotropic  $^{13}\text{C}$  HF constant is extremely sensitive to the amplitude of the  $2s$ -orbital, which is more difficult to be calculated accurately compared to other orbitals.



**FIG. 2.** (a) 488-atom H-terminated 4H-SiC(0001) unit cell including a single  $P_{bc}$  center used for first-principles calculations. (b) 503-atom H-terminated Si(111) unit cell for calculating the  $P_b$  center. In (a) and (b), blue, brown, and small white balls depict the Si, C, and H atoms, respectively. The vacuum thickness is about 18 Å for each structure. The Si(111) cell was constructed on the algorithm proposed in Ref. 33. The calculated three-dimensional wave functions related to DB states of the C adatom and surface Si atom are also drawn with the isosurface of about 30% of maximum amplitude. The visualization of crystal structures and wave functions was performed using VESTA. (c) Total-energy calculations on 4H-SiC(0001) unit cells with/without a  $P_{bc}$  center under either lateral lattice expansion or compression. The vertical axis indicates relative changes in the calculated total energy, and the horizontal axis denotes relative changes in the lateral lattice constant of unit cells. Zero of lattice constant was set at the optimized lattice constant of the H-terminated 4H-SiC slab.



In Fig. 2(c), we examine the effect of a top SiO<sub>2</sub> layer on the 4H-SiC(0001) surface through the intentional introduction of an in-plane strain into the 4H-SiC unit cell. Here, we optimized the internal atomic positions by the HSE06 functional with the varying in-plane lattice constants. The horizontal axis indicates the introduction of either a tensile strain or compressive strain along two lateral directions. In the C-adatom structure shown in Fig. 2(a), the bond length between the C adatom and three Si atoms is expanded by 6% (1.99 Å) compared to the normal C–Si length (1.88 Å). Therefore, the C-adatom structure should become more stable when it is compressed along the lateral directions. In fact, the energy gain of creating a C-adatom increases under compressive strain, as shown in Figure 2(c). Namely, the C-adatom structure has a tendency to shrink; in other words, it intrinsically involves a local compressive strain. Accordingly, the formation of the C adatoms (the  $P_{bc}$  centers) can locally cancel out the oxidation-induced tensile strain.<sup>26</sup> We emphasize that such a strain-induced formation mechanism is just similar to that proposed for the  $P_b$  center at the Si(111)/SiO<sub>2</sub> interface.<sup>7,11</sup>

The spin density of the  $P_b$  center at the Si(111)/SiO<sub>2</sub> interface was found to be typically  $2\text{--}3 \times 10^{12} \text{ cm}^{-2}$ ,<sup>7,9–11</sup> which is approximately 50% smaller than that of the  $P_{bc}$  center ( $3\text{--}4 \times 10^{12} \text{ cm}^{-2}$ ,<sup>17,18</sup>) at the 4H-SiC(0001)/SiO<sub>2</sub> interface. This ratio is similar to that of the atomic densities between the Si(111) and 4H-SiC(0001) surfaces:  $7.8 \times 10^{14}$  and  $1.2 \times 10^{15} \text{ cm}^{-2}$  for their top Si atoms, respectively. In Ref. 18, we demonstrated hydrogen passivation of the  $P_{bc}$  center, providing with another similarity to the  $P_b$  center.

Since the above spin density is just comparable to the free-carrier density in the inversion layer of 4H-SiC MOSFETs ( $< 9 \times 10^{12} \text{ cm}^{-2}$ ),<sup>25</sup> the  $P_{bc}$  center has non-negligible impacts on the performance of the MOSFETs. Actually, we observed that the  $P_{bc}$  center was diminished by 1/10 or less after post oxidation anneal (POA) with NO, which simultaneously increased  $\mu_{FE}$  over  $30 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ .<sup>18</sup> The physical reasons why the  $P_{bc}$  center affects  $\mu_{FE}$  are because (1) this center reduces the amount of mobile electrons via electron capture and (2) charged  $P_{bc}$  centers (charged DBs) increase Coulombic scattering. In fact, an increase of  $\sim 2 \times 10^{12} \text{ cm}^{-2}$  was observed in the free-carrier density after NO POA,<sup>25</sup> which is comparable to the density of  $P_{bc}$ . However, the  $P_{bc}$  center cannot account for the total amount of electron traps ( $\leq 8 \times 10^{12} \text{ cm}^{-2}$ ) and other traps should also be present. The electronic level of  $P_{bc}$  will also be important for  $p$ -channel 4H-SiC MOSFETs, because of its amphoteric nature likewise the  $P_b$  center. Its exact location is being examined experimentally and theoretically. At least, we estimate that its neutral DB level (spin-1/2 state) is located in the midgap region because the  $P_{bc}$  center became EDMR-active under a negative gate bias [c.f., Fig. 1(a)].

In summary, we established a benchmark model of a typical interface defect in 4H-SiC(0001)/SiO<sub>2</sub> systems. In this most studied wideband-gap-semiconductor MOS interface, the  $P_{bc}$  center (carbon DB) is intrinsically formed in association with the oxidation-induced strain. We unambiguously identified that this center is just a carbon version of the famous  $P_b$  center in Si-MOS systems, based on the first full-analysis on <sup>13</sup>C HF interaction of an interfacial C atom.

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