

Be and Be-related impurities in diamond: density functional theory study

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First-principles density functional simulations were employed to investigate the geometries, electrical properties, and hyperfine structures of various beryllium-doped diamond configurations, including interstitial (Be_i), substitutional (Be_s), and beryllium-nitrogen (Be-N) complexes. The incorporation of Be into the diamond lattice is more favorable as a substitutional dopant than as an interstitial dopant, although both processes are endothermic. Interstitial Be could potentially exhibit motional averaging from planar to axial symmetry with an activation energy of 0.1 eV. The most stable Be_s configuration has T_d symmetry with a spin state of $S = 1$. Co-doping with nitrogen reduces the formation energy of $\text{Be}_s\text{-N}_n$ ($n = 1 - 4$) complexes, which further decreases as the number of nitrogen atoms increases. This is attributed to the smaller covalent radius of nitrogen compared to carbon, resulting in reduced lattice distortion. $\text{Be}_s\text{-N}_3$ and $\text{Be}_s\text{-N}_4$ co-doping introduces shallow donors, while Be_s exhibits n -type semiconductivity, but the deep donor level renders it impractical for room-temperature applications. These findings provide valuable insights into the behavior of beryllium as a dopant in diamond and highlight the potential of beryllium-nitrogen co-doping for achieving n -type diamond semiconductors.

Key words: diamond, beryllium, nitrogen, n -type, p -type, first principle

1. Introduction

Diamond is widely used in several fields due to its remarkable properties. Consequently, it is challenging to exploit diamond in electronic device technology, which is known to dope both natural and synthetic diamonds. Diamond with p -type conductivity has been observed for B-doped diamond by ion implantation and gas-phase doping [1–7]. However, doping diamonds to obtain n -type semiconductors remains a challenge. Nitrogen, as the dominant impurity in natural and synthetic diamonds, is a relatively deep donor (1.7 eV below the conduction band minimum). Phosphorus is a promising candidate for an n -type dopant with a donor level (0.6 eV below the conduction band minimum [8]), although with low ionization fractions at room temperature in addition to low phosphorus solubility. Despite a reasonable concentration of P being reached [9], intrinsic defects compensate the introduced carriers, and many P atoms are not on the substitutional site, which can influence the number of carriers.

Sulfur has been reported to generate a shallow donor state in CVD diamonds [10–12], although the energy levels remain controversial. Prins [13] reported that oxygen incorporated by the ion-implantation technique yields shallow n -type diamond with an activation energy of approximately 0.32 eV. However, he suggested that the generation of electronic devices above 600°C deactivates the oxygen donors. Czelej et al. [14] showed that doping diamond with arsenic and antimony introduces shallow donor levels in the band gap at 0.5 eV below the conduction band minimum. Most of the potential dopants highlighted previously possess either high activation energy or high formation energy, thereby impeding the effectiveness of doping and overall performance of diamond post-doping.

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Co-doping is a strategic approach involving the utilization of a minimum of two dopants, offering a viable solution to the issue of compensation. Several researchers have attempted to achieve *n*-type diamonds using two types of dopants (co-doping), mainly B-O [15], B-N [16], Li-N [17], and the effect of hydrogen on doped diamond [18–20]. However, none of these materials yield *n*-type semiconductors. Hu et. al. [21] showed that incorporating phosphorus with boron can improve the mobility and conductivity and lead to a higher consistency in the lattice structure. Theoretical studies have shown that typical transition metal impurities such as titanium, vanadium, and chromium affect both the structural and electronic properties. The formation and transition energies of these impurities are crucial for understanding their impact on the semiconducting properties [22, 23] of the host material.

Beryllium-doped diamond was successfully obtained by microwave plasma-assisted chemical vapor deposition (MPCVD) [24]. Beryllium has also been introduced via ion-implantation [25], providing a further evidence for the possibility of incorporating Be into diamonds. As there is no complete understanding of Be doping in diamonds, there is a great motivation to pursue this issue further.

2. Method

First-principles calculations were conducted using the plane-wave pseudopotential software called AIMPRO [26, 27] within the framework of density functional theory (DFT). The structures were optimized using a conjugate gradient scheme until the total energy changed by less than 10^{-5} a.u. In the simulation of the structures investigated in this research, 216-atom simple-cubic supercells with a side length of $3a_0$ are typically utilized. This ensured that the Be atoms were closer to one another than any of the periodic images, except for the calculation of reorientation barriers using climbing nudged elastic bands, where 64 lattice sites were used for the calculation because of the computational cost.

The self-consistent modelling code utilized in this study relies on density-functional theory for modelling the candidate structures by employing a generalized gradient approximation [28]. Sampling of the Brillouin zone was carried out using the Monkhorst-Pack scheme [29] using a uniform mesh of $2 \times 2 \times 2$ special *k*-points. The expansion of Kohn-Sham eigenvectors employed a Gaussian *n*-type orbital basis. The treatment of carbon and beryllium involved fixed linear combinations of *s*- and *p*-orbitals augmented with a set of *d*-functions to account for polarization, resulting in 22 functions per atom. Nitrogen was treated using separate sets of *s*-, *p*-, and *d*-Gaussians of four different widths, yielding 40 functions per atom. The determination of the matrix elements of the Hamiltonian involved a plane-wave expansion of the density and Kohn-Sham potential with a cutoff of 300 a.u., leading to well-converged total energies with respect to the charge density basis. Diffusion barriers were determined by applying the climbing nudged elastic band approach, as described in previous works [30, 31]. Hyperfine interactions were obtained by reconstructing the all-electron wave functions in the core region [32, 33]. Electrical levels were obtained by reference to a marker systems [34]. The donor levels are obtained in comparison to N_s^0 with a level at $E_c - 1.7$ eV and the acceptor levels are obtained in comparison to B_s^0 with a level at $E_v + 0.37$ eV. The formation energy of *X* in the charge-state *q* was calculated using [35]

$$E^f(X, q) = E^t(X, q) - \sum_i \mu_i + q(E_v(X, q) + \mu_e) + \alpha_M \frac{q^2}{L\epsilon}. \quad (2.1)$$

Here, $E^f(X, q)$ represents the formation energy of system *X* in a specified charge state *q*. $E^t(X, q)$ denotes the total energy of system *X* in the same charge state *q*, derived from computational methods, such as DFT. μ_i are the chemical potentials of the atomic species, with the sum over the atoms in the system, E_v is the energy of the valence band top, μ_e is the electron chemical potential relative to the valence band top and α_M is a geometric term (Madelung constant), *L* is the length scale of the system (supercell dimension) and ϵ is the static dielectric constant of the medium. In this study, we investigated the chemical potential of Be from the hexagonal close-packed structure of pure Be bulk, whereas the chemical potential of nitrogen was based on NH₃.

3. Results

3.1. Formation energy and solubility

To investigate the complexity of the formation of the Be-doped diamonds, we computed the defect formation energy.

Table 1. Formation energies of substitutional and interstitial Be-doped in diamond. $E_s^f(X)$ and $E_i^f(X)$ represent the formation energy of substitutional and interstitial Be, respectively

Structure	$E_s^f(X)$	$E_i^f(X)$
Be-doped	4.62 eV	10.28 eV

Table 1 lists formation energies of substitutional and interstitial defects in Be-doped diamond denoted $E_s^f(X)$ and $E_i^f(X)$, respectively. The formation energies of the two configurations are quantified at 4.62 eV and 10.28 eV, respectively. This observation suggests that the incorporation of a beryllium atom into the diamond lattice is more favorable when occurring as a substitutional dopant. Importantly, the formation energy corresponding to $E_i(X)$ reaches a considerable value of 10.28 eV, which signifies that the process of introducing dopants into the diamond structure possesses significant challenges for a solitary Be atom. Such findings align with the conclusions drawn by Zhou et. al. [36]. The reason is that the covalent bond radius of the Be atom (0.96 Å) is larger than that of C atom (0.77 Å).

Table 2. Defect formation energies of $\text{Be}_s\text{-N}_1$, $\text{Be}_s\text{-N}_2$, $\text{Be}_s\text{-N}_3$ and $\text{Be}_s\text{-N}_4$ complexes. $E^f(X)$ represents the defect formation energy.

Structure	$E^f(X)$
$\text{Be}_s\text{-N}_1$	+0.28 eV
$\text{Be}_s\text{-N}_2$	-4.07 eV
$\text{Be}_s\text{-N}_3$	-4.35 eV
$\text{Be}_s\text{-N}_4$	-4.64 eV

On the other hand, we found that Be could be incorporated more easily in the presence of nitrogen. The four structures (Be-N_n , $n = 1, 2, 3$ and 4) calculation results in table 2 clearly illustrate that the formation energies of the structures are low endothermic for single nitrogen and exothermic for the other. The low formation energies of these impurities indicate that nitrogen and beryllium atoms exist as a whole in diamond instead of as individual dopants. The covalent radius of nitrogen (0.734 Å), indicating a smaller lattice distortion, results in less internal strain, which contributes to the construction of doped structures with low formation energy.

3.2. The interstitial Be, Be_i

Beryllium atoms are placed at various interstitial positions in the lattice, including the bond center (BC), antibonding (AB), hexagonal (H), and tetrahedral (T_d) sites, as well as at random positions. To establish convergence, all atoms in the cell were allowed to move freely during the geometry optimization. Moreover, we varied the basis set and included or excluded Be 1s electrons in the pseudopotential. However, no significant differences were observed.

In contrast to previous work [37], we found that among the six different structures studied, the structure shown in figure 1(a) is the most stable. The C-Be-C bond was heavily distorted from the [111] symmetry axis. Since the atom is squeezed between two carbon atoms in normal lattice sites, the Be atom breaks a C-C bond and resides in an off-axis interstitial site in the [111] direction; consequently, the original D_{3d} symmetry is reduced to C_s symmetry during geometric relaxation (denoted $\text{Be}_{i,oa1}$). We found that the energy of D_{3d} symmetry configuration was higher than C_s configuration by 1.54 eV. The Be atom has formed bonds with two nearest-neighbor C atoms, with one Be-C bond being shorter than the others with lengths of 1.44 Å and 1.49 Å, respectively. The broken C-C bond is dilated by approximately 52%

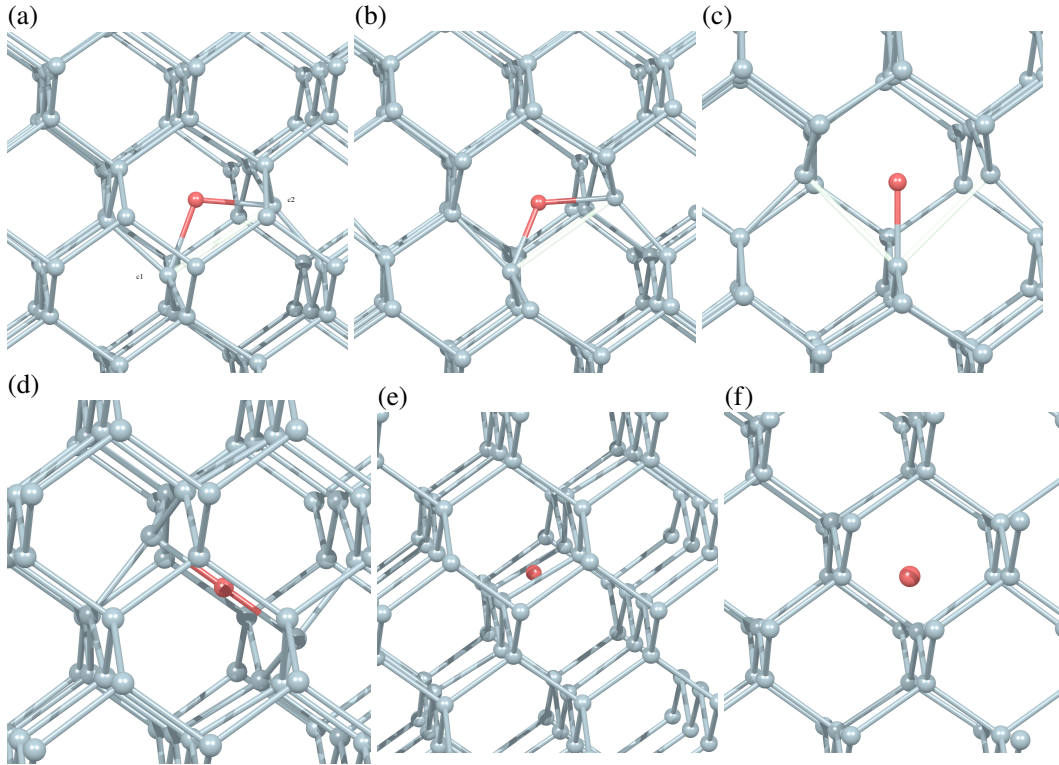


Figure 1. (Colour online) Schematic structures of the substitutional Be configurations. Grey and red spheres represent C and Be, respectively (a) off-axis C_s , (b) off-axis C_2 , (c) C_{2v} , (d) $BC-D_{3d}$, (e) $H-D_{3d}$ and (f) T_d . Transparent sticks indicate broken bonds.

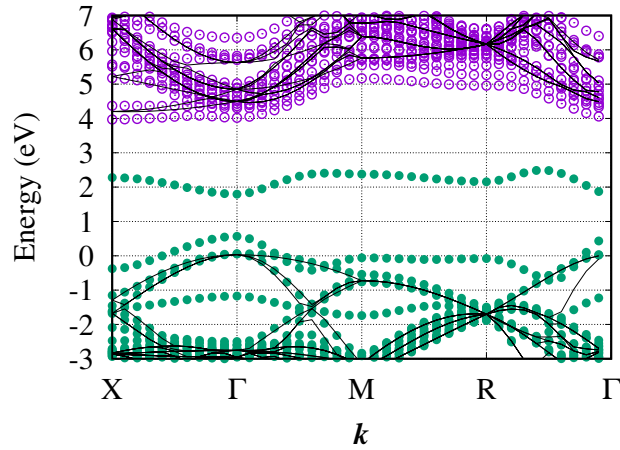


Figure 2. (Colour online) The Kohn-Sham band structure in the vicinity of the band gap for Be_i 64 supercell. Filled and empty circles show filled and empty bands, respectively, with the bands from the defect-free cell superimposed in full lines for comparison. The energy scale is defined by the valence band top at zero energy ($E_v = 0$ eV).

(2.34 Å). The band structure (figure 2) is suggestive of a donor level (a'' orbital) near the middle of the band gap ($E_v + 2.18$ eV), which is fully occupied, whereas the a' orbital is almost resonant with the valence band edge.

The next most stable configuration is characterized by the beryllium (Be) atom in the off-axis

interstitial arrangement ($\text{Be}_{i,oa2}$), as depicted in figure 1(b). In this configuration, the Be atom relocates to form equidistant bonds with two adjacent carbon atoms, each measuring 1.45 Å. The resulting triangular structure, with the Be atom at the vertex, is displaced outside the (110) plane, achieving C_2 symmetry. This configuration is less stable than $\text{Be}_{i,oc1}$ by 0.11 eV.

The results indicate a motional averaged structure for $\text{Be}_{i,oa1}$ defect as shown in figure 3(a), the Be atom orbits about the symmetry axis. The barrier between the six equivalent distortions [figure 3(b)] from D_{3d} symmetry was 0.11 eV. The calculations suggest that at room temperature, there should be motional averaging from C_s symmetry to trigonal D_{3d} .

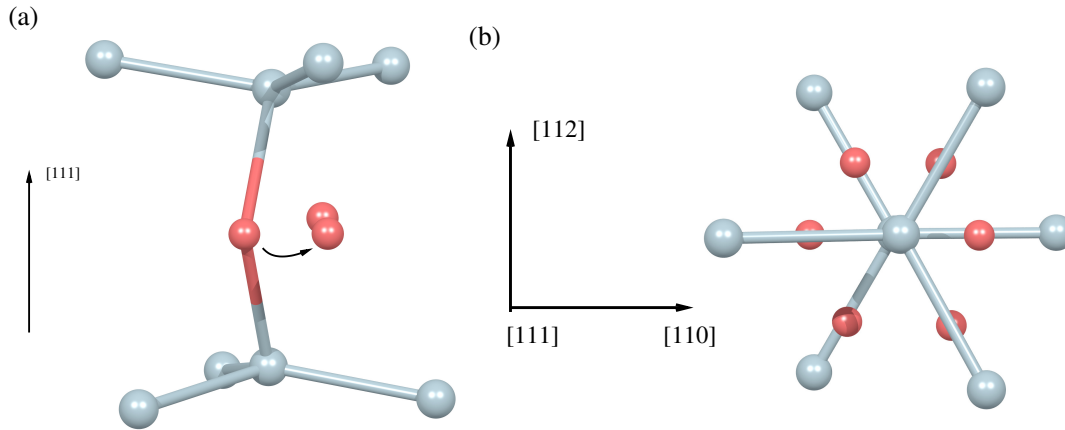


Figure 3. (Colour online) Geometry structures of the interstitial Be defects. (a) and (b) describes the bond centered configuration $\text{Be}_{i,oa1}$ with different orientation.

The structure shown in figure 1(c) exhibited C_{2v} symmetry. The Be atom forms a bond and resides at the mid-point between the three coordinated C atoms. This structure is higher in energy than that of the C_s configuration ($\text{Be}_{i,oa1}$) by 1.1 eV.

The structure in figure 1(d) shows that the Be atom sticks to the center of the C-C bond to undergo D_{3d} symmetry. The energy is higher than $\text{Be}_{i,oa1}$ by 1.54 eV. In the structure where the Be atom forms a non-bond in a hexagonal configuration (D_{3d} point group) [figure 1(e)], the energy is higher than that of $\text{Be}_{i,oa1}$ by 2 eV. In contrast to the previous work [37], we found that the structure in figure 1(f), which exhibits T_d point group, is higher than that of $\text{Be}_{i,oa1}$ by 3.1 eV. The donor level was situated at 1.2 eV below the conduction band minimum. Yan et. al. [37] suggested that T_d is an n -type metal conductivity characteristic which can readily be refuted. The relative energies are listed in table 3, which disagree with previous theoretical calculations [38].

Table 3. Relative energy of relaxed structures with respect to C_s structure in eV.

Symmetry	Spin configuration	Relative energy
C_2	$S = 0$	0.11 eV
C_{2v}	$S = 0$	1.11 eV
$D_{3d}(\text{BC})$	$S = 0$	1.54 eV
$D_{3d}(\text{H})$	$S = 0$	2.00 eV
T_d	$S = 0$	3.14 eV

In the neutral charge state, the structure is EPR-inactive. However, in the presence of shallow acceptors, charge transfer is expected to occur, which gives rise to an EPR-active defect. Hyperfine tensors for the most stable configuration in the positive charge state are listed in table 4 and there are no hyperfine values for interstitial Be in the literature thus far. In the positively charged state, the formation of the Be-C bond was weakened, with most of the electron density localized at the nearest carbon neighbors, leading to small anisotropic hyperfine tensors for Be.

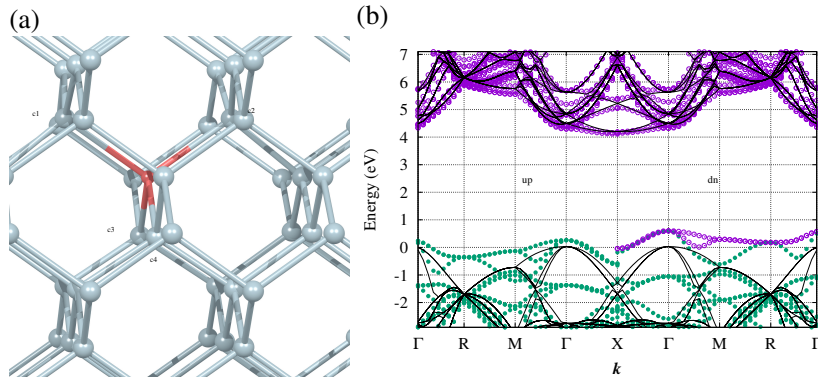
Table 4. Calculated hyperfine tensors (MHz) of Be and the two nearest neighbor ^{13}C in interstitial Be, where θ is relative to $[001]$ and ϕ is measured from $[100]$ toward $[010]$ in xy-plane.

Species	A_1		A_2		A_3	
	C_s , charge= +1, $S = 1/2$					
Be	5	(90, 315)	1.2	(165, 45)	-1.6	(75, 45)
C ₁	238	(56, 45)	113	(146, 45)	112	(90, 315)
C ₂	254	(56, 45)	102	(146, 45)	101	(90, 315)

3.3. The substitutional Be, Be_s

We also examined the stability and electronic characteristics of the substitutional dopants Be_s , because the interstitial lithium within the diamond lattice may exhibit mobility and is likely to be localized at carbon vacancies [39, 40]. As the elements are located in the same period as lithium, it is conceivable that beryllium interstitial impurities can also be accommodated at the vacancy sites.

Series of structures are determined. In contrast to Yan et. al. [37], we find that Be_s has T_d symmetry and is the most stable one [figure 4 (a)] with the spin state of the system being 1, the energy difference between the optimized structures with lowest energy, and that constrained to $(C_{3v}, S = 0)$, $(C_{2v}, S = 0)$ and $(T_d, S = 0)$ are found to be marginally higher by 0.09 eV, 0.10 eV and 0.12 eV, respectively. The Be_s -C bond length was 1.67 Å. The band-gap is shown in figure 4(b). The empty bands being 0.71 eV above the valence band top suggests that Be has double acceptor. A previous study [37] showed that Be_s induces a shallow acceptor level in the band gap. However, they reported neither a method that was used nor the location of the electrical levels. For $S = 0$ configuration, the acceptor level is at 0.60 eV above the valence band top. Tests utilizing 216-atom cells produce qualitatively analogous outcomes for shallow acceptor defects; however, the energy levels are marginally lower within the band gap. This defect has three metastable structures, all of which possess acceptor levels located at 0.71 eV above the valence band.

**Figure 4.** (Colour online) (a) Schematics for Be_s (T_d). Grey and red spheres represent C and Be, respectively. (b) Band structure for Be_s configuration. Filled and empty circles show filled and empty bands, respectively. The energy scale is defined by the valence band top at zero energy.**Table 5.** Calculated hyperfine tensors (MHz) of Be and the four nearest neighbor ^{13}C in substitutional Be. θ and ϕ are given as indicated in table 4

Species	A_1		A_2		A_3	
	$T_d, S = 1$					
Be	-4	(90, 0)	-4	(90, 90)	-4	(0, 0)
C ₁ ,C ₂ ,C ₃ ,C ₄	57	(55, 225)	17.2	(45, 90)	17.2	(66, 333)

In the neutral charge state, the structure is EPR-inactive. However, the acceptor level in the lower half of the bandgap is likely to be negatively charged in materials containing nitrogen-donors. The small hyperfine tensors on the Be atom indicate that the probability density of the two unpaired electrons is localized on the nearest-neighbor carbon atoms, as illustrated in table 5.

3.4. The $\text{Be}_s\text{-N}_n$ complexes ($n = 1, 2, 3$ and 4)

We attempted to co-dope Be with nitrogen impurities. Four sets containing one, two, three, and four nitrogen atoms were introduced around the substitutional Be atom to replace the original nearest-neighbor carbon atoms denoted $\text{Be}_s\text{-N}_1$, $\text{Be}_s\text{-N}_2$, $\text{Be}_s\text{-N}_3$ and $\text{Be}_s\text{-N}_4$, respectively.

$\text{Be}_s\text{-N}_1$ relaxed into a C_{3v} symmetry as shown in figure 6(a), where the Be-C and Be-N bond lengths are 1.67 Å and 1.60 Å, which are respectively 8.4% and 3.9% longer than the C-C bonding. Our calculations show that the formation energy of $\text{Be}_s\text{-N}_1$ decreases (+0.28 eV) compared to single-element doping at substitutional or interstitial sites. One possible explanation is that the atomic radius of the nitrogen atoms is smaller. $\text{Be}_s\text{-N}_1$ doping introduces an acceptor level lying at 0.85 eV above the valence band top. In the neutral charge state, the $(\text{Be}_s\text{-N}_1)$ complex has an odd number of electrons, rendering it EPR active with $S = 1/2$. The calculation hyperfine tensors for the N, Be and the three carbon atoms nearest neighbor to Be are listed in table 6. The unpaired electron probability density is localized on the three carbon atoms neighboring the Be atom.

Table 6. Calculated hyperfine tensors (MHz) of $\text{Be}_s\text{-N}_1$. θ and ϕ are given as indicated in table 4

Species	A_1		A_2		A_3	
	$C_{3v}, S = 1/2$					
Be	-0.2	(125.3, 135)	-5.8	(53.3, 135)	-5.8	(90, 45)
N	-1.6	(125.3, 135)	-1.2	(144.7, -45)	-1.2	(90, 45)
C ₁ ,C ₂ ,C ₃	27.6	(116.8, 120.3)	29.3	(45, 180)	84.2	(57, 49.5)

Interestingly, when the number of N atoms increased to two, the formation energy of $\text{Be}_s\text{-N}_2$ became negative (-4.07 eV). Increasing the number of N atoms results in less strain, as the covalent radius of the nitrogen atom is smaller than that of carbon. $\text{Be}_s\text{-N}_2$ relaxed to C_{2v} symmetry, as shown in figure 6(b). The Be-C and Be-N bond lengths are 1.63 Å and 1.64 Å, which are 5.8% and 6.5% longer than the C-C bonds, respectively. The ground state of the neutral complex would have $S = 0$, and thus would be EPR-inactive. Moreover, it possesses a very deep acceptor at $E_v + 4.91$ eV. Therefore, it is not possible for the complex to be ionized.

When the number of N atom increases to three, the formation energy of $\text{Be}_s\text{-N}_3$ impurity is even lower (-4.35 eV), and it is 8.97 eV and 4.63 eV lower than that of $\text{Be}_s\text{-N}_1$ and Be, respectively. Surprisingly, in contrast to Sun study [41], geometry optimization of $\text{Be}_s\text{-N}_3$ resulted in a structure with C_1 symmetry. As shown in the figure 6(c), the distances from Be to the two four-fold coordinated N atoms, three-fold coordinated N atom and C are 1.65 Å 1.56 Å and 1.63 Å, respectively, which are 7.1%, 1.3% and 5.8% longer than the original C-C bond.

$\text{Be}_s\text{-N}_3$ is also found to possess a metastable structure with C_s symmetry; this configuration is only +0.11 eV higher in energy than the C_1 configuration. in contrast to the results of a previous study [41, 42]. The band gap indicates a shallow donor level at 1 eV below the conduction band minimum which is lower than that of N. The hyperfine tensors are presented in table 7. The unpaired electron density was largely localized on C-N antibonding orbital as illustrated in figure 5, providing a hyperfine tensor magnitude close to that of the P1 center. The broken N-C bond dilation was similar to that of P1 center in the diamonds.

Finally, when the number of N atoms increased to four, the formation energy of $\text{Be}_s\text{-N}_4$ impurity reached -4.64 eV. $\text{Be}_s\text{-N}_4$ structure exhibited C_s symmetry [figure 6(d)], in contrast to a previous study [41]. The distances from Be to the three four-fold coordinated N atoms and three-fold coordinated N atom are 1.65 Å and 1.63 Å, respectively, which are 7.1% and 5.8% longer than the original C-C bond. The band-gap level of $\text{Be}_s\text{-N}_4$ is higher than that of $\text{Be}_s\text{-N}_3$, which is 1.16 eV below the conduction

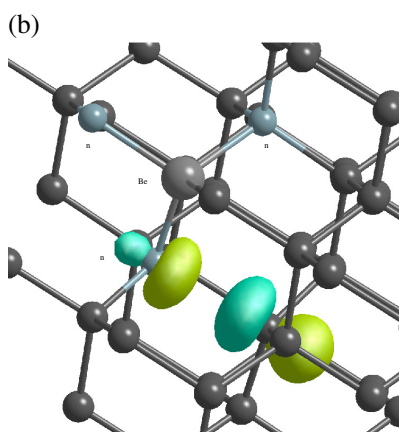


Figure 5. (Colour online) Unpaired electron Kohn-Sham functions for Be-N₃ complex.

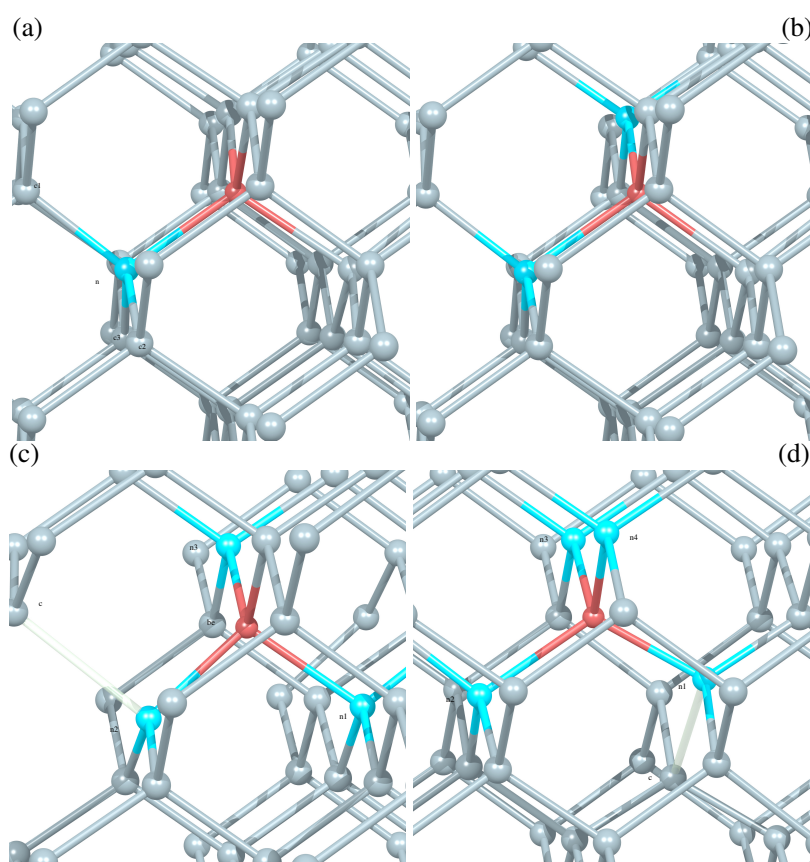


Figure 6. Schematic structures of Be-N complexes. Grey, blue and red spheres represent C, N and Be, respectively. (a) Be_s-N₁, C_{3v} symmetry and (b) Be_s-N₂, C_{2v} symmetry, (c) Be_s-N₃, C_1 symmetry and (d) Be_s-N₄, C_s symmetry. Transparent sticks indicate broken bonds.

band minimum. Midgap acceptors such as vacancies [43] may ionize these defects without the need for illuminations. The effect of ionizing Be-N₄ is a reduction in the broken N-C dilation from %40 in the neutral state to %29 in the positive charge state compared to the C-C bond in a perfect diamond. We also report the hyperfine interactions for Be, N and radical C atoms, although to-date, there are no experimental data with which to make a comparison. The unpaired electron density was localized in an N-C antibonding orbital similar to that of the Be-N₃ complex.

Table 7. Calculated hyperfine tensors (MHz) of Be_s-N₃. θ and ϕ are given as indicated in table 4

Species	A_1		A_2		A_3	
	$C_1, S = 1/2$					
Be	-0.2	(50, -33)	1.5	(73, 72)	1.9	(45, -180)
N ₂	87.2	(73, -56)	87.3	(140, 12)	129.1	(46, 55)
C	178.4	(62, 157)	178.5	(48, -83)	362.6	(45, 56)

Table 8. Calculated hyperfine tensors (MHz) of (Be_s-N₄)⁺¹. θ and ϕ are given as indicated in table 4

Species	A_1		A_2		A_3	
	$C_s, S = 1/2$					
Be	-0.1	(114.5, 135)	1.5	(24.6, 135)	2	(90 - 135)
N ₁	86.1	(143.5, 135)	86.2	(90, 45)	127.2	(53.5, 135)
C	175.9	(90, 45)	176	(144, 135)	360	(54.1, 135)

4. Conclusions

First-principles calculations were conducted to investigate the formation energy, solubility, and electronic properties of Be-doped and Be-N co-doped diamonds. The formation energy of substitutional Be defects (4.62 eV) is lower than that of interstitial Be defects (10.28 eV), suggesting that Be incorporation is more favorable as a substitutional dopant. However, the high formation energies indicate significant challenges in introducing Be dopants into the diamond structure. Co-doping with nitrogen was found to considerably reduce the formation energy, with Be-N complexes having low endothermic or exothermic formation energies depending on the number of N atoms. Among the interstitial Be configurations, the off-axis interstitial configuration with C_s symmetry Be_{i,oa1} was found to be the most stable. Substitutional Be (Be_s) introduces a double acceptor level 0.71 eV above the valence band top. Be-N co-doping with increasing number of N atoms (1 to 4) progressively lowers the formation energy, with Be-N₃ and Be-N₄ complexes exhibiting shallow donor levels at 1.0 eV and 1.16 eV below the conduction band minimum, respectively. Hyperfine tensors were calculated for various configurations to aid in future experimental identification of these defects.

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Берилій та пов'язані з ним домішки в алмазі: дослідження методом функціоналу густини

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Для дослідження геометрії, електричних властивостей та надтонких структур різних конфігурацій алмазів, легованих берилієм, включаючи міжвузлові (Be_i), замісні (Be_s) та берилій-азотні (Be-N) комплекси, було застосовано першопринципне моделювання методом функціоналу густини. Включення Be в алмазну ґратку в якості замісної легуючої речовини є більш сприятливим, ніж міжвузловий легант, хоча обидва процеси є ендотермічними. Міжвузловий Be може потенційно проявляти динамічне усереднення від площинної до осьової симетрії з енергією активації 0.1 еВ. Найстійкіша конфігурація Be_s має симетрію T_d зі спіновим станом $S = 1$. Спільне легування азотом знижує енергію утворення комплексів $\text{Be}_s\text{-N}$, яка ще більше зменшується зі збільшенням кількості атомів азоту. Це пояснюється меншим ковалентним радіусом азоту у порівнянні з вуглецем, що призводить до зменшення спотворення кристалічної ґратки. Спільне легування $\text{Be}_s\text{-N}_3$ та $\text{Be}_s\text{-N}_4$ вводить поверхневі донори, тоді як Be_s демонструє напівпровідність n -типу, але глибокий донорний рівень робить його непрактичним для застосувань при кімнатній температурі. Отримані результати дають важливе розуміння поведінки берилію як легуючої домішки в алмазі та підкреслюють потенціал спільного легування берилієм і азотом для отримання алмазних напівпровідників n -типу.

Ключові слова: алмаз, берилій, азот, n -тип, p -тип, першопринципне моделювання
