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Original Research

Assessing Electronic Structure Features of Fullerene-Like BN and BP Nanocages

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Abstract: Electronic structures of representative models of boron nitride (BN) and boron phosphide (BP) nanocages were assessed in this work by employing density functional theory (DFT) calculations. The models were found achievable along with optimization calculations and they were stabilized to be analyzed for the electronic features. The frontier molecular orbital (FMO) features were evaluated including exact energies for the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) levels. The models were found suitable and their features were found comparable to distinguish them for further applications. Not only the exact levels of HOMO and LUMO but also their distances were different and other related parameters such as energy gap, energy of Fermi level, chemical potential, and chemical hardness were indicating the specific features for the models. Indeed, the BP nanocage was found more suitable regarding a higher conductivity rate and a lower chemical hardness in comparison with the BN nanocage. On the other hand, both models were found measurable by variations of electronic structure features for developing their further applications.

Keywords: Conductivity; Density functional theory; Electronic structure; Fullerene; Nanostructure.

Introduction

Electronic structures features are very important regarding their dominant roles in the materials characterizations and developments [1]. In this regard, assessing such features are very important for learning about the ability of materials for customizing in desired applications and purposes [2]. By the innovation of nanostructures, they were found very interesting regarding their electronic structures to make them semiconductors or conductors for further applications [3]. Accordingly, several ideas were arisen how to identify a correct structure for a specified application in the terms of electronic structure assessments [4]. The pure carbon nanostructures were indeed the pioneers of generating many more architectural types of nanostructures in both of compositions and shapes [5]. The members of elements of groups three and five of periodic table of element were those candidates of producing heterogeneous nanostructures [6]. Boron; as a famous element of group 3, has already attracted so many attentions of researchers to study its pure system or in combination with other elements such as those nitrogen and phosphor of group five [7-10]. Accordingly, the structures of boron nitride (BN) and boron phosphide

(BP) were become very popular based on their unique features for working in different aspects such as conductors/semiconductors or sensors/adsorbents [11-15]. To this point, we did this work to assess the electronic structure for representative models of BN and BP nanocages. We performed density functional theory (DFT) calculations and were investigated their features based on the evaluated properties of optimized models.

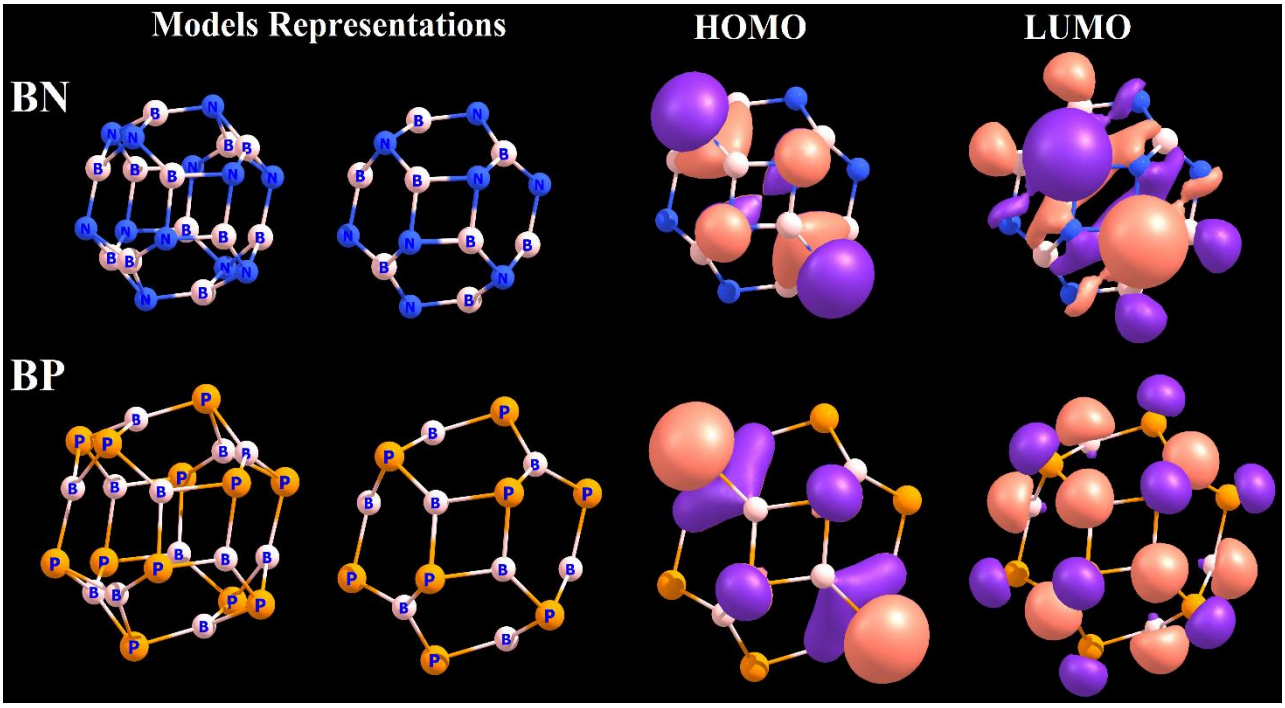

Figure 1: Models of BN and BP nanocages and their HOMO-LUMO patterns.

Materials and Methods

Representative models of boron nitride (BN) and boron phosphide (BP) nanocages (Figure 1) with the formulas $B_{12}N_{12}$ and $B_{12}P_{12}$ are assessed in this work regarding their electronic structures features. Forts of all, geometries of the models were optimized to obtain their stabilized structures in correspondence to their minimized energy state. Next, the models were involved in further calculations to investigate their electronic based features. For the molecular scales, evaluating the characters of frontier molecular orbitals (FMO) are very important because of the dominant roles of the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) levels for determining the tendency of molecule for participating in electronic transferring system. In this case, the models were analyzed and their features were characterized by evaluating the exact values of energies of HOMO and LUMO levels and their related features including energy gap (E_{Gap}), energy of Fermi level (E_{Fermi}), chemical potential (C_{Pot}), and chemical hardness (C_{Hard}). All the evaluated parameters were summarized in Table 1. These parameters could help to recognize the molecular models regarding their chemical reactivity especially for the cases of electron transferring. As HOMO shows the electron involving level and LUMO shows the electron vacant level, the occurrence of electron transferring could be indeed managed by these two levels. The additional parameters could show the importance of such models for involving in the electron transferring processes not only inside the molecular model but also in contributing to other molecular models and systems. In addition to such quantities, graphical representations of HOMO-LUMO distribution patterns (Figure 1) and density of states (DOS) diagrams (Figure 2) will be also complementary for approaching the purpose of electronic structures of BN and BP nanocages. The calculations of this work were done by employing the B3LYP/6-31G* DFT method as implemented in the Gaussian program to use the computational tools for investigating the chemicals [16-20].

Results and Discussion

The models of this work were investigated for assessing the electronic structures features of BN and BP nanocages based on DFT calculations. The models were optimized and their properties were evaluated for evaluating their chemical properties especially regarding the FMO related features. In this case, the optimized models were exhibited in Figure 1 including the models representations and their HOMO-LUMO distribution patterns for both of BN and BN nanocages. First of all, it was shown that the bond distance of BN was shorter than that of BP, with these distance 1.44 Å and 1.91 Å respectively. So, BP model was indeed larger than BN model regarding the bond distances at the same number of involving atoms; $B_{12}N_{12}$ and $B_{12}P_{12}$. To this point, the models were available based on their optimized structures at the minimized energy state. Next, the models were analyzed by their FMO features as shown by the visualized patterns for HOMO and LUMO levels. As found by such patterns the directions of distributions were the same for the investigated models; however, the concentrations were indeed different based on their features. In this regard, the models were found available based on such parameters and their features were indicating difference of BN and BP models based on such issues. To more explain such issues, the models were assumed to be different regarding such electronic features in addition to the already found different BN and BP bond distances. To explain more details, the illustrated DOS diagrams were shown in Figure 2 to show properties of molecular orbitals prior to or after than each of HOMO and LUMO levels, respectively.

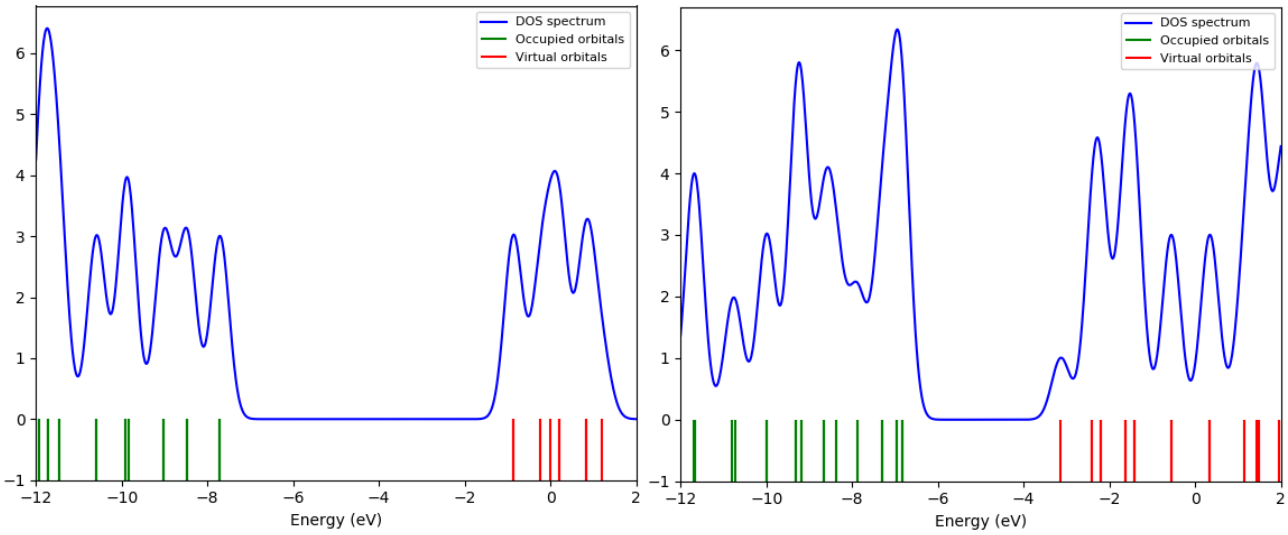

Figure 2: DOS diagrams of BN and BP nanocages.

There is an important parameter so called “conductance rate” for the conducting materials, in which it is directly proportional to the distance of HOMO-LUMO levels. It is very obvious with the illustrated DOS diagrams that the distances of HOMO and LUMO levels are different for the investigated models, then the models will be different in the terms of conductance rates. The model goes to a higher conductivity if the distance is shorter and the model goes to a lower conductivity if the distance is longer. In such a HOMO-LUMO energy distance dependency, it would be very helpful to find a clear insight for deciding about the investigated materials regarding their conductivity issues. For the investigated models, the BP nanocage was found with a higher conductivity level in comparison with the BN nanocage with a lower conductivity based on the evaluated plane-gap of DOS diagrams, in which the feature is obvious by eye. In other words, the models could be measurable regarding the fluctuations of electronic molecular orbitals features to be distinguished from each other or to be applicable for various and specific applications. To quantitatively discuss this claim, the results of FMO related parameters were obtained and they were summarized in Table 1.

Table 1: Evaluated FMO features of optimized BN and BP nanocages (All units are in eV).

Model	HOMO	LUMO	E_{Gap}	E_{Fermi}	C_{Pot}	C_{Hard}
BN	-7.71	-0.86	6.85	-4.28	-4.28	3.42
BP	-6.83	-3.13	3.70	-4.98	-4.98	1.85

The evaluated FMO results of optimized BN and BP nanocages were summarized in Table 1, in which the quantitative comparisons of electronic features could be learnt from them. The exact levels of HOMO and LUMO were different for both models and their distances were also different. The values of E_{Gap} indicated a significant difference between the energy distances of HOMO-LUMO levels. It was also obvious from the graphical representations of patterns of Figure 1 that the models were in different modes of such distributions. Additionally, the models were different regarding the values of E_{Fermi} and C_{Pot}, which are very dominant for determining the models regarding their electron transferring features. Accordingly, the value of C_{Hard} indicated a lower hardness for BP than BN in agreement with the obtained results of E_{Gap}. On the other hand, the models were also measurable regarding their electronic features for being customized in the specific applications. Hence, learning details of such systems could be helpful for providing more insights into their further applications.

Conclusion

The obtained results of electronic structures of BN and BP indicated dominant differences between the models. Their optimized structures indicated longer bond distances for the BP model in comparison with the BN model. Additionally, the models were assessed based on the evaluated electronic features, in which the levels of HOMO and LUMO and their related parameters indicated a possibility of recognition for the systems. More results were obtained based on the variations of energy distances of HOMO and LUMO and their related parameters even in the terms of graphical representations. In accordance with the conductivity rate, the models were also analyzable based on such systems and they were distinguishable for employing in different applications. As a final remark, the models were useful to be customized based on their electronic structures features for working in different purposes and applications.

Disclosure Statement

The author(s) did not report any potential conflict of interest.

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