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A DFT Study of the Photocatalytic and Photovoltaic Properties of BX (X=N, P)

[1]Shehroz Abdullah, [2]Ghulam Murtaza

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Shehroz Abdullah
Materials Modeling Lab, Department of Physics, Islamia College Peshawar, Pakistan
Ghulam Murtaza
Materials Modeling Lab, Department of Physics, Islamia College Peshawar, Pakistan

ABSTRACT

In this work we have used Density Functional Theory (DFT) to explore BX monolayers (X = N, P) in photocatalysis and photovoltaic systems. Such materials exhibit high stability and tunability, which is important to high energy conversion. Boron Nitride (BN) is a high bandgap material and thus it is a good choice of high-temperature insulator, whereas Black Phosphorus (BP) is a low bandgap material and can be used in low energy optoelectronics such as photodetectors and solar cells. Using DFT-calculation, it has been found that variations occur in the band structure, light absorption, electronic transition and charge carrier dynamics. Compared with BP which has more ample bonding properties, a high thermal conductivity is observed in BN. Optical properties, such as dielectric functions, and absorption coefficients, are sought to point out the superiority of each material. Their photocatalytic and photovoltaic can be improved by use of materials doping and heterostructure integration. As capitalized on by the research, BX monolayers will be very useful in sustainable energy applications, especially in splitting the water and harvesting the sun. Still, the additional study is required to evaluate their scalability and implement-ability. These are potential materials that can be the future green technologies.

INTRODUCTION

The recent occurrences in photocatalytic and photovoltaic research have revealed the two-dimensional (2D) materials, especially the BX (X = N, P) monolayers, as possible candidates for the conversion of energy as an effective process. This material has attracted a lot of interest by virtue of tunable electronic characteristics, stability, and their potential uses in sustainable energy systems. The BX monolayers have distinct layered structures that make them a broad platform in energy application, including photocatalysis and photovoltaics. Their tunability of electronic properties by heterostructure integration or doping have also provided access to widening their range of efficiency in energy conversion. Energy systems installed with these materials have in the recent years solved key problems of efficiency, scalability and costs [1]. Theoretical works have played an important role in the determination of structure, electronic and optical properties of BX monolayers especially on the ones implemented using density functional theory (DFT). The studies give critical information on the stability and performance of BX monolayers in different conditions which would enable optimization of the properties of monolayers towards desired goal of energy applications. DFT allows demonstrating that BX monolayers have outstanding electronic stability required in high-performance photocatalysis/photovoltaics. Moreover, doping with such elements as nitrogen, phosphorus and others has proven to change their electronic band structure, thereby optimizing their photocatalytic and photovoltaic effects. With such use of doping in maximizing their electronic properties, BX monolayers are a preferable entrée in energy systems [2]. Besides doping, use of other materials in the form of heterostructures has also been suggested in a bid to optimize the photocatalytic and photovoltaic characteristics of BX monolayers. The heterostructure uses synergistic effect of various materials, enhancing the charge separation, light absorption, and efficiency of the materials. This method has been found to demonstrate a boosted photocatalytic activity of BX monolayers through enchantment of charge monographer and mitigation of recombination charges. BX monolayers when stacked together with other 2D derivatives or semiconductor substrates can provide a more energy efficiency and scalable platform to energy harvesting situations proving the scalability of multi-material systems in high energy applications [3].

The optical properties of BX monolayers are also outstanding (very high light absorption and appropriate bandgap structure) qualifying them as good candidates to be used in photovoltaics. DFT simulations give optical properties which indicate that BX monolayers could be able to absorb sunlight efficiently and transform its energy into electricity. Their wide tunable bandgap gives the possibility to optimize the light absorption in the visible spectrum to help the efficiency of solar cells. BX monolayers also have promise in photocatalysis, especially on water splitting as a source of hydrogen as fuel an important technology in renewable energy production. These photocatalytic effects make them more appealing to the methods of producing sustainable energy sources [4].

BX monolayers are a sub-set of 2D materials with a significant potential of photocatalysis and photovoltaics. They can be highly optimized by doping and heterostructure combinations making them a perfect candidate in next generation energy conversion applications. Their structural stability and performance, their potentialities regarding optimization, have been theoretically studied, mainly with the DFT, and gave valuable information. It is a topic of future research and needs to be studied about their scalability and potential application in practical areas. Even as world demands renewable energy technologies, BX monolayers are in a position to contribute in enhancing the solar energy and photocatalytic systems [5].

COMPUTATIONAL METHODOLOGY

In our study, we utilized the plane-wave approach within Density Functional Theory (DFT), implemented through the CASTEP code. The simulation model is based on a two-atom graphene-like unit cell, comprising one carbon (C) atom and one germanium (Ge) atom located at the A and B positions within a honeycomb lattice. To achieve computational efficiency, we adopted Ultrasoft pseudopotentials (USP), as proposed by Vanderbilt, enabling calculations at the lowest feasible cutoff energy for the plane-wave basis set. For exchange-correlation effects, the Generalized Gradient Approximation (GGA) with the Perdew-Burke-Ernzerhof (PBE) functional was employed, using an energy cutoff of 500 eV for the expansion of plane-wave functions. A periodic boundary condition was applied in the plane directions, with a vacuum spacing of 20 Å along the perpendicular direction to minimize interactions between periodic images in the c-direction. We employed a $21 \times 21 \times 1$ K-point grid for Brillouin zone sampling, following the Monkhorst-Pack method. The convergence criteria for self-consistent field (SCF) iterations were set as follows: 5.0×10^{-6} eV/atom for total energy, 0.01 eV/Å for the maximum force, 0.02 GPa for maximum stress, and 1.0×10^{-5} Å for the maximum displacement during geometry optimization [6-8].

RESULT AND DISCUSSION

STRUCTURAL PROPERTIES

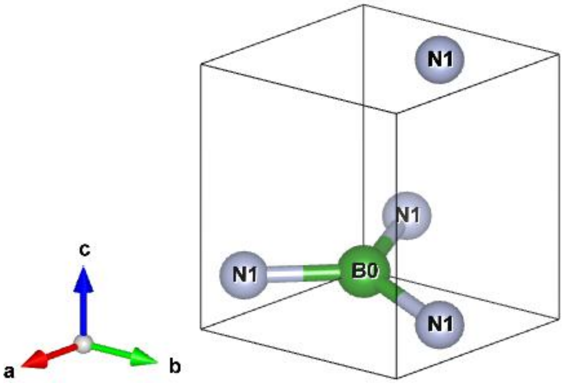
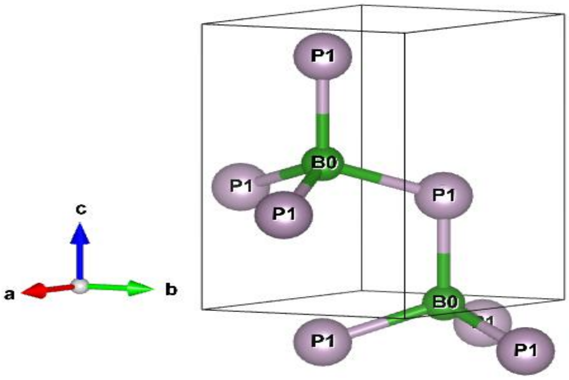


Fig 1(a) BN



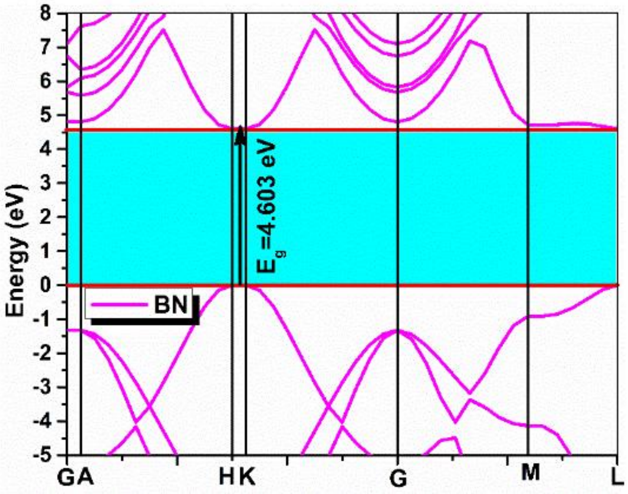
Fig(b) BP

he first graph is a diagram of the Boron Nitride (BN) hexagonal crystal structure which has boron (B) and nitrogen (N) atoms alternating on a hexagonal lattice. These atoms combine to form each unit cell with the center of each hexagon having a B atom surrounded by N atoms. The bonding is very strong with covalent type of bond which exists between boron and nitrogen causing the structure to possess a high in plane anisotropy whereas the interlayer interaction is much weaker, i.e., like graphite. This loose interlayer binding enables the use of BN in such applications as lubricants and high-temperature insulator because the layers can simply glide past one another [9]. The crystallographic axes (a, b, and c) indicating the orientation of the unit cell present in the graph are also important to determine the directional nature of the cuisine. The second illustration shows the molecular structure of the Black Phosphorus (BP) that is composed of phosphorus (P) atoms in a puckered bilayers arrangement.

It is formed by the covalent bonding of the atoms in a two-dimensional lattice and then with a weak van der Waals bond between the layers. It is the puckered structure that imparts BP its truly anisotropic nature, with a tunable bandgap, whose value can be defined according to the height used. The capacity of BP to show a direct gap is an indication that despite being similarly composed with BN the latter similarity does not mean that the former does not have any uses especially in the field of electronics and optoelectronics. Both its electronic characteristics and especially the number of layers is critical to the applications in next-generation devices such as transistors and photodetectors. Both of these two materials are two-dimensional and anisotropic however, these two materials possess quite different structure and electronic behavior, thus; they have different technological application, i.e. an insulator in the case of BN and electronic devices in the case of BP [10,11].

ELECTRONIC PROPERTIES

The band structure of BN (boron nitride) in the first graph suggests that the band gap of this material is direct with an approximate value of 4.6 eV labeled by the horizontal cyan band. It indicates that BN is an insulating material in accordance to its application in a number of electronic and optoelectronic components where it is needed to have good thermal stability and insulating property. A large energy offset between the conduction band and valence is evident as in wide band gap semiconductors. These band structures can be determined by DFT calculations and in fact, calculations of materials such as BN makes use of generalized gradient approximation (GGA). The kind of analysis will be significant in the light-absorbing capability as well as emitting of light in the material, its conducting electricity and functioning in high-temperature conditions [12].



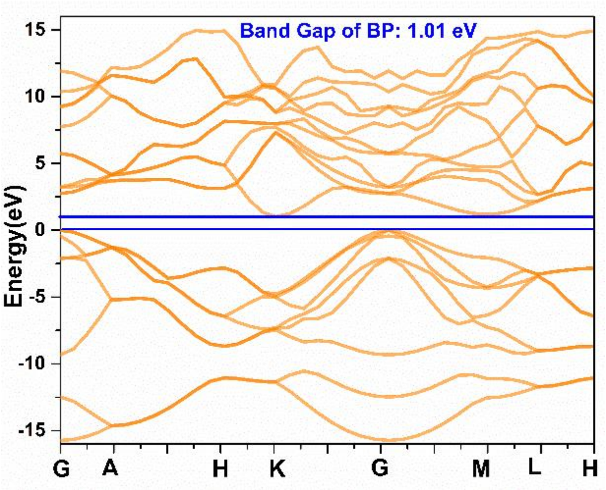


Fig2(a) Band structure of BN　　*Fig 2(b) Band structure of BP*

The second graph is aligned towards the band structure of the BP (black phosphorus) whereas the blue line reveals the band gap of about 1.01 eV. BP has smaller gap compared to BN making it fall under the semiconductor category. The material is of great interest to electronic devices that require the band-gap to be easily tuned, e.g. field-effect transistors and optoelectronic components, since the band-gap band-gap can be adjusted by variation of the layer thickness. The non-direct gap indicated in the graph and a hallmark of BP indicates more intricate optical characters and higher potential of device applications. DFT calculations of BP particularly using the hybrid functionals allow a better understanding of its electronic structure and can help design devices that can take advantage of its anisotropy. The band structures are calculated by DFT and play a reference role in relating the electronic properties of material in a practical way. The band gap values and the character of conduction and valence bands are decisive in making devices that can be based on its electrical and optical characteristics peculiar to each of the materials [2,3].

The initial graph indicates the Density of States (DOS) of Boron Nitride (BN) and the y-axis shows the Density of states per energy (in states per eV) and the x-axis shows the energy (in eV). The DOS tells us useful details regarding the electronic structure of BN. The feature close to the Fermi level hinted by the vertical green line at 0 eV shows the sharp peak distinctive of the band gap of the material which emphasizes that BN is an insulator or a wide-band gap semiconductor. The existence of more than one peak in both the negative region of the energy and the positive region of the energy indicates that different electronic states other than the conduction band and valence band may have partaken in lowering the overall potential of the electronic and have contributed to it accordingly. This property is important in its electronics properties of the material and in its use in electronics and optoelectronics. Very similar effects can be seen in other semiconducting materials including graphene and hexagonal boron nitride where the bonds between the boron and nitrogen atoms give its unusual electronic properties [15].

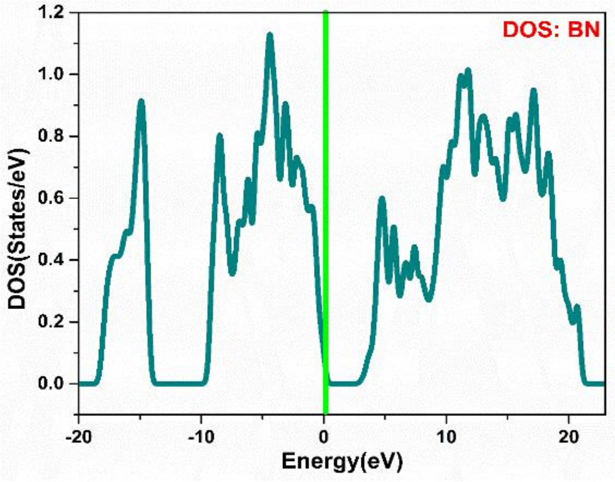


Fig 3(a) DOS BN

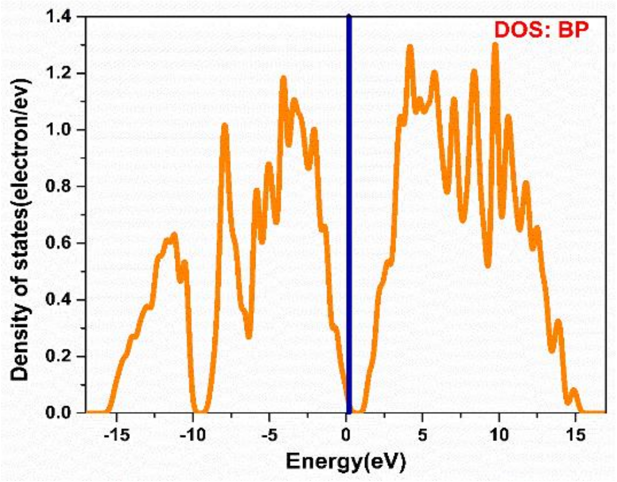


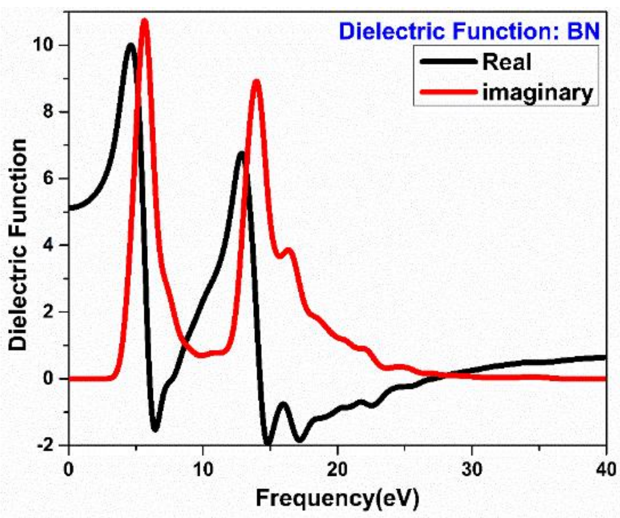
Fig3(b) DOS BP

The second graph indicates the DOS of Boron Phosphide (BP) but the variable presented on x-axis is energy and DOS (electron/eV) on y-axis. As the graph shows there is a sharp rise at the Fermi level which is the vertical blue line at 0 eV and so the graph shows the typical band structure of BP. The large values of density of states at both positive and negative energy hints at there being both a conduction and a valence band and similar to BN, BP has semiconducting properties and contains a band gap. The DOS of BP is however more dotted symmetric and wider than that of BN and it means that there is a better overlap of the valence and conduction bands. This characterization is representative of a potentially behavioral electronic signature especially in regard to its utilization in high-performance electronics and optoelectronics where the conduction and the valence band properties balance is a key element to device behavior. The tendencies that are traced in these DOS plots indicate that, although there can be similarities of the electronic structure of BN and BP like having a band gap and state distribution, the asymmetry and the width of the peaks show that they differ in their band structure and might acquire different applications in technological spheres [16].

OPTICAL PROPERTIES

DIELECTRIC FUNCTION

In the first graph we have the graph of Dielectric functional Boron Nitride (BN) reflecting both the real (black line) and imaginary (red line) parts of the dielectric functional versus the frequency (in eV). The real part of the dielectric function is the main factor that contributes to the capacity of a material to store some energy, and the imaginary part is associated with energy loss related to absorption. Here the actual dielectric function will have large peaks at certain frequencies, which are the electronic transitions of the material, and demonstrates how BN will react to an external electric field. The imaginary component of the dielectric function indices exhibits strong peaks too, which define the energy absorption spectrum of BN, on the doorway frequencies of the band gap. Observation of absorption peaks signifies inter band transition in the electronic structure of the material and can be explained due to the interaction of the material electrons with the incident electromagnetic waves. These trends reflect trends in an insulating material with a wide band gap, in which the peaks are at higher frequencies, as is also in BN. The analysis is based on Density Functional Theory (DFT) that offers an accurate account of the electronic structure and response to mediums forming dielectrics under different conditions [17].



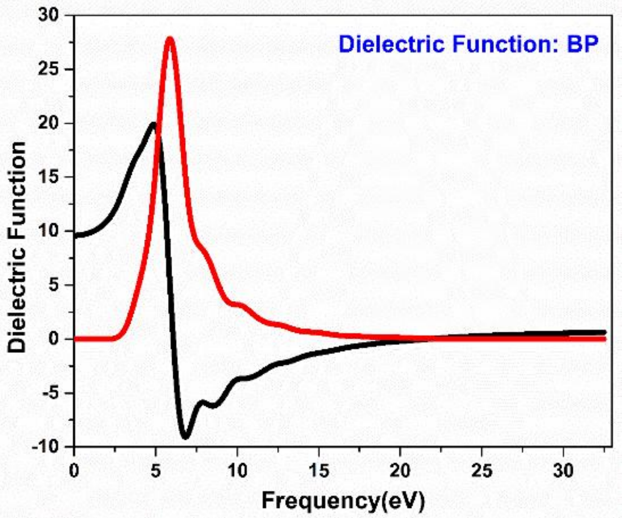


Fig 3(a) Dielectric Function of BN ***Fig3(b) Dielectric Function of BP***

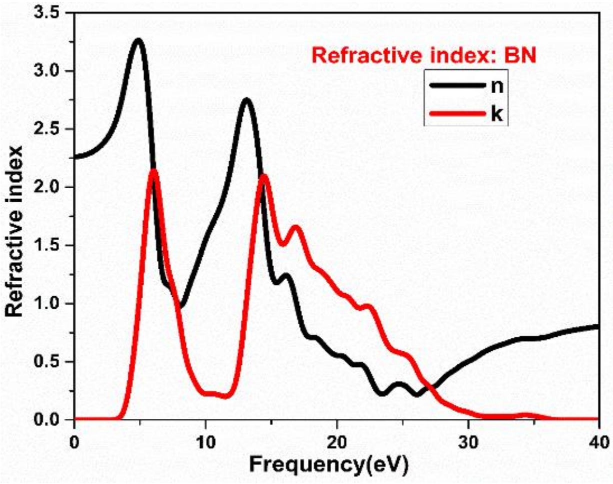
The second figure shows the Dielectric function of Boron Phosphide (BP) which is again the real and imaginary part of dielectric Function plotted against the frequency on the x-axis. The maximum part of BP real dielectric-constant exceeds that of BN by far, particularly at low frequencies which means stronger electronic transitions in this substance. The absorbed energy is sharply peaked too, indicating that BP admits a more intense absorption at some frequencies range. It is representative of smaller band gap than BN and so transitions occur at lower photon energies. The divergences between BN and BP in their dielectric behavior, including the locations and intensities of each peak, are noteworthy, in their digression towards understanding their possible functionality in the optoelectronics and high frequency systems.

DFT is also used to further explain the nature of such electronic transitions and absorption lines through modelling the electronic states of the material involved and making inferences in regards changes in polarization and energy loss processes upon interaction with a photon. The variations of the peaks and their strength are a direct consequence of band structures and electronic structures of the materials under calculation in DFT simulations. Such dielectric characteristics are critical in the modeling of the behavior of materials in a number of applications including fabrication of high performance electronic and photonic devices [18].

REFRACTION

Figure 1 depicts the refractive index of Boron Nitride (BN) down to the real (black and fake, marked as n) and the imaginary (red and imaginary, marked as k) part of the refractive index as a function of frequency (in eV) on the x-axis. The real part of refractive index (n) gives information on how well the material bends light and it it has a maximum at certain frequencies particularly between 5-10eV which correspond to the absorption peaks in dielectric function and Density of States (DOS). n The real part has several peaks, which shows a strong electronic transition indicating a coupling of light with the electronic structure of the material and hence is a property of band gap. The imaginary part (k) is the absorption of the material with sharp peaks that are associated with the high energy absorption areas mostly at the same frequencies as nnn. Such behavior is in agreement with an insulating medium like BN where the effect of absorption and refraction is confined in the band gap of a material. The overall behavior of the BN reflects that it has a wide band gap and low absorption at low frequencies and it had more interactions at high photon energies. It is an analysis based upon Density Functional Theory (DFT) and assists in explaining the interaction of BN with light to such a degree as to be used in high-frequency and/or optic applications [19].

The second figure is the graph of refractive index of Boron Phosphide (BP) real part only (black line) and imaginary part only (red line). The trend of BP seems identical to that of BN but with greater peak on its real and imaginary sides, more so at the lower frequencies. A downward spike of the real part (n) is at about 4-5 eV which is smaller than that of BN making BP possess a smaller band gap. This conduct opines that BP has the capacity to communicate with lower energy photons than BN and therefore the potential is made better to be used in optoelectronic applications, where such communications are instrumental. BP The imaginary part (k) of BP shares the same trend with the real part but is stronger at the lower frequencies, just as the material has a stronger absorption in the lower frequencies. This implies that BP efficiently takes light compared to the BN at lower energies and this is probably because BP has a narrower gap band making electronic transitions at low photon energies. The data of the refractive index modeled via DFT can help to better understand the optical properties of BP, which have a great potential in such applications as light-emitting diodes (LEDs) and high-efficiency photodetectors.The discrepancies between BN and BP, as represented in the refractive index, can demonstrate how the electronic construction of the materials, especially their band gap, affects the optical properties of the specific compounds. The large band gap of BN leads to reduced absorption and refractive effects at lower energies; but the band narrower of BP will give rise to greater optical interactions at lower photon energies [20].



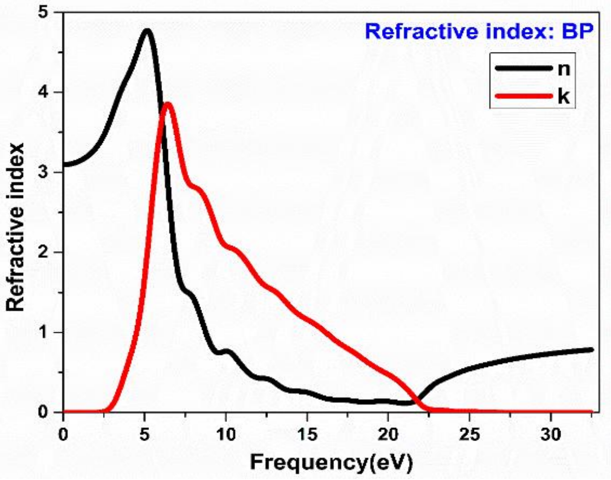


Figure 4a: Refractive index of BN

Figure 4b: Refractive index of BN

PHONON CALCULATIONS

The first example is the dispersion of phonon of the crystal Boron Nitride (BN) and demonstrates the frequency of the phonon (in THz) of the various symmetrical points in the Brillouin zone, namely between the points G, A, HK, G, M and L. This graph reveals the behavior of a phonon which are quantized oscillations of the atomic lattice along various wave vectors in the reciprocal space of materials. The intense spikes at the phonon branches are optical and acoustic phonons in BN with the acoustic phonons having frequency zero at the Gamma (G) point and rising in frequency as wave vector increases. The optical branches instead are higher up in the frequency and never cross zero at the Gamma point as is characteristic of insulating materials such as BN. A high range of frequencies, up to 50THz can be found in phonon modes, which refers to BN as having quite stiff bonds, which makes it very conductive to heat. It was obtained from the calculation of a phonon dispersion using Density Functional Theory (DFT), which gives key information on thermal and mechanical properties of BN, which is vital to realize its employment in high-performance product areas, including thermal management in electronic products [21].

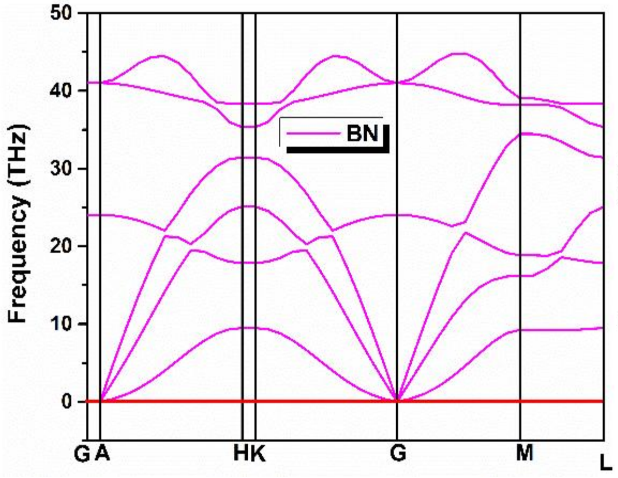


Figure 5a: Phonon Calculations for BN

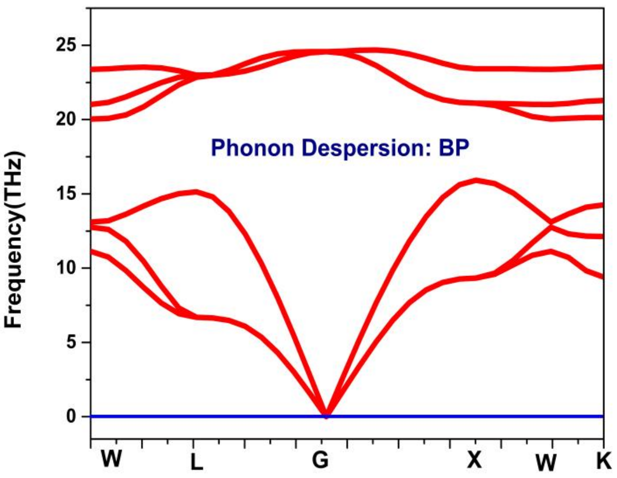


Figure5b: Phonon Calculations for BP

The second figure indicates the phonon dispersion of Boron Phosphide (BP) in which the frequency in THz is plotted against the wave vectors W, L, G, X, and K in the Brillouin zone. BP phonon frequencies are much lower than BN phonon frequencies and the uppermost phonon frequencies attain values of approximately 25 THz. The acoustic phonons once more originate at zero-frequency at Gamma, but the optical branches occur at higher frequencies. But, BP exhibits a strong phonon softening at the Gamma point, the low frequency branches show a dramatic dip, indicating that the bonding characteristics of BP are even more flexible than it is the case in BN. This softens to show a reduction in thermal conductivity which may mean that BP would be more practical in usages where the controlling of heat is less important and where a high level of eye sight or electronic usage is required. The differences between BN and BP are clear in their phonon dispersion and thus the properties of the two materials are different with regard to vibrations and hence their application in optoelectronic devices where phonons and charge carrier interactions are of importance. Being able to increase the thermal conductivity, BN has a better atomic interaction and thermal conductivity at higher phonon frequencies, which will be useful in application where heat dissipating is essential. BP on the other hand has lower thermal conductivity and softer phonons which would perhaps render it more applicable to electronic applications where weaker thermal transport is desirable i.e. in the use of optoelectronics and interfaces involving light-matter coupling [22].

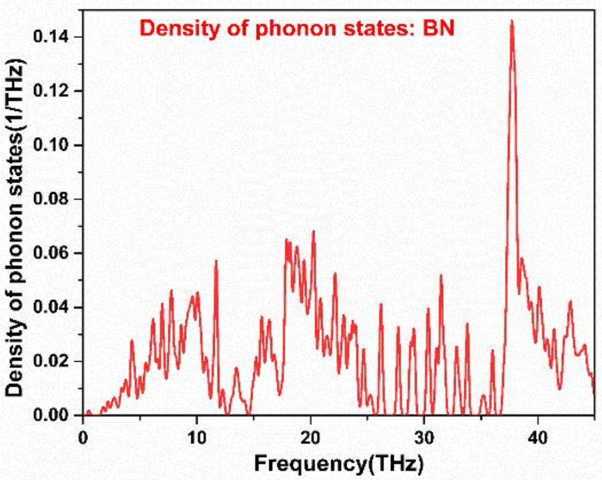


Figure 6a: DOS of Phonon States BN

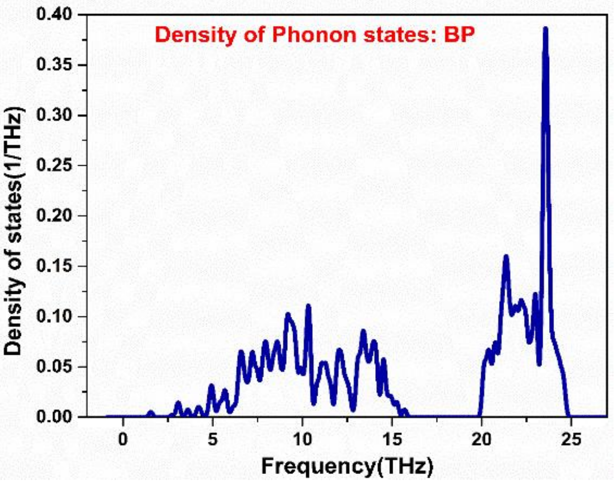


Figure 6b: DOS of Phonon States BN

The Density of Phonon States (DOP) of Boron Nitride (BN) graph is shown in the first graph where DOP is plotted against the frequency (in THz) on the x- and y-axis respectively. The graph displays a set of high-value peaks at certain frequencies, which means that there are definite phonon modes in BN. The existence of these peaks is a direct result of the vibrational nature of BN and does play a big role in explaining its thermal and mechanical properties. The peaks in the state density at particular frequencies, especially at the list of 20-40 THz, report to the phonon modes of the optical phonons of the material. The peak near 40 THz is quite sharp and indicates a possibility of a large density of states there which may be very crucial in the thermal conductivity of BN since phonon scattering in this range can significantly affect the flow of heat. The relatively higher states of phonons density in BN show that the material has rigid bonds with the ability to conduct adequate heat; hence, making it a very suitable material in high performance application areas wherein management of heat is substantive. This phonons state distribution is the result of Density Functional Theory (DFT) calculations and all the necessary information concerning the vibrational characteristics of BN and its applications in thermally conductive treatments like electronics and heat dissipation substrates [23]. The second figure shows Density of Phonon States (DOP) of Boron Phosphide (BP), where the frequency (in THz) is plotted in the x-axis and the DOP (in states/THz) in the y-axis. The phonon states distribution is wider in BP including a lot of peaks in the area of 0-25 THz, and the overall density of states is lower as in case of BN. The sharpest peak at approximately 20 THz implies that BP possesses a rich density of the optical phonon mode as compared to BN; however, the range is more dispersed, which implies that BP is characterized by more manageable atom bonds and relatively lower rigidness. This reduced stiffness is indicated in the distribution of phonon states as the rate of peak frequency is reduced, meaning that the interaction between atoms is less. The Delocalization of phonon states is broader in BP and this indicates toward a less-efficiently heat conducting material than in the case of BN. This property also makes BP a possible candidate for use where thermal conductivity is not a principal requirement (as with optoelectronics or light-emitting devices), where management of heat can take a secondary interest to the interaction of the material with light. Phonon state distribution, which was based on the calculations conducted with DFT, allows identifying BP as an excellent material to consider in instances that involved efficient absorption of light sources and low thermal conductivity. The analysis of the comparison of BN and BP show some major differences in the vibrational features and thermal features. These raise and sharper peaks at BN prove that it has an entity that holds stronger atomic bonds, and collectively has an increased thermal conductivity, and broader peaks at BP which shows the entity has more flexible bonding and a lower thermal conductivity. The variations play a key role in hailing the materials to be used in particular applications whereby black phosphorus (BP) is more suitable to applications involving electronics devices that need significant heat dissipation, and BN is most appropriate to applications involving optoelectronic devices where low thermal conductivity and effective interaction of light are needed [24].

OPTICAL CONDUCTIVITY AND ABSORPTION COEFFICIENT

The first couple of graphs are frequency dependent conductivity of Boron Nitride (BN), in which the real (solid black) and imaginary (dashed red) conductivity are plotted against frequency (in eV). The actual term of the conductivity (sigma real) is the capability of the material to conduct electricity, displaying acute peaks in special frequencies. The first sharp rise is at approximately 10 eV, this is the sensitivity of the material concerning the external electric fields; it is the electronic transition between the valence and conduction band. Low conducting component of the real conductivity implies that at these frequencies BN will act like insulator or show a large resistive effect. Energy dissipation part, the imaginary part (sigma imaginary) of the conductivity, has about the same frequency dependences, peaks about the same frequencies as well. The fact that the imaginary part has the highest values near 10 eV tells that there is strong absorption of energy at these photon energies, the very consequence of interband transitions in the electronic structure of the material. These Density Functional Theory (DFT) based conductivity curves bring another valuable information of the electronic and optical properties of BN, which is insulator at low frequencies and can absorb the high energy photons efficiently. Such behavior qualifies BN to be applied in electronic and optoelectronic devices especially in those situations where high resistive effects are desired at low operating energies and high photon absorption energy[25].

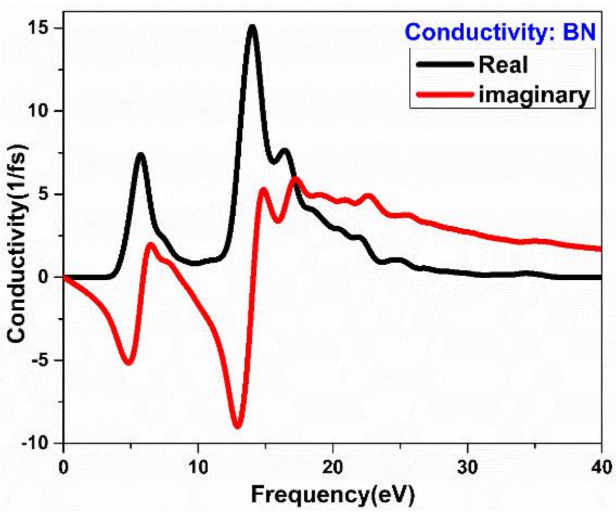


Figure 7a: Conductivity of BN

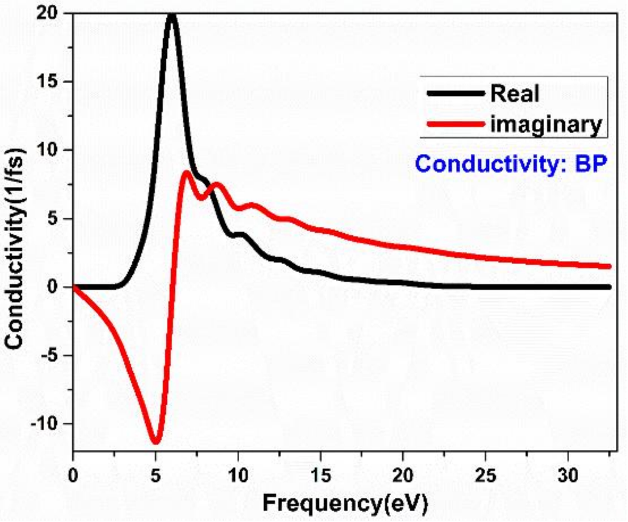


Figure 7b: Conductivity of BP

The second graph displays frequency-dependent conductivity of Boron Phosphide (BP) and has both real (black) and imaginary (red) components as functions of frequency (eV). BP has the same kind of behavior as BN, only difference is that the position and magnitude of the conductivity peaks in BP is slightly different. BP has the highest value of the real conductivity (sigma real) around 5 eV implying that BP is more conductive than BN at low photon energies. This implies that BP band gap is smaller and hence electron transitions can occur at lower energies as compared to that of BN where more significant photon energies are required to drive electrons into the conduction band. The imaginary component (imaginary) of BP too has peaks, although a great deal of absorption is taking place as much as photon energies go as low as 5 eV. This implies that BP has a higher potential to absorb lower energy range of photons than BN, which is congruent with the smaller band gap referred to BP. The conductivity data based on DFT indicate the applicability of BP in optoelectronics especially in equipment where an efficient absorption of energy is required at low photon energies (examples include photodetectors and light-emitting diodes LEDs). The position of the peaks of BN and BP differences in their conductivity behavior and the capability in conducting and absorbing energy is the main point of their difference. Due to large band gap, BN has high resistivity and low absorption at low frequencies whereas BP, due to slighter band gap, is highly conducting and absorbing to low-energy photons. These properties which are based on DFT are fundamental in ascertaining the potential usage of these materials in different electronic and optoelectronic stages where the control of the energy absorption, conduction as well as the dissipation is significant [26].

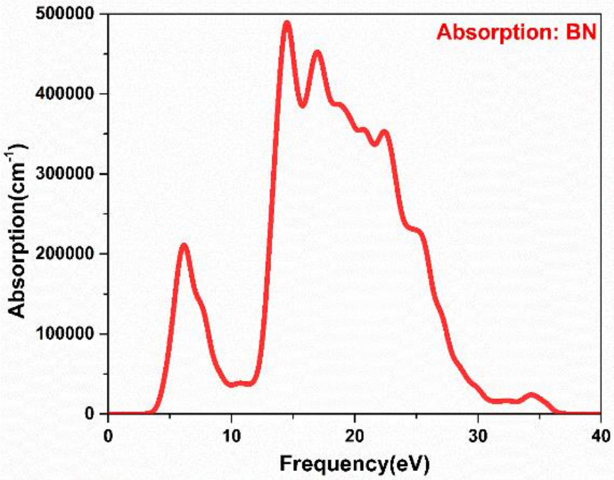


Figure 8a: Absorption of BN

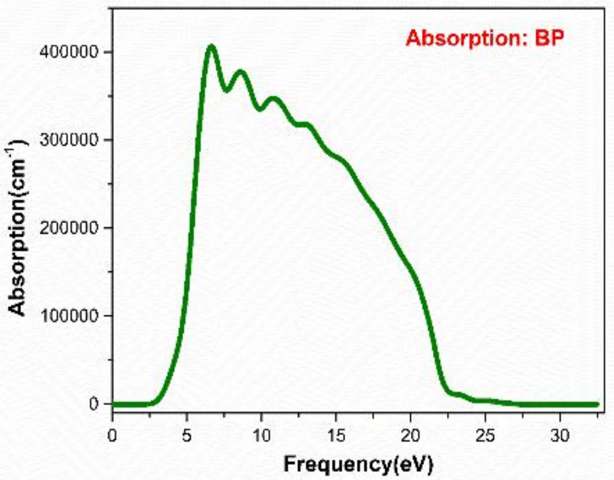


Figure 8b: Absorption of BN

The red graph is an absorption spectrum of Boron Nitride (BN) and the absorption frequency (in cm 1) is plotted versus frequency (in eV). A sharp peak at 10 eV is observed in the graph followed by other small peaks at higher frequencies to 30 eV. The highly pronounced sharp peak at about 10 eV indicates a high absorption of light at the said energy that can be given by the light interband transitions between valence and conduction levels in line with the wide band gap of BN. The absorption tail to the high frequencies is a sign that BN still absorbs light at the high photon energies but not as effectively as it does at lower frequencies. This kind of absorption behavior predicted by Density Functional Theory (DFT) is typical of semiconductors or, more precisely, wide band semiconductors which tend to have transitions mostly at higher energies, and at lower energies the material is transparent. An example of such a material is the BN as it has a wid band gap. The general form of the absorption spectrum is characteristic to insulators indicating only a minimum amount of absorption that is performed by lower-energy photons whereas photons with an energy larger than their band gap are absorbed efficiently. Such properties indicate that BN would be appropriate in high-energy fields, i.e. ultra-violet (UV) photodetectors, and as sensors that necessitate use of wide-band gap semiconductors in optical filtering [27]. The second figure is the absorption spectrum of Boron Phosphide (BP) and this is also given as absorption (in cm1) versus frequency (in eV). In BP, the peak of absorption value is rather high at 5 eV, which is much lower than the absorption peak of BN. This implies that a band gap value of BP is smaller than BN that allows it to absorb photons with less energy. At the same time, the absorption tail of BP also shows a longer wavelength range of tail Absorption, but there is a lower pyro peak than BN, which means that BP has a higher absorption probability at low energy and a relatively lower energy of the photon. The computed narrower band gap of BP enables transitions to lower energies, which makes it an improved app-contributed in the visible and near-infrared ranges of the spectrum, e.g., the light-emitting diodes (LEDs), the solar cells, and the photodetectors. The BP absorption spectrum displays the features of a narrow gap semiconductor, much stronger light absorption at lower energy incident photons than at higher frequencies. This qualifies BP in optoelectronic applications in lower energy devices. The comparison provided of the BN and BP in the optical properties of their absorption spectrum notes the impact of the band gap of the material on the optical characteristics. The wide band gap of BN means that it is strongly absorbing at higher photon energies so that it would be most suitable in UV based applications whereas BP as a material has a closer band gap that would absorb more efficiently at low energy photons that is desirable in visible and near-infrared applications. Such information obtained by DFT calculations is very important in designing and optimizing materials to be used in particular optoelectronic application [28].

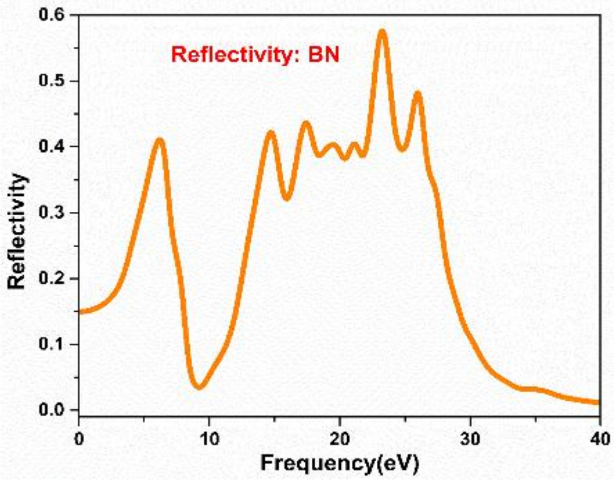


Figure 9a: Reflectivity of BN

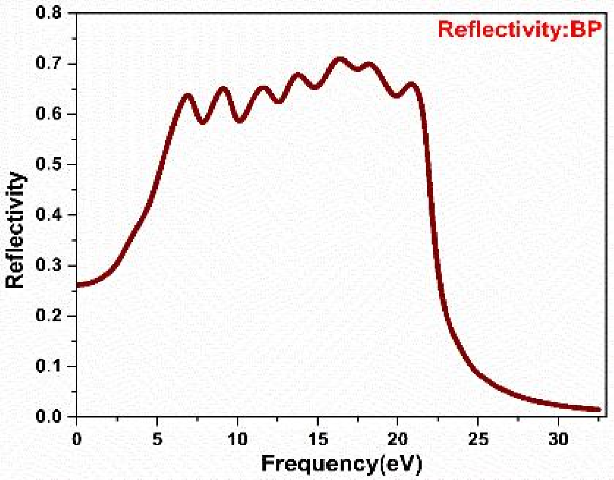


Figure 9b: Reflectivity of BP

In the first graph, reflectivity of Boron Nitride (BN) has been plotted on frequency (in eV). Reflectivity is defined by some sharp peaks, mostly between 5 and 20 eV. In turn, these peaks refer to the behavior of the material to reflect light powerfully at certain frequencies that are the response of the material regarding its electronic transitions. The relationship between reflection property in BN and its electronic structure is explicit; according to Density Functional Theory (DFT). The wide bandgap of BN has the result that light at elevated levels of photon energy is highly reflected, as is typical of the wide-band gap semiconductors that are capable of reflecting a large quantity of incident electromagnetic energy. With the increased frequency, reflectivity is instead slowly decreased, especially at above 20 eV, indicating a diminished efficiency of reflectivity at a higher photon problem energy. This activity means that BN has a special utility in optical coatings and UV filtering where it is necessary to have high reflectance at some specific wavelengths. The large reflectivity of BN in UV/vis range portrays the insulation property and the capability to reflect high energy photons efficiently which is very vital in several photonic and optoelectronic applications [29]. The reflectivity of Boron Phosphide (BP) is given in the second graph where the reflectivity is plotted in terms of frequency (in eV). BP has a much broader and stronger reflectivity peak than BN with its maximum reflectivity at about 5 eV and the reflectivity falling steadily above 20 eV. The reflectivity of BP is stronger in lower photon energy range (approximately 5 eV), as the band gap of BP is narrower than that one of BN. It indicates that BP scatters light more effectively at lower photon energies as is common in materials with band gap narrower in width. The pronounced loss of reflectivity above 20 eV indicates that BP does not reflect well the high-energy photons in comparison with the BN and it is associated with its narrow band gap and electronic structure. The simulations used DFT to determine that the electronic structure of BP offers transitions at lower photon energies hence more appropriate in applications involving visible light and near-infrared radiation hybrids. The property qualifies BP as a viable material in optoelectronic application in LEDs, photodetectors, and solar cells where high reflectivity in the visible and near-infrared spectrum is desired. The difference between BN and BP spectra of reflectivity indicates the role of the band gap in the reflection of light. WHFSE of BN has a wider band gap and therefore happens to reflect more at higher photon energy, whereas BP has a narrow band gap and therefore reflects more at lower photon energy. Such properties are crucial in the optimization of materials in the optoelectronic uses that pertain to certain necessities of light reflection and absorption properties [30].

PHOTOCATALYTIC CALCULATIONS

The figure shown demonstrates the electronic band structure of two separately two-dimensional materials Black Phosphorus (BP) and Boron Nitride (BN) calculated using the

Density Functional Theory (DFT) techniques. The energy spectrum, in his plot, is given as a function of the wavevector in terms of the high-symmetry directions of the Brillouin zone. It is important to note that the horizontal lines, denoted in blue and green, respectively, are majorly highlighted at the energy levels of the conduction band minimum (CBM) and the valence band maximum (VBM). These turning points supply the upper and lower limits to the electronic states of the material, and on these the band gap can be extrapolated. Both BP and BN have different electronic properties, and their band gap is largely different, and it is larger in BP than in BN. The red bars in the graph represent the corresponding values of the electronic band gaps and this gives an evident visual distinction of the two materials. The BP material exhibits a direct band gap, which makes it a good product in optoelectronics such as photodetectors and transistors since light absorption and emission are useful properties. On the other hand, its wide band gap makes BN insulating in nature, which makes it a great choice as a high-temperature and high-voltage candidate where dielectric stability is imperative.

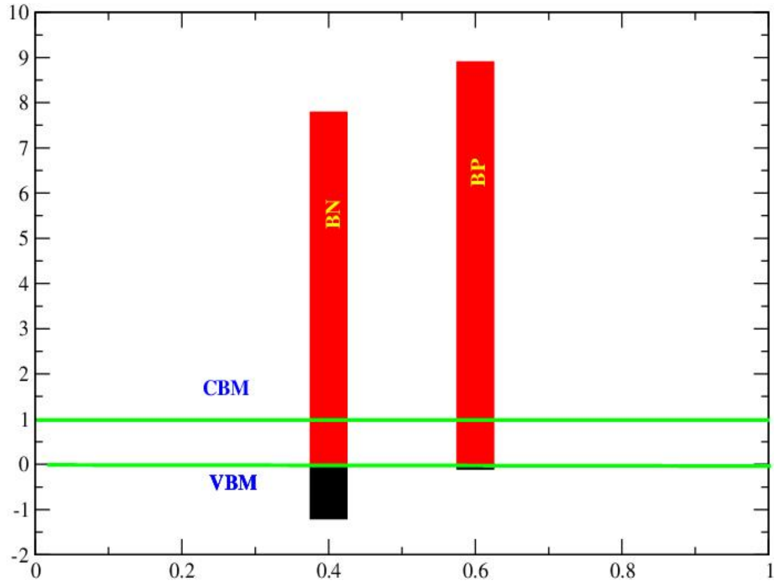


Figure 10: Photocatalytic Properties of BX (X=N, P)

DFT calculations are used to gain crucial information in the electronic structure of these materials and by solving the Kohn-Sham equations the electronic structure of materials including the band gaps can be determined at the atomic level. In these first-principles calculations one can gain in depth insights into the nature of the electronic states of the materials, information crucial in their technological optimization, extending from flexible electronics to high-performance semiconductors. With regard to DFT, these outcomes validate the fact that BP has a relatively small band gap which is favorable in the applications of low power and high-speed devices, and highly stable around extreme conditions, which BN is compatible in terms of insulating applications. The computer-based algorithms employed in calculating such band structures provide an exact, predictive system of designing the next-generation materials to the many cutting-edge technological applications [31-36].

CONCLUSION

In this study we present an in-depth first-principles study of photocatalytic and photovoltaic properties of BX monolayers (X = N, P) using Density Functional Theory (DFT). The findings demonstrate the outstanding prospects of these materials in energy conversion technology especially photocatalysis, and photovoltaics to provide a new mechanism to solving the worldwide energy crisis. The application of Boron Nitride (BN) and Black Phosphorus (BP) monolayers, despite their structural, electronic, and optical properties, can become a potentially necessary way in the next generation energy systems. The high-bandgap, electronically very stable BN suits to high-temperature, high-voltage, and insulating applications. The band structure obtained using the DFT explains why it is usable in ultraviolet (UV) photodetectors, electronic devices and high-performance insulation materials which is attributed to insulating behavior and strong dielectric properties. BP, on the other hand, is well suited to the low energy optoelectronic applications such as photodetectors, solar cells, and light-emitting diodes, with this narrower direct bandgap. The tunable electronic properties and efficient absorption of visible to near-IR spectra of BP make it a significant material to energy conversion techniques that run at lower energies of photons than the current state. DFT simulations play important roles in the optical, phonon and electronic properties of these materials and how their performance can be enhanced by doping and integration of heterostructures. Their difference in phonon properties, high thermal conductivity in BN and more flexible bonding properties of BP enhances further the application specific to each material in the energy systems where thermal management is a vital part of efficiency of the whole system. The dielectric properties, such as the dielectric function, refractive index, absorption spectra and reflectivity signal the material superiorities of each material in various applications in energy collection and conversion. The findings provide a direct route to have control over the electronic properties of BX monolayers so as to optimize their usability in photocatalytic water splitting, solar energy harvesting and any other sustainable energy technology. BX monolayers are a revolutionary type of new two-dimensional materials that have a huge prospect of propelling photocatalytic and photovoltaic applications. Their optimal dependence on application along with unique properties in the electronic, optical, and thermal attributes make them one of the best-placed research and development in the renewable-energy space in future. More other experimental confirmation, scaling of the materials, and implementation in real systems will be essential in the realization of the full potential of the materials. The current work forms a strong theoretical starting point, which shows the future efforts of taking advantage of BX monolayers to devise efficient, sustainable, and scalable energy conversion systems.

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