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Structural and Electromagnetic Analysis on Silicon-doped Boron Nitride Nanostructures for Gas Sensing: A Physico-chemical Study

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Abstract

It was studied how nitrogen-based gases containing NO, NO_2, and N_2O attach to a special kind of nanostructure called Si-doped boron nitride (BN) nanocage (B_5N_{10}). Our findings show that when these gases stick to the Si-doped BN, they form stable compounds, especially when the gas is right in the center of the cage. Using nuclear quadrupole resonance analysis, it was found that silicon-doped BN has the least change in electric potential and the highest negative charge on the atoms. Nuclear magnetic resonance results also showed how effectively the silicon atoms in the BN structure can accept electrons when toxic gases are attached, and how strong the bonds are between the silicon and the gas molecules. Additionally, the adsorption of gas molecules can create a spin polarization on the BSiN surface, suggesting these materials can be used as magnetic surfaces to detect gases. Through IR analysis, the adsorption of NO_2, NO, and N_2O showed the most changes and the strongest tendency for gas molecules to stick to the surface. Based on the results of the standard Gibbs free energy change for adsorption, the effectiveness of Si doping in BN nanocages for adsorbing gas molecules depends on the strength of the covalent bonds between the gas molecules and the BSiN structure. Finally, the best selectivity for gas molecule adsorption in the doped BN nanocage, from highest to lowest, is: BSiN(NO_2) > BSiN(N_2O) > BSiN(NO). These results indicate that the new BSiN catalyst is a good material for creating effective catalysts.

Keywords

nanostructure, air pollution, gas sensor, doping silicon, boron nitride, quantum calculations

1 Introduction

Nitrous oxide, or N_2O, is a key greenhouse gas that comes mostly from human actions like farming, burning fuel, treating wastewater, and industrial activities [1]. Even though it's present in small amounts in the air, it traps more heat than other gases like carbon dioxide or methane. Also, N_2O is the main way nitrogen oxides get into the stratosphere, and these nitrogen oxides can damage the ozone layer either directly or through complex chemical reactions [2–4]. Because of this, there is worry about too much N_2O being released into the atmosphere. In recent years, many efforts have been made to reduce N_2O levels. Some examples include using less nitrogen-based fertilizer [5], reducing the use of fuels that contain nitrogen in cars and other sources, and developing methods to break down or change N_2O into other substances [4–6].

Boron nitride (BN) nanomaterials are used because they have great qualities like being eco-friendly for absorbing pollutants and having semiconducting properties [7–10]. These materials often behave like semiconductors, making them a good substitute for carbon nanotubes. The properties of boron and nitrogen, which are next to carbon in the periodic table, make boron nitride a topic of many studies [11–13]. In recent years, many studies have looked into how chemical pollutants can be removed using different types of boron nitride nanostructures as materials for cleaning water [14–16]. Scientists have explored various forms of boron nitride-based nano adsorbents, including nanoparticles, fullerenes, nanotubes, nanofibers, nanoribbons, nanosheets, nanomeshes, nanoflowers, and hollow spheres. These materials are being considered because

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they have great properties like a big surface area, flexible structures, strong chemical and mechanical resistance, lots of structural flaws, and many active sites where reactions can happen [17, 18].

Boron nitride analogues of gamma-graphyne, known as BN-yne, have been shown to be stable through first-principles calculations and quantum mechanical molecular dynamics simulations [19, 20]. The partially polar B-N bonds in BN-yne can create an additional dipole moment, making its surface more reactive towards gas molecules. Studies using density functional theory (DFT) show that the energy required to adsorb hydrogen onto BN-yne is about 0.1 eV, which is much higher than on graphyne [21]. It is important to improve the surface reactivity of BN-yne for practical use.

Recently, scientists compared how well silicon-doped boron nitride nanosheets (Si/BNNs) work compared to regular boron nitride nanosheets (BNNs) when sensing common toxic gases like carbon monoxide, carbon dioxide, hydrogen cyanide, nitrous oxide, nitric oxide, nitrogen dioxide, ozone, and sulfur dioxide. To understand how these materials perform in sensing, they used a method called ab initio calculations based on DFT. The results showed that adding silicon to BNNs greatly improved their ability to detect gases because the silicon atoms had extra free electrons. The study also found that the best sensing ability of Si/BNNs was for O_3, followed by NO, SO_2, CO, NO_2, N_2O, HCN, and CO_2. These findings can help in creating better sensors for toxic gases that are more effective, selective, and stable [22].

The researchers used spin-polarized density functional theory calculations to check if a single silicon atom doped boron nitride graphyne-like nanosheet (Si@BN-yne) could be used to reduce nitrous oxide (N_2O).The calculations showed that adding silicon to boron nitride graphene is energetically favorable, and the resulting Si@BN-yne is both dynamically and thermodynamically stable. They also studied how water and oxygen molecules attach to the Si@BN-yne nanosheet. Their findings suggest that the new Si@BN-yne material can be a good catalyst for removing nitrous oxide from the environment [23].

This research focuses on evaluating how adding silicon atoms affects the performance of a B_5N_{10} nano detectors in detecting gases. It also looks into how well the detector can remove harmful gases such as nitric oxide, nitrogen dioxide, and nitrous oxide during the process of adsorption.

2 Theoretical insights, applied material and method

2.1 Adsorption of gas molecules on Si–BN

The goal of this study is to remove harmful gases like NO, NO_2, and N_2O from the air using an environmentally friendly method with a Si-doped BN nano-detector (Fig. 1). Boron nitride nanocages were created with a silicon atom added, which helps improve the ability of the detector to sense gases. In our research, we used the CAM–B3LYP–D3/EPR-3 and LANL2DZ levels of theory to analyze and understand the sample properties.

Fig. 1 shows how gas molecules like NO, NO_2, and N_2O are adsorbed onto the BSiN surface, forming complexes such as BSiN(NO), BSiN(NO_2), and BSiN(N_2O) in a nano-detector. This process was studied using molecular modeling. The charge distribution in these complexes was calculated using Bader charge analysis [24]. The ability of

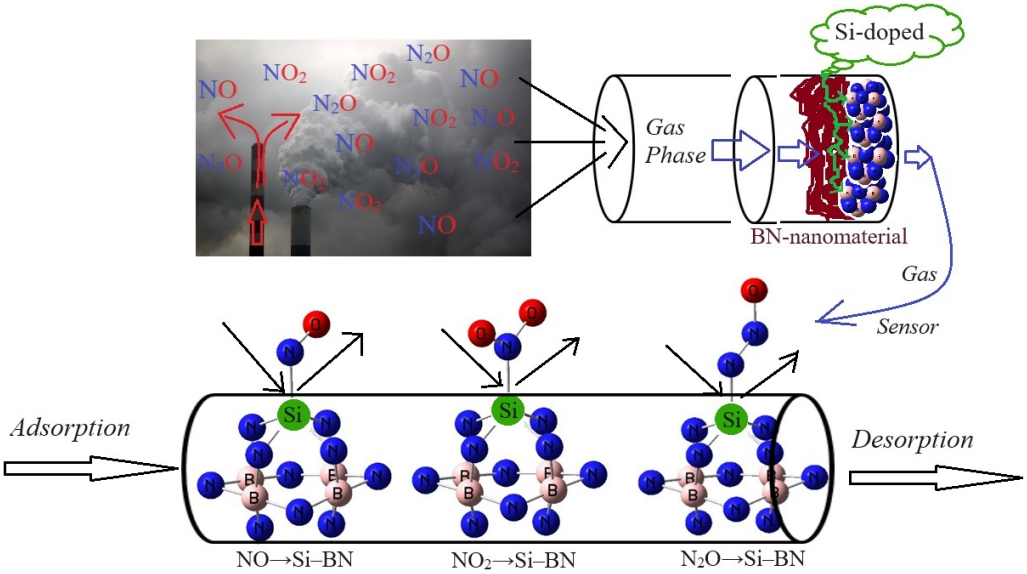


Fig. 1 Application of Si–BN for adsorption of gas molecules of NO, NO_2, N_2O and formation of complexes: BSiN(NO), BSiN(NO_2), and BSiN(N_2O) using CAM–B3LYP–D3/6-311+G (d,p), LANL2DZ calculation

the Si–BN to trap NO, NO_2, and N_2O molecules was confirmed through the formation of N→Si bonds, as shown in Fig. 1. No matter which gas molecule is involved, the boron nitride nano-detector adjusts itself to hold the molecule by improving its sensitivity through the use of different silicon doping atoms, as depicted in Fig. 1.

2.2 Application of density functional theory approach

Hohenberg–Kohn functions made the electronic density a key variable for electronic and structural calculations. Basically, the use of density functional theory became important only after W. Kohn and L. J. Sham introduced their well-known set of equations, called the Kohn–Sham (KS) equations [25–30].

Looking at the electronic density in the KS image shows a big decrease in quantum computing. This means the KS method makes it easier to study systems that can't be handled by traditional *ab-initio* methods. Kohn and Sham introduced a solution that uses single-electron orbitals to handle the kinetic energy in a simple and fairly accurate way. They found a way to calculate a correction term separately. Therefore, you start with a model of M that has electrons that don't interact with each other, connected to an external potential v_s, and with a Hamiltonian [29, 30]:

$$\hat{H}_s = -\sum_i^M \frac{1}{2}\vec{V}_i^2 + \sum_i^M v_s\left(\vec{r}_i\right) = \sum_i^M \hat{h}_s;$$
$$\hat{h}_s = -\frac{1}{2}\vec{V}_i^2 + v_s\left(\vec{r}_i\right). \tag{1}$$

By representing the single particle orbitals ψ_i all electronic densities physically acceptable for the system of "non-interacting" electrons are written in Eq. (2):

$$\rho\left(\vec{r}\right) = \sum_i^M \left|\psi_i\left(\vec{r}\right)\right|^2. \tag{2}$$

Finally, the total energy could be measured by the KS method due to Eq. (3):

$$E[\rho] = \sum_i^M n_i \left\langle \psi_i \left| -\frac{1}{2}\vec{V}^2 + v_{ext}\left(\vec{r}\right) + \frac{1}{2}\int \frac{\rho\left(\vec{r}'\right)}{\left|\vec{r}-\vec{r}'\right|}\, d\vec{r}' \right| \psi_i \right\rangle$$
$$+E_{xc}[\rho] + \frac{1}{2}\sum_\beta^N \sum_{\alpha\neq\beta}^N \frac{\vec{Z}_\alpha \vec{Z}_\beta}{\left|\vec{R}_\alpha - \vec{R}_\beta\right|}. \tag{3}$$

Therefore, the precise exchange energy functional is described by the Kohn–Sham orbitals in lieu of the density which is cited as the indirect density functional. This research has employed the penetration of the hybrid functional of three-parameter basis set of B3LYP (Becke, Lee, Yang, Parr) within the conception of DFT upon theoretical computations [31, 32]. The popular B3LYP (Becke, three-parameter, Lee–Yang–Parr) and exchange-correlation functional becomes based on Eq. (4) [33–35]:

$$E_{XC}^{\text{B3LYP}} = (1-\alpha)E_x^{\text{LSDA}} + \alpha E_x^{\text{HF}}$$
$$+b\Delta E_x^{\text{B}} + (1-c)E_c^{\text{LSDA}} + cE_c^{\text{LYP}}, \tag{4}$$

where $\alpha = 0.20$, $b = 0.72$, $c = 0.81$ shows a generalized gradient approximation: the Becke exchange functional [36] and the correlation functional of Lee et al. [37] for B3LYP and E_c^{LSDA} is the VWN local spin density approximation to the correlation functional [38], and LSDA is the local spin density approximation. In addition, E_x^{HF} is Hartree–Fock exact exchange functional, E_x^{B} is a Becke exchange potential, E_c^{LSDA} is the difference between the Hartree–Fock exchange energy and the LSDA, and E_c^{LYP} is Lee–Young–Parr correlation potential.

In this article, the potential energy surface (PES) using DFT calculations have been computed applying Gaussian 16, Revision C.01 software [39]. The input $\vec{Z}$-matrix for adsorption of NO, NO_2 and N_2O molecules in air by the BSiN has been designed with GaussView (6.06.16) [40] using basis sets of 6-311+G (d,p) for silicon and oxygen, EPR–3 for nitrogen and LANL2DZ for boron atoms with multiplicity of +1 and convergence on root-mean-square (RMS) density matrix = 1.00D-08 and convergence on maximally mixed state (MAX) density matrix = 1.00D-06.

In this study, how gas molecules interact with BSiN was modeled and looked at. Based on DFT analysis, it was found that the ability of BSiN to attract gas molecules depends mostly on the electronegativity of its functional groups and how well the BSiN interacts with the gas molecules.

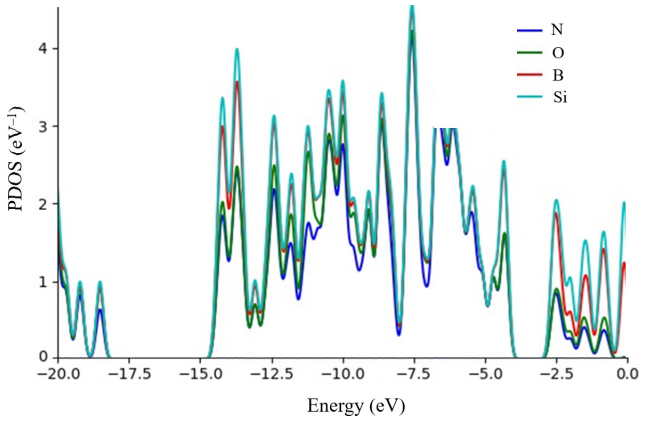
3 Results and discussion

The main gases causing air pollution are NO, NO_2, and N_2O. The study looked at how well a boron nitride nano-detector, which has been mixed with silicon, works for detecting these gases. It was found that the gas molecules bond with boron and nitrogen in a chemisorptive way. This bonding behavior is shown through how the doping atoms, B_5N_{10}, are spread out evenly, and the detector has a single layer structure.

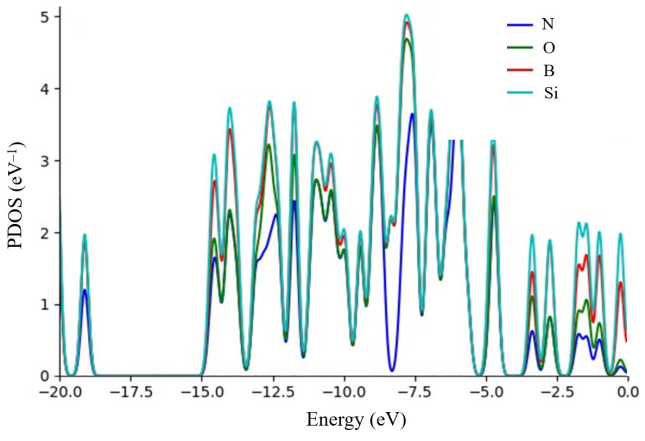
3.1 Projected density of states and electronic evaluation

The electronic structures of gas adsorption, including NO, NO_2, and N_2O, using Si-doped B_5N_{10} as a sensor to detect and capture gas molecules in the air have been shown using the CAM–B3LYP–D3/6-311+G (d,p) and LANL2DZ

levels of theory. Fig. 2 (a) to (c) shows the projected density of states (PDOS) for BSiN(G) when gas molecules are adsorbed. The presence of energy states from the *p*-orbitals of Si, N, and O within the gap of BSiN makes the system reactive. From Fig. 2, it is clear that after gas molecules are trapped, there is a strong contribution from the *p*-orbitals in the unoccupied energy levels. The partial PDOS curve shows that the *p*-states of nitrogen atoms in the gas molecules and the *p*-states of the silicon atom in BSiN overlap due to the conduction band (Fig. 2 (a) to (c)). This leads to a clear adsorption behavior in BSiN(G), because of the strong interaction between the *p*-states of nitrogen atoms in the gas molecules and the *p*-states of silicon in the BSiN complexes.



(a)



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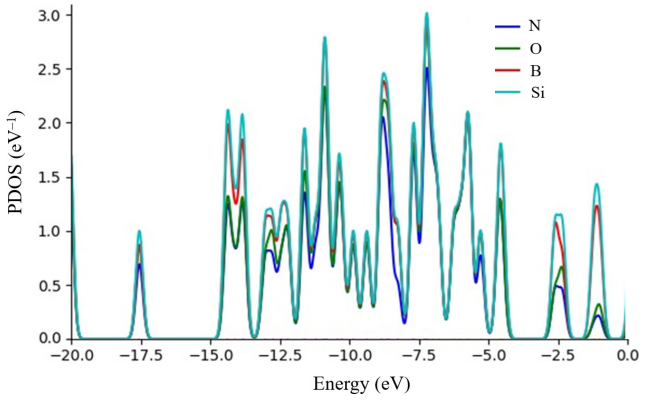

(c)

Fig. 2 PDOS (eV^{-1}) of gas molecules of NO, NO_2, N_2O adsorbed on Si–BN including (a) BSiN(NO), (b) BSiN(NO_2), and (c) BSiN(N_2O) complexes by CAM–B3LYP–D3/6-311+G (d,p), LANL2DZ

Fig. 2 (a) to (c) shows that the BSiN(NO), BSiN(NO_2), and BSiN(N_2O) complexes, through gas molecule adsorption, have the most contribution in the middle of the conduction band between –5 to –10 eV. The contribution from boron and nitrogen states becomes larger and similar to each other. Adsorbing NO, NO_2, and N_2O affects the interfacial electronic properties of B_5N_{10}, helping to select these cations. In BSiN(NO) (Fig. 2 (a)), there is a sharp peak around –7.5 eV for the Si atom. In BSiN(NO_2) (Fig. 2 (b)), there is a strong peak around –9 eV, along with a peak at –7.5 eV for the Si atom. In BSiN(N_2O) (Fig. 2 (c)), the Si graph shows a sharp peak around –7.5 eV.

3.2 Insight into nuclear quadrupole resonance

In the case of electric field gradient (EFG) at the nucleus in NO, NO_2, and N_2O, it is determined by the valence electrons that are twisted as they attach to the close nuclei of BSiN, which trap gas molecules. The nuclear quadrupole resonance (NQR) frequency where transitions happen is unique to BSiN(G) complexes (G = NO, NO_2, N_2O) (Table 1) [41–44]. In this study, the electric potential, which is the amount of energy needed to move an electric potential from one place to another within an electric field, has been calculated for BSiN(NO), BSiN(NO_2), and BSiN(N_2O) complexes (Table 1).

In Table 1, the Bader charge and electronic potential properties of Si-B, N in BSiN, and N and O in gas molecules trapped on doped-boron nitride nanocages have been studied. The results show that as the negative charge on different atoms increases, the electric potential from NQR calculations also increases. Additionally, the silicon atom (Si, atomic number 15) acting as a doping element in the BN nano-detector has the greatest potential to accept electrons from the nitrogen (N, atomic number 7) in molecules like NO, NO_2, and N_2O that are adsorbed on the BN nano-detector (Table 1). Moreover, in Fig. 3 (a) to (c), the electric potential of nuclear quadrupole resonance for various atoms such as Si/B, N in BSiN, and N and O in gas molecules trapped on doped-boron nitride nanocages has been drawn. These potentials were calculated using the CAM–B3LYP–D3/EPR-3 and LANL2DZ methods.

In Fig. 3 (a), it was seen that the BSiN(NO) material shows a good ability to catch NO gas with high sensitivity,

Table 1 The electric potential E_p and Bader charge Q through NQR calculation for BSiN(NO), BSiN(NO_2), and BSiN(N_2O) complexes using CAM–B3LYP–D3/EPR–3, LANL2DZ calculation

	BSiN(NO)			BSiN(NO_2)			BSiN(N_2O)	
Atom	Q (e)	E_p (a.u.)	Atom	Q (e)	E_p (a.u.)	Atom	Q (e)	E_p (a.u.)
Si_{15}	1.0996	−1.75968	Si_{15}	1.1638	−1.73984	Si_{15}	1.1201	−1.75314
N_1	−0.1906	−18.2495	N_1	−0.1173	−18.1461	N_1	−0.2528	−18.2554
O_2	−0.0846	−22.2135	O_2	−0.1327	−22.24	N_2	0.0998	−18.1806
B_3	0.0273	−11.2791	B_3	0.0359	−11.272	B_3	0.0245	−11.2753
N_4	0.0080	−18.2831	N_4	0.0108	−18.2776	N_4	−0.0089	−18.2677
N_5	0.0060	−18.2656	N_5	−0.0004	−18.2554	N_5	−0.0107	−18.2589
B_6	0.0310	−11.2787	B_6	0.0370	−11.2719	B_6	0.0325	−11.2758
B_7	0.0303	−11.2793	B_7	0.0359	−11.2719	B_7	0.0315	−11.2755
B_8	0.0316	−11.2788	B_8	0.0370	−11.2719	B_8	0.0331	−11.2764
N_9	−0.0205	−18.269	N_9	−0.0168	−18.2634	N_9	0.0115	−18.2797
N_{10}	0.0066	−18.2652	N_{10}	−0.0004	−18.2554	N_{10}	−0.0113	−18.2595
N_{11}	−0.2401	−18.2808	N_{11}	−0.2250	−18.2703	N_{11}	−0.2417	−18.2743
N_{12}	−0.2300	−18.2805	N_{12}	−0.2321	−18.2707	N_{12}	−0.2344	−18.277
N_{13}	−0.2316	−18.2817	N_{13}	−0.2250	−18.2703	N_{13}	−0.2346	−18.2762
N_{14}	−0.2309	−18.2802	N_{14}	−0.2320	−18.2707	N_{14}	−0.2366	−18.2776
N_{16}	−0.0204	−18.2692	N_{16}	−0.0166	−18.2634	N_{16}	0.0105	−18.2811
N_{17}	0.0082	−18.2832	N_{17}	0.0108	−18.2776	N_{17}	−0.0071	−18.2666

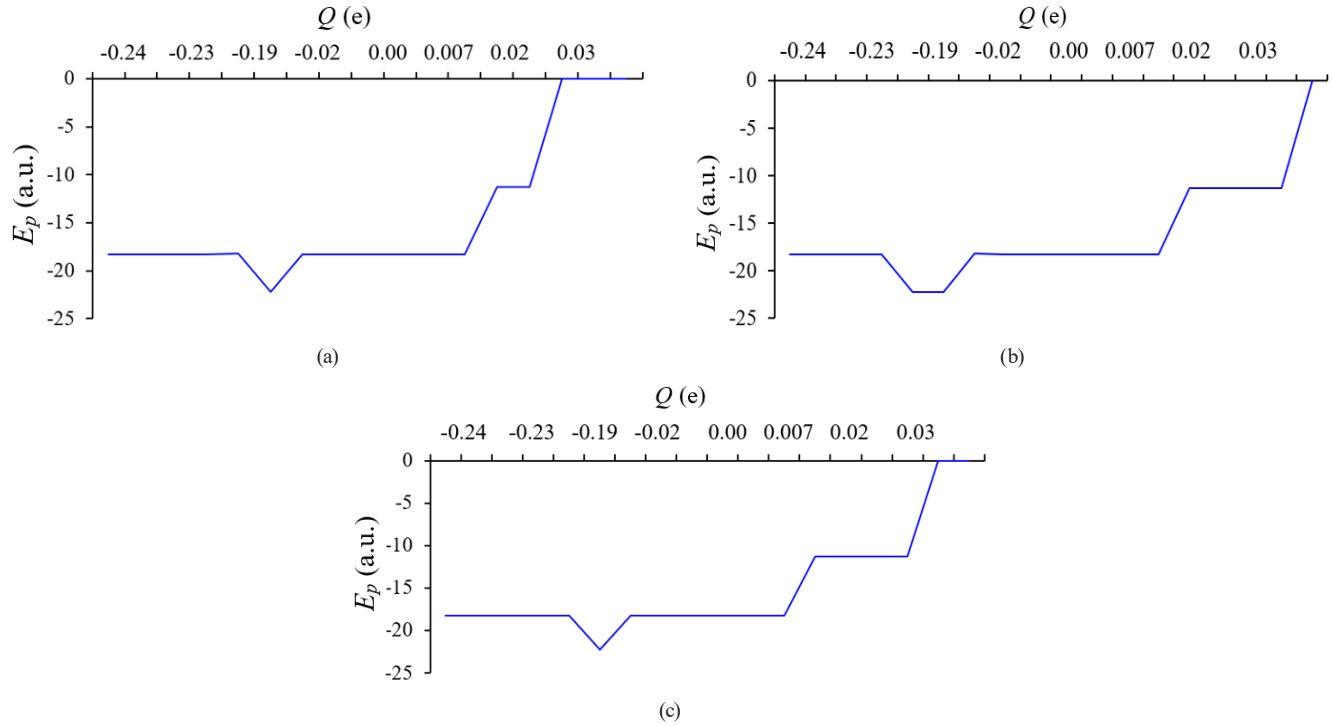

Fig. 3 Electric potential (E_p) *versus* Bader charge Q (e) through NQR calculation for (a) BSiN(NO), (b) BSiN(NO_2), and (c) BSiN(N_2O) complexes by CAM–B3LYP–D3/EPR–3, LANL2DZ

as shown by the R^2 value of 0.9827. Similarly, in Fig. 3 (b), the BSiN(NO_2) material demonstrates a similar ability to capture NO_2 gas with a slightly lower R^2 value of 0.9743. In Fig. 3 (c), the BSiN(N_2O) material was found to be effective in capturing N_2O gas, with an R^2 value of 0.9006. The curves for BSiN show waves caused by these gas molecules. The peaks in the electric potential change are visible when NO_2, NO, and N_2O are trapped on BSiN, showing that nitrogen and oxygen atoms are better at accepting electrons compared to silicon, which is part of the BN nano-detector.

The silicon in the BN nano-detector, being a semiconductor, shows better sensitivity when it accepts electrons from NO, NO_2, and N_2O during the adsorption process. The BSiN material, with an average atomic charge of 1.1 coulombs, behaves similarly in the process of removing gas molecules. It is well known that the ability to capture gas molecules is connected with BSiN, meaning that the gas molecules absorbed in the Si-doped nanocage can enter through a different path compared to the original nanocage.

3.3 Analysis of nuclear magnetic resonance spectra

Based on the results, the nuclear magnetic resonance (NMR) spectra of BSiN shows how well it can act as a sensor for absorbing harmful gas molecules like NO, NO_2, and N_2O. This helps determine how effectively BSiN can detect and remove these dangerous gases from the air in an environmentally friendly way. From the DFT calculations, the chemical shielding (CS) tensors were determined in the principal axis system to calculate both the isotropic chemical shielding (CSI) and anisotropic chemical shielding (CSA) [45]:

$$\sigma_{iso} = \left(\sigma_{11} + \sigma_{22} + \sigma_{33}\right)/3, \tag{5}$$

$$\sigma_{aniso} = \sigma_{33} - \left(\sigma_{22} + \sigma_{11}\right)/2. \tag{6}$$

The NMR data for the isotropic shielding (σ_{iso}) and anisotropic shielding tensors (σ_{aniso}) of gas molecules that are trapped in BSiN and form complexes like BSiN(NO), BSiN(NO_2), and BSiN(N_2O) have been calculated using the Gaussian 16, Revision C.01 software package [39], and the results are shown in Table 2.

In Table 2, the NMR data shows that significant amounts of NO, NO_2, and N_2O were adsorbed onto the BSiN, which acts as a selective sensor for detecting gas molecules in the air. The changes in chemical shift anisotropy were seen for nitrogen atoms, oxygen molecules (O_2) when NO or N_2O were adsorbed, and for O_2 when NO_2 was adsorbed on the BSiN. A weak signal was observed near the parallel edge of the nanocage pattern, which might be caused by the non-spherical distribution of these complexes due to boron binding. It is interesting that adding silicon to the BN nano-detector can improve the stability of the nanocage, leading to better magnetic alignment of the complexes. The results also show that silicon can be adjusted to achieve the best alignment of the nanocage when a magnetic field is applied.

In fact, when NO, NO_2, and N_2O are absorbed, they can create spin polarization on the BSiN surface, which suggests that these surfaces could be used as magnetic scavenging surfaces for gas detection. The shielding effects, both isotropic and anisotropic, change depending on how many electrons are being accepted by the gas molecules that get trapped on the atom-doped boron nitride nanocage. Fig. 4 shows the same pattern of shielding for boron and nitrogen. However, there is a big difference when silicon is used as a doping atom, especially when it interacts

Table 2 Data of NMR shielding tensors for selected atoms of BSiN(NO), BSiN(NO_2), and BSiN(N_2O) complexes using CAM–B3LYP–D3/6-311+G (d,p), LANL2DZ calculation

BSiN(NO)			BSiN(NO_2)			BSiN(N_2O)		
Atom	σ_{iso}	σ_{aniso}	Atom	σ_{iso}	σ_{aniso}	Atom	σ_{iso}	σ_{aniso}
Si_{15}	14.62	12.52	Si_{15}	13.41	10.65	Si_{15}	28.77	17.21
N_1	192.56	384.90	N_1	351.76	362.40	N_1	78.93	567.22
O_2	483.66	446.82	O_2	1640.67	1363.15	N_2	625.27	512.88
B_3	82.97	83.28	B_3	86.75	83.11	B_3	76.10	120.90
N_4	632.16	715.69	N_4	667.28	729.72	N_4	1209.22	2081.44
N_5	460.89	248.70	N_5	449.04	212.10	N_5	2524.64	3080.04
B_6	82.84	84.06	B_6	87.42	81.72	B_6	84.99	95.13
B_7	83.55	82.75	B_7	86.74	83.16	B_7	89.80	100.23
B_8	82.66	83.30	B_8	87.42	81.75	B_8	88.32	97.13
N_9	336.67	513.56	N_9	313.33	635.74	N_9	278.88	3989.46
N_{10}	457.73	296.56	N_{10}	448.95	211.72	N_{10}	1756.26	2124.54
N_{11}	461.37	425.06	N_{11}	444.08	395.29	N_{11}	220.22	1341.21
N_{12}	468.95	388.36	N_{12}	449.18	406.40	N_{12}	309.98	1116.88
N_{13}	499.78	451.39	N_{13}	444.94	395.52	N_{13}	361.77	1430.73
N_{14}	465.66	387.06	N_{14}	449.40	407.20	N_{14}	265.39	1247.17
N_{16}	329.86	536.87	N_{16}	313.06	636.08	N_{16}	539.06	3707.21
N_{17}	611.84	711.69	N_{17}	666.68	729.12	N_{17}	1376.43	2295.01

with nitrogen in NO, NO_2, and N_2O during the adsorption process on the BN nano-detector.

In Fig. 4 (a) to (c), gas molecules of NO, NO_2, N_2O in the complexes of BSiN(NO) (Fig. 4 (a)), BSiN(NO_2) (Fig. 4 (b)), and BSiN(N_2O) (Fig. 4 (c)) denote the fluctuation in the chemical shielding during ion trapping. Fig. 4 (a) to (c) shows the gap chemical shielding between silicon doping of BSiN and gas molecules. The yield of electron accepting for doping atoms on the BSiN through gas molecules adsorption approves the possibility of covalent bond between silicon and these NO, NO_2, N_2O towards toxic gas removal from air. In the NMR spectroscopy, it has been observed the remarkable peaks around interaction of NO, NO_2, N_2O molecules through adsorbing on the BSiN during toxic gas detection and removal from air; however, there are some fluctuations in the chemical shielding behaviors of isotropic and anisotropy attributes. Therefore, the authors believe that the extracted results would be useful in the design of BSiN based doped nanomaterials for increasing the adsorption of gas molecules in addition to the structural studies using solid-state and solution NMR techniques.

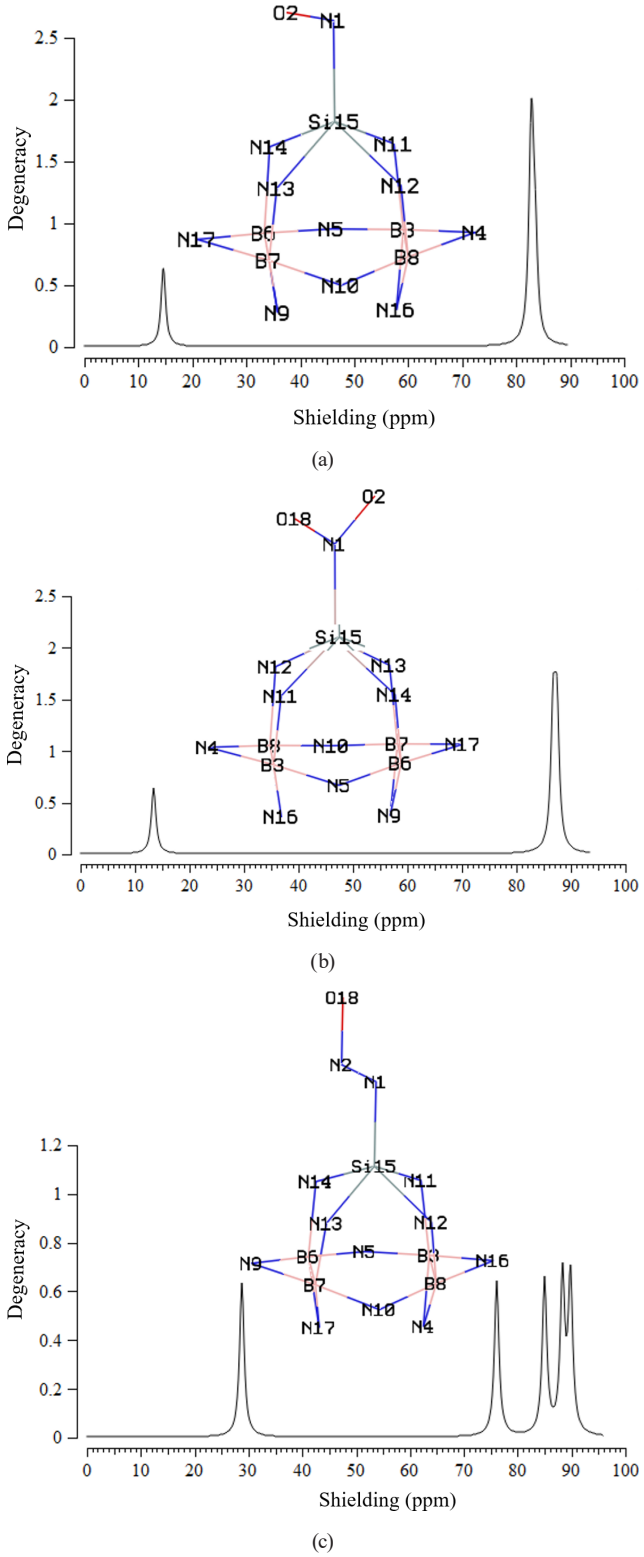

Fig. 4 The NMR spectra for (a) BSiN(NO), (b) BSiN(NO_2), and (c) BSiN(N_2O) complexes using CAM–B3LYP–D3/6-311+G (d,p), LANL2DZ

In Fig. 4 (a) to (c), the gas molecules NO, NO_2, and N_2O in the complexes BSiN(NO) (Fig. 4 (a)), BSiN(NO_2) (Fig. 4 (b)), and BSiN(N_2O) (Fig. 4 (c)) show changes in chemical shielding during ion trapping. Fig. 4 (a) to (c) also shows the difference in chemical shielding between the silicon-doped BSiN and the gas molecules. The ability of the doping atoms in BSiN to accept electrons through the adsorption of gas molecules supports the possibility of forming covalent bonds between silicon and these NO, NO_2, N_2O molecules, which can help remove toxic gases from the air. In NMR spectroscopy, clear peaks were found around the interaction between NO, NO_2, N_2O molecules and the BSiN material during gas detection and removal. However, there are some changes in the chemical shielding behavior, both isotropic and anisotropic. The authors think these findings could be helpful in designing BSiN-based doped nanomaterials to improve gas molecule adsorption, as well as in structural studies using solid-state and solution NMR techniques.

3.4 Infra red spectroscopy and thermodynamic factors

The IR calculations have been done to study how BSiN absorbs NO, NO_2, and N_2O molecules when detecting toxic gases in the air. As a result, several clusters were simulated, including BSiN bonded with NO (Fig. 5 (a)), BSiN bonded with NO_2 (Fig. 5 (b)), and BSiN bonded with N_2O (Fig. 5 (c)). These simulations were carried out using the CAM–B3LYP–D3/6-311+G (d,p) and LANL2DZ methods.

Fig. 5 (a) shows the frequency range from 200 to 1100 cm^{-1} for BSiN(NO) with sharp peaks at 652.05, 682.12, 685.59, and 1047.31 cm^{-1}. Fig. 5 (b) shows the frequency range from 100 to 1100 cm^{-1} for BSiN(NO_2) with sharp peaks at 411.31, 451.64, 563.66, 596.34, 685.50,

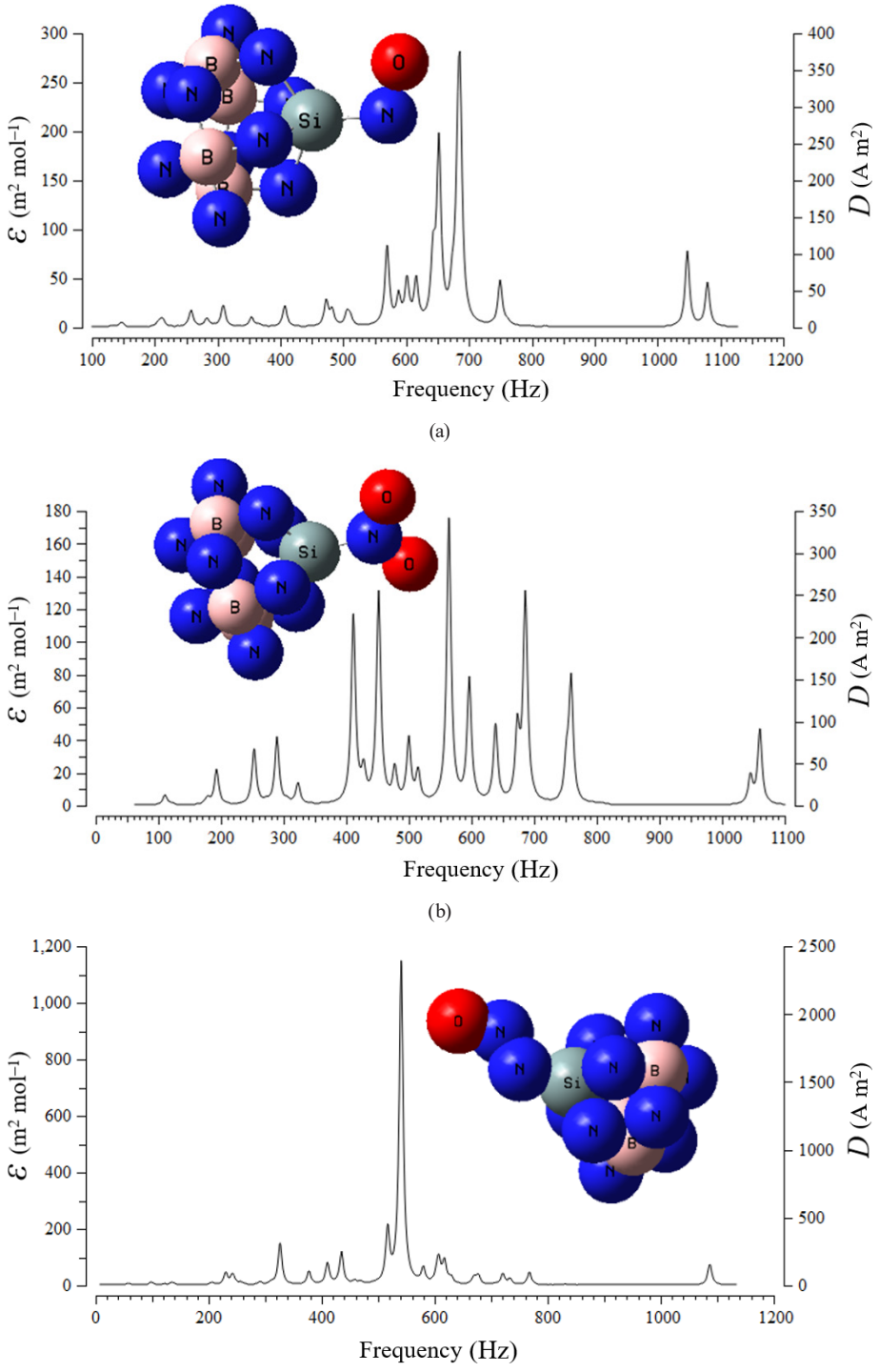

Fig. 5 The frequency (cm^{-1}) changes through the IR spectrums for (a) BSiN(NO), (b) BSiN(NO_2), and (c) BSiN(N_2O) complexes using CAM–B3LYP–D3/6-311+G (d,p), LANL2DZ. ε (m^2 mol^{-1}) is the absorbance unit and D (A m^2) is the dipole strength *via* the esu or electrostatic unit, which is a unit of charge in the Gaussian unit system

and 758.87 cm^{-1}. Fig. 5 (c) shows the frequency range from 200 to 1100 cm^{-1} for BSiN(N_2O) with sharp peaks at 326.33, 410.18, 435.01, 516.74, and 540.63 cm^{-1}. From the IR spectroscopy, the adsorption of NO_2, NO, and N_2O shows the most fluctuations when detected using a doped BN nano-detector with a Si atom. The IR spectra of NO, NO_2, and N_2O adsorbed on BSiN show that the structure of the main complex is related to the electron behavior of the doped Si on the BN nano-detector. Table 3, which includes thermodynamic data, suggests that BSiN, due to its ability to adsorb NO_2, N_2O, and NO, may be more effective at detecting and removing gas molecules from polluted air.

Table 3 The thermodynamic characters of BSiN(NO), BSiN(NO_2), and BSiN(N_2O) complexes using CAM–B3LYP–D3/6-311+G (d,p), LANL2DZ calculation

Compound	Dipole moment (A m^2)	$\Delta E^0 \times 10^{-3}$ (kcal/mol)	$\Delta H^0 \times 10^{-3}$ (kcal/mol)	$\Delta G^0 \times 10^{-3}$ (kcal/mol)	S^0 (cal/K × mol)
BSiN(NO)	1.1293	−489.207	−489.206	−489.239	108.794
BSiN(NO_2)	2.5583	−536.378	−536.377	−536.411	111.937
BSiN(N_2O)	1.7382	−523.518	−523.518	−523.552	114.612

Thermodynamic parameters for the adsorption of gas molecules with BSiN have been calculated using the DFT method. It was found that, for a specific number of nitrogen donor sites in NO, NO_2, and N_2O, the stability of the complexes, due to the presence of silicon doping atoms, follows this order: BSiN(NO_2) is more stable than BSiN(N_2O), which in turn is more stable than BSiN(NO) (as shown in Table 3).The thermodynamic data in Table 3 helps identify the highest efficiency of silicon doping in BN nano-detectors for gas molecule adsorption, based on the standard adsorption Gibbs free energy change $\left(\Delta G^0_{ads}\right)$, which depends on the covalent bonding between the gas molecules (NO, NO_2, N_2O) and the BSiN material, making it a strong sensor for removing air pollutants.

The adsorption process of NO, NO_2, N_2O molecules on the BSiN is affirmed by the ΔG^0_{ads} quantities:

$$\Delta G^0_{ads} = \Delta G^0_{\mathrm{BSiN}(G)} - \left(\Delta G^0_G + \Delta G^0_{\mathrm{BSiN}}\right);\ G = \mathrm{NO}, \mathrm{NO}_2, \mathrm{N}_2\mathrm{O}. \quad (7)$$

Table 3 has shown that the key role of doped atom of Si during interaction between the adsorbates of NO, NO_2, N_2O molecules as the electron donor and the adsorbent of BSiN as an electron acceptor.

4 Conclusion

This research investigated doping silicon on the boron nitride nanocage to improve its ability to detect toxic gases, which helps in cleaning polluted air. The research tested how well the BSiN material can separate different gas molecules, like NO, NO_2, and N_2O, by looking at the electrical forces between the gas molecules and the BSiN. The Si atom is found to be the active catalytic site for chemisorbed and dissociated NO, NO_2, and N_2O molecules due to the localization of a significant positive charge and spin density. The electrical and heat-related properties of the BSiN were studied using a method called density functional theory. The results showed that the gas molecules stick to the Si–BN in a stable way, with the strongest attachment happening right in the middle of the BSiN structure. The ability of the doped boron nitride nanocage to pick up different gases is in this order: BSiN (NO_2) is the best, followed by BSiN (N_2O), and then BSiN (NO). This research suggests that using metals, nonmetals, and metalloids as doping elements in nanomaterials can help create better sensors for removing pollution. Based on these exciting results, BSiN is recommended as a very effective, inexpensive, and eco-friendly catalyst for removing NO, NO_2, and N_2O from waste gases.

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