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ABSTRACT
In recent work, we have investigated the electronic and optical properties of pristine and functionalized Si$_2$BN quantum dots (QDs) using first-principles calculations. Due to the edge functionalization, Si$_2$BN QDs have binding energies of $-0.96$ eV and $-2.08$ eV per hydrogen atom for the adsorption of single and double hydrogen atoms, respectively. These results reveal the stability and the bonding nature of hydrogen at the edges of Si$_2$BN QD. In particular, the charge transfer between hydrogen and other atoms is explicitly increased. The electronic band structure of pristine Si$_2$BN QD shows a metallic behavior with a finite number of electronic states in the density of states at the Fermi level. The frequency-dependent optical properties, such as refractive index, extinction coefficient, absorption coefficient, electron energy loss spectra, and reflectivity, are computed for both the parallel and perpendicular components of electric field polarization. The higher absorption was found in the infrared regime. The present study shows that the functionalization of Si$_2$BN QD by two hydrogen atoms is energetically stable. It offers a promising application of Si$_2$BN QD, which can be used in optical nanodevices such as photodetectors and biomedical imagination.

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INTRODUCTION
In all of the available alternative energy sources such as solar batteries and fuel cells, hydrogen is the substantial reassuring candidate to fulfill rapidly enhancing demand as an alternative. To conserve the environment from the harmful effects of fossil fuel, to meet the requirement of more energy, and to store hydrogen have become the hottest topics of investigation for the researchers working in the field around the globe nowadays. Carbon-based materials are recommended as a potential application for hydrogen storage media, viz., carbon nanotube, fullerenes, and graphene. All these materials offer an advantage of a quite high surface area, thermal stability, and easily amenable absorption capacity.1–4 In recent years, much attention has been focused on the wide application potential of graphene, and more efforts are made to explore other applications of graphenelike materials. Among those, graphene is a planar layer exfoliated from graphite and has a consistent focus of research due to its structural, chemical, and electronic properties.5 In the recent development of materials science, a rapid expansion of research in the direction of discoveries of materials for sustainable and renewable energy is observed. Hydrogen is assumed to be one of the most important elements for future energy strategies due to its strong efficiency, abundant availability, and environmental friendliness.6–8 Because of its 2D nature, the Si$_2$BN monolayer can be pliable and strong. It could be like other properties of 2D materials that indicate superior and high
electron flexibilities, which have tunable electronic band structure and high thermal conductivities. Moreover, the presence of Si atoms in the monolayer of Si$_2$BN will make the surface more reactive. Therefore, it is a very interesting material candidate for hydrogen storage.\textsuperscript{3–14} In all of these materials, such as 2D graphene, the Si$_2$BN monolayer has garnered a lot of attention for its potential use and application of hydrogen storage.\textsuperscript{14} After taking inspiration from the above work, we have performed a detailed study on the structure, electronic, and optical properties of functionalized graphenelike solid Si$_2$BN QD.

It was previously reported that the Si$_2$BN monolayer has superior carrier mobilities for electrons and shows a higher capacity for Si$_2$BN QD, which was large enough to avoid the interaction between the Si$_2$BN QDs in the neighboring periodic images, we take only the Γ-point to sample the Brillouin zone. The frequency-dependent optical properties are calculated by random phase approximation (RPA).

The frequency-dependent complex dielectric function $\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$ is known to describe the optical properties of materials, where $\varepsilon_1$ and $\varepsilon_2$ are the real and imaginary parts of complex dielectric functions,\textsuperscript{26} respectively.

$$\varepsilon_1(\omega) = 1 + \frac{2}{\pi} \int_0^\infty \frac{\alpha'\varepsilon_2(\alpha')d\alpha'}{(\alpha'^2 - \omega^2)}$$

$$\varepsilon_2(\omega) = \left(\frac{4\pi^2}{m^2\alpha^2}\right) \sum_k \int \left[(i|M|)^2f(1-f)\right.\left.\times \delta(E_{jk} - E_{ik} - \omega)d^2k\right]$$

The absorption coefficient, extinction coefficient, reflective index, electron energy loss spectrum, and reflectivity are calculated from the following relations:

$$\alpha(\omega) = \sqrt{2}\omega[\varepsilon(\omega) - \varepsilon_1(\omega)]^{1/2},$$

$$K(\omega) = \left[\frac{\sqrt{\varepsilon_1(\omega)^2 + \varepsilon_2(\omega)^2} - \varepsilon_1(\omega)}{2}\right]^{1/2},$$

$$n(\omega) = \left[\frac{\sqrt{\varepsilon_1(\omega)^2 + \varepsilon_2(\omega)^2} + \varepsilon_1(\omega)}{2}\right]^{1/2},$$

$$L(\omega) = \frac{\varepsilon_2(\omega)}{\varepsilon_1(\omega)^2 + \varepsilon_2(\omega)^2},$$

$$R(\omega) = \frac{|\sqrt{\varepsilon(\omega) - 1}^2}{|\sqrt{\varepsilon(\omega) + 1}|^2},$$

where $\varepsilon(\omega) = \sqrt{\varepsilon_1(\omega)^2 + \varepsilon_2(\omega)^2}$ is the relative dielectric constant.

**RESULTS AND DISCUSSIONS**

**Structural properties**

The optimized structure of graphenelike pristine Si$_2$BN (PSi$_2$BN) with the unit cell having a hexagonal symmetry is shown in Fig. 1. The optimized bond length of PSi$_2$BN is 1.46 Å between B–N atoms, 2.24 Å between Si–Si atoms, 1.76 Å between Si–N atoms, and 1.95 Å between Si–B atoms, respectively. We obtained the optimized lattice parameters $a = 6.35$ Å, $b = 6.45$ Å, and $c = 18$ Å for PSi$_2$BN, which is consistent with the previously reported work.\textsuperscript{12,15,16} In previously work, the values of formation energy of the PSi$_2$BN monolayer are $-50.82$ eV with HSE-functional and $-45.39$ eV with PBE-functional,\textsuperscript{2,27} which show that the Si$_2$BN monolayer material is energetically more stable structure.

Also, Figs. 1(b) and 1(c) show the relaxed structure of edge functionalization (EF) of the Si$_2$BN quantum dot (QD) by double hydrogen (Si$_2$BNQD2) and single hydrogen (Si$_2$BNQD1), respectively. The Si$_2$BNQD2 has a length of 2.29 nm and a width of 2.03 nm as shown in Fig. 1(b). Additionally, Fig. 1(c) shows the top and side views of Si$_2$BNQD1 of 2.34 nm length and 2.15 nm width.
During the formation of Si2BNQD2, the bond length is slightly changed and the corresponding bond length is 2.24 to 2.17 Å (Si–Si), 1.95 to 1.70 Å (Si–B), 1.76 to 1.21 and 1.94 Å (Si–N), and 1.46 to 1.45 and 1.61 Å (B–N), while in the case of Si2BNQD1, the bond length is 2.24 to 2.10 and 2.25 Å (Si–Si), 1.95 to 1.68 and 1.97 Å (Si–B), 1.76 to 1.57 Å (Si–N), and 1.46 to 1.20 and 1.49 Å (B–N). To better understand the stability and bonding nature of hydrogen at the edges of Si2BN, we have calculated the binding energies of Si2BNQD, which are calculated as follows:

\[ E_b = E_{Si2BN+H/H_2} - E_{Si2BN} - \mu_{H/H_2} \]  

where \( E_{Si2BN+H/H_2}, E_{Si2BN}, \) and \( \mu_{H/H_2} \) are the total energy of Si2BN with the hydrogen atom, the total energy of Si2BN without hydrogen, and the chemical potential of hydrogen. The evolution of binding energies is \(-0.96 \text{ eV} \) and \(-2.08 \text{ eV} \) per hydrogen atom for single and double hydrogen atoms functionalized at the edges of Si2BN, respectively. This is a favorable binding energy. It means that the double hydrogen atom functionalization at the edges of Si2BN is energetically more stable.

### Electronic properties

The electronic band structure and partial density of states (PDOS) are shown in Fig. 2. The electronic band structure shows the metallic behavior of PSi2BN. However, despite the significant reduction in symmetry, PSi2BN still retains the inversion symmetry that causes the material to be metallic. Here, PDOS is to understand the orbital contribution at the Fermi level \( E_F \); the main contribution to the states at \( E_F \) comes from the \( p \)-states of “Si,” “B,” and “N” atoms. The contribution of the \( p \)-orbital of Si is much higher than that from the \( p \)-orbital of “B” and “N” atoms. The contribution of the \( s \)-orbital of all atoms “Si,” “B,” and “N” in total DOS is higher near the Fermi level. The finite numbers of electronic states are found at the Fermi level, therefore, it shows conducting behavior.

Furthermore, we have calculated PDOS of Si2BNQD2 and Si2BNQD1 to understand the contribution of different orbitals to the electronic states so that we have drawn partial density of states, as shown in Fig. 3. It can be clearly seen from the partial density of states (PDOS) of Si2BNQD2 that the states have the contribution of the \( p \)-orbital, i.e., all the three \( p \)-orbitals of “Si,” “B,” and “N.” However, the contribution of the \( p \)-orbital of the “Si” atom is much higher than that of the \( p \)-orbital of “N” and “B” atoms. The contribution of the \( s \)-orbital of “H,” “Si,” “B,” and “N” atoms is higher near the Fermi level. We have also calculated the PDOS of Si2BNQD1 to understand the orbital contributions and it consists of more discrete peaks. The contribution of \( p \)-orbitals of “Si,” “B,” and “N” atoms is more dominant at the Fermi level as compared to \( s \)-orbitals of these atoms. Additionally, the \( s \)-orbital of “H” atoms has less contribution to the conduction of electrons at the Fermi level.
level. The lower side of the density of states and the contribution of the s-orbital of atoms "H" and "Si" are higher in the range of ~3.65 eV to 3.29 eV. "B" and "N" atoms are higher near the Fermi level in the PDOS as shown in Fig. 3.

**Optical properties**

Additionally, we have also analyzed the frequency-dependent optical properties and made interpretations in terms of electronic band structures and the projected density of states. The imaginary part of the dielectric function (real transition occurs between the occupied and unoccupied electronic states) is calculated by Eq. (2). The dielectric function is directly related to the electronic band structure. The real part of the dielectric function is connected to the stored energy within the medium, while the imaginary part is associated with the dissipation of energy into the medium. Figures 4(a) and 4(b) show the computed parallel and perpendicular component of the real part Re ε(ω) and the imaginary part Im ε(ω) of the complex dielectric function. The real and imaginary parts of the complex dielectric functions are calculated in the electric field polarized parallel (E||X) and perpendicular (E⊥Z) to the material. The spectrum of PSi2BN and Si2BNQD consists of numerous precise peaks that can be traced to dipole-allowed transition between states near the Van Hove singularities (VHSs) 28,29.

From the real part of the dielectric function, information about the electronic polarizability of the material can be acquired. The value of the real part of the dielectric function is negative near to 1.25 eV (E||X) for PSi2BN. This indicates the metallic character of PSi2BN in the polarization direction (E||X) of the electromagnetic (EM) spectrum. The maximum electronic polarizability is in the (E||X) direction, and very less polarization is in the (E||Z) direction. Figure 4(a) shows the values of the static dielectric constant for PSi2BN, Si2BNQD2, and Si2BNQD1 in the polarization direction (E||X) are 18.74, 8.80, and 5.54, respectively, while the values of the static dielectric constant for PSi2BN, Si2BNQD2, and Si2BNQD1 in the polarization direction (E⊥Z) are 1.55, 1.29, and 1.04, respectively. Furthermore, we found that the polarization is very high in the pristine case as compared to Si2BNQD2 and Si2BNQD1. The polarization value of the PSi2BN system in the x-direction is two times larger than Si2BNQD2, while it is three times larger than Si2BNQD1. The electronic polarization of Si2BNQD2 and Si2BNQD1 systems is reduced as compared to the PSi2BN system.

It is evident from Fig. 4(b) that the imaginary part of the dielectric function depends on the direction of polarization of light, and it strongly depends on interband transition from valence band maximum (VBM) to conduction band minimum (CBM) after the absorption of light. The imaginary part of the dielectric function shows the absorption of light. In the imaginary part of the dielectric function, the absorption peaks occur in the range of 0.59 eV–8.42 eV for PSi2BN, 0.55 eV–6.43 eV for Si2BNQD2, and of 0.55 eV–6.27 eV for Si2BNQD1 in a parallel polarization direction (E||X), whereas for the perpendicular polarization direction (E⊥Z), the imaginary part...
of the dielectric function peaks rises in the range of 4.43 eV–9.75 eV (PSi2BN), 3.47 eV–9.83 eV (Si2BNQD2), and 7.66 eV–9.83 eV (Si2BNQD2). The first absorption peaks start in the infrared (IR) region for each case in the polarization direction (E||X) and show a very high intensity, which behaves like a redshift. The high absorption peak is found at 0.60 eV. It means that the material is more sensitive in the IR region.

In the imaginary part of the dielectric function Im $\varepsilon(\omega)$, there are many peaks found at 0.59 eV, 2.68 eV, 6.31 eV, and 8.46 eV in the polarization direction (E||X) and 4.4 eV, 6.05 eV, 6.91 eV, 8.12 eV, and 9.71 eV in the polarization direction (ELZ) for the PSi2BN system. For PSi2BN, all these peaks in the imaginary part are mainly associated with the four possible electronic transitions from $\pi$ (occupied states) $\rightarrow \pi^*$ (unoccupied states), $\pi \rightarrow \sigma^*$, $\sigma \rightarrow \sigma^*$, and $\sigma \rightarrow \pi^*$ between band edges near the special points in the first BZ. In the case of QD, the interband transition peak appears at 0.55 eV, 4.29 eV, 5.46 eV, and 6.45 eV for (E||X) and 4.56 eV, 5.60 eV, 7.19 eV, 8.90 eV, and 9.77 eV in (ELZ) for the Si2BNQD2 system, while for the Si2BNQD1 system, the peaks occur at 0.55 eV, 5.08 eV, and 6.29 eV in (E||X) and 7.66 eV and 9.83 eV in the (ELZ) polarization direction. The peaks shifted toward the lower photon energy side, which is associated with interband transitions from $\pi \rightarrow \pi^*$ (valence band to conduction band), while some of the peaks that appear at a higher energy side are mainly associated with the interband transition from $\pi \rightarrow \sigma^*$, $\sigma \rightarrow \sigma^*$, and $\sigma \rightarrow \pi^*$. The maximum intensity in the absorption spectra is found to be 0.59 eV, 0.55 eV, and 0.55 eV for PSi2BN, Si2BNQD2, and Si2BNQD1 in the polarization direction, respectively. There is a noticeable absorption peak at 0.59 eV, 0.55 eV, and 0.55 eV in the polarization direction (E||X) for PSi2BN, Si2BNQD2, and Si2BNQD1 systems, while there is no distinct absorption peak below 3.01 eV, 3.01 eV, and 3.01 eV for (E||X) and (E⊥X) for PSi2BN system, while for the Si2BNQD1 system, the peaks occur at 0.55 eV, 4.29 eV, 5.46 eV, and 6.45 eV; and the highest absorption peak is located at the energy of 0.71 eV, while in the polarization direction (ELZ), the absorption peaks occur at energies of 0.71 eV, 2.48 eV, 6.57 eV, and 8.56 eV, and the highest absorption peak is located at the energy of 0.71 eV, while in the polarization direction (ELZ), the absorption peaks occur at energies of 4.47 eV, 6.09 eV, 6.93 eV, 8.38 eV, and 9.77 eV; however, the high intensity absorption peak appears at 9.77 eV photon energy.

For Si2BNQD2, we noticed that the absorption peaks are located at energies of 0.63 eV, 4.21 eV, 5.52 eV, and 6.55 eV and the highest absorption peak is at 0.63 eV (IR region), which is slightly shifted to the lower photon energy site as compared to PSi2BN in the polarization direction (E||X), while for the polarization direction (ELZ), the absorption peaks are located at 4.58 eV, 5.68 eV, 7.23 eV, 8.88 eV, and 9.85 eV, and the maximum absorption peak corresponds to the energy of 7.23 eV. In the case of Si2BNQD1, the absorption of the system has two large peaks, first near the energy of 0.65 eV and the other around 6.35 eV, and the highest absorption peak is at the energy of 0.65 eV (E||X). For the (ELZ) direction, the absorption peaks are at energies of 4.45 eV, 8.40 eV, and 9.81 eV and the maximum absorption peak corresponds to the energy of 9.81 eV. We found that similar absorption peaks start from the IR region like graphene.30 The very high intensity of absorption peaks is found in the IR region; therefore, it is very sensitive in the IR region. Due to this, it can be used as an IR photodetector.

The calculated extinction coefficient and the refraction index of PSi2BN and Si2BNQD are depicted in Fig. 6. The local maximum of the extinction coefficient of PSi2BN is 4.33 and 1.24 for the parallel and perpendicular polarization directions, respectively. The maximum refractive index is 4.33 at 0.0 eV photon energy.

In the (E||X) polarization direction, the refractive index n(ω) in the IR region quickly decreases with energy, while it is stable in the UV region and becomes constant after 13.59 eV, as shown in Fig. 6. In the (ELZ) direction, it decreases monotonically even into near UV, where after oscillations, it decreases into far UV and becomes constant after 13.44 eV. For the PSi2BN system, the spectrum curves of the refractive index n(ω) decrease rapidly with an increase in photon energy in the UV region and become constant after 14.54 eV of both phases in the (E||X) and (ELZ) polarization directions. The maximum refractive index is 1.62 at 5.86 eV and 1.40 at 5.30 eV for both directions of the electric field. The PSi2BN to be used as an inner layer coating between the UV absorbing layer and the substrate could be validated due to high refractive indices. The first and maxima extinction coefficients are located at 0.68 eV for (E||X) and 9.77 eV for the (ELZ) direction. These energies cause the photons to be absorbed very fast, i.e., their depth path will be curtailed. The second main peak of the extinction coefficient is around 6.5 eV [see Fig. 6(a)], and these peaks in the
The extinction coefficient reflects the maximum absorption in the medium. Each peak in the extinction coefficient has better absorption of light as presented in Fig. 6(a).

The spectrum curve of the refractive index $n(\omega)$ of Si$_2$BNQD$_2$ and Si$_2$BNQD$1$ systems under parallel and perpendicular polarization directions rapidly decreases with an increase in photon energy in the UV region and becomes constant after 10.00 eV. In the (E||X) direction, the refractive index $n(\omega)$ decreases very fast with energy in the IR region, while in the UV region, it decreases steadily and gives a saturation state after 10.00 eV. However, in the (E$\perp$Z) direction, it decreases monotonically even into near UV, where after oscillations, it decreases into far UV and becomes constant after 10.60 eV. The maximum refractive index is 1.25 at 3.42 eV and 1.22 at 3.03 eV in the (E||X) and (E$\perp$Z) directions for the Si$_2$BNQD$_2$ system, respectively. The maximum extinction coefficient is at 0.65 eV and 7.21 eV for Si$_2$BNQD$_2$ in the polarization direction (E||X) and (E$\perp$Z), respectively. The corresponding peaks in the extinction coefficient have maximum absorption spectra, as shown in Fig. 5.

The different properties of materials can be optimized by the contribution of the electron energy loss spectrum $L(\omega)$ (EELS).

The loss spectrum arises both from the excitation of single electrons in a medium, just as it happens with the absorption of photons. It is found that some of the energy can be released in discrete amounts from a fast electron traversing in the material, represented by $L(\omega)$, and excitation of electrons by the other electrons in a medium. Plasmon excitations can be identified from the excitation of collective oscillations of the free conduction electrons in a metal by analyzing the $L(\omega)$ spectrum. The plasma frequency is known as the highest peaks in the $L(\omega)$ spectra that represent the characteristics associated with the plasma oscillations and the corresponding frequency. The plasma oscillations will successfully screen the electric field in the UV regime. The electromagnetic radiation incident is along the parallel to the z-direction, then it is reflected from the material’s surface and will increase in reflective intensity. Thus, the peaks in $L(\omega)$ also correspond to the trailing edges in the reflection spectra.

Generally, EELS describes the energy losses when the electron travels inside the materials. The EELS is represented in Fig. 7(a), which is a function of photon energy. The calculated energy loss spectrum $L(\omega)$ of the PSi$_2$BN system is depicted in Fig. 7(a). For the polarization direction parallel to PSi$_2$BN, Si$_2$BNQD$_2$, and Si$_2$BNQD$1$ systems, there are a lot of photon energy losses above 7 eV and resonance occurs visible to the UV regime. While the electromagnetic radiation incident is along the parallel to the z-direction,
the energy loss starts from 3 eV. For the (E||X) direction, the energy loss function comprises more individual peaks in each system. Si₂BNQD will significantly reduce the electron energy loss function in the UV region, as shown in Fig. 7(a).

The reflectivity of Si₂BN for both the directions is as depicted in Fig. 7(b), which describes how much light is reflected from the material with an amount of light incident on the material. In the lower photon energy below 1.18 eV for the Si₂BN system, the reflectivity in the (R||X) direction is higher than the (RLZ) direction due to the stronger optical excitations in the (E||X) case. The maximum reflectivity is found to be 93%, 88%, and 72% close to 1 eV on the x axis for SPSi₂BN, Si₂BNQD2, and Si₂BNQD1 systems, respectively. Most of the electromagnetic radiation is reflected in Si₂BN in parallel to the x-direction, while in Si₂BNQD, it is to reduce the reflection of EM light. We have also noticed that when the electric field is parallel to the Si₂BN system, the reflectivity is more at lower energy and transmission is less at this energy range. It can be observed that there are numerous peaks in the reflectivity curves up to 1.18 eV. In the low energy region for the Si₂BNQD2 system (below approximately 0.77 eV), the reflectivity in the (R||X) direction is higher than the (RLZ) direction, mainly owing to the stronger optical excitations in the (E||X) case. In the electric field perpendicular to the Si₂BNQD1 system, the reflectivity is very less in the whole photon energy region, whereas the reflectivity is relatively more at the energy range between 0.74 eV and 6.43 eV in the electric field parallel to the Si₂BNQD1 system. It is also found that the reflectivity is more at lower energy and transmission is less at this energy range in the electric field parallel to the Si₂BNQD1 system. It can be observed that there are multiple peaks in the reflectivity curves up to 7.24 eV. The maximum reflectivity reaches the higher values of 36% and 41% for (E||X) and (ELZ) directions, respectively. By taking cognizance of the above description, the Si₂BN material is much better for the IR light absorber; therefore, it is very useful in the IR photodetector.

CONCLUSIONS

In conclusion, a detailed investigation of the electronic and optical properties of PSi₂BN, Si₂BNQD2, and Si₂BNQD1 was performed by density functional theory (DFT). The Si₂BNQD2 shows it to be energetically more stable as compared to Si₂BNQD1. The electronic band structure of PSi₂BN, as well as Si₂BNQD2 and Si₂BNQD1, shows metallic behavior. Optical anisotropy is observed from parallel and perpendicular light polarization directions in PSi₂BN, Si₂BNQD2, and Si₂BNQD1 systems. We have also investigated the dielectric function, refractive index, absorption spectrum, extinction coefficient, reflectivity, and electron energy loss spectra. The calculated static refractive index is 4.33 (PSi₂BN) (E||X), 2.96 (Si₂BNQD2) (E||X), 2.35 (Si₂BNQD1) (E||X), 1.24 (PSi₂BN) (ELZ), 1.13 (Si₂BNQD2) (ELZ), and 1.03 (Si₂BNQD1) (ELZ) for different polarization directions. The higher refractive index is found in the UV part of the electromagnetic spectrum, allowing applications as an inner layer coating under UV absorbers. This indicates the great potential for applications in IR photodetector and optoelectronic devices.

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