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# DFT Investigation of AlP-Doped BN Nanotube for CO Gas Capturing

**Hesamaldin Zahedi**
*Department of Applied Chemistry, Faculty of Pharmaceutical Chemistry, Tehran Medical Sciences, Islamic Azad University, Tehran, Iran*

**Mohammad Yousefi**
*Department of Chemistry, Yadegar-e Imam Khomeini (RAH) Shahr-e Rey Branch, Islamic Azad University, Tehran, Iran*

**Mahmoud Mirzaei**✉
*Biosensor Research Center, School of Advanced Technologies in Medicine, Isfahan University of Medical Sciences, Isfahan, Iran*

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**ABSTRACT.** Density functional theory (DFT) calculations were performed to investigate monoxide carbon (CO) gas capturing at the surface of aluminum phosphorous (AlP) doped boron nitride (BN) nanotube to create CO@AlPBN model. All singular models of this work were optimized first to obtain minimized energy structures. Subsequently, the CO capturing was explored in an additional optimization process at the surface of AlPBN model. Geometrical and electronic properties were evaluated for the optimized models to achieve the purpose of this work. The results indicated that the AlPBN model could work better than BN model for contributing to interactions with CO gas. The obtained results of capturing process approved this achievement. For detection of the gas captured model, UV spectrum could help by shifting the peak of CO@AlPBN model to longer wavelengths than raw AlPBN model. And finally, the AlPBN model could be considered for further investigations for the CO gas capturing purposes.

**KEYWORDS.** Boron nitride; Aluminum; Phosphorous; Carbon monoxide; Gas capturing; DFT.

**INTRODUCTION.** Since the innovation of carbon nanotubes (CNTs) in 1991, several attempts have been dedicated to investigate various features of this novel material.[1, 2] Moreover, numerous investigations have been performed to create other types of nanostructures in addition to available CNTs, which have been seen to be geometrical-dependent for electronic properties.[3] Among the research results, combinations of boron and nitrogen have been seen to make other useful nanostructures such as boron nitride (BN) nanotubes, which have been seen always semi-conductor independent of restricting geometrical factors.[4] Indeed, BN nanotubes have become popular very soon because of their ionic structures in comparison with non-ionic CNTs especially for applications in water media.[5] The investigations have been continued more and more to show the characteristic features of BN nanotubes for applications in several fields of science and engineering.[6-10] In addition to pure nanotubes, atomic doped models have been also seen very much important in order to new electronic features of impure nanotubes.[11-13] Several types of atomic-doped BN nanotubes have been investigated to this time

✉ Corresponding author; *E-mail address*: mdmirzaei@pharm.mui.ac.ir (M. Mirzaei).

employing computational and experimental methodologies.[14-16] One of the expected applications of nanotubes is their role for capturing gases in environment as a detector, a sensor or a container.[17] Therefore, this feature has been always an interesting topic for researchers to see such application for nanotubes. In addition to regular gases in environment, some of them are poisonous and breathing them is very much dangerous for human life safety. Carbon monoxide (CO) is one of irregular gases in environment, in which its breathing may kill a person very soon.[18] In the countries using natural gases for heating resources of homes, this poisonous CO could make dangerous situations for normal living. Therefore, it is an important task to make a sensitive detector or sensor for early detection of this gas in the living environment.[19] This capability of CO capturing has been already investigated for pure BN nanotubes.[20]

To this point, this work was established to investigate aluminum-phosphorous (AlP) doped BN nanotube for CO capturing through quantum chemical computations (Fig. 1). AlP was doped instead of a BN bond in the nanotube and the new structure (AlPBN) was investigated for the purpose of gas sensing (CO@AlPBN). In addition to experiments, computer-based methodologies could always provide insightful information for the investigated materials and systems especially for those of complicated nanostructures.[21-27] Moreover, such computer-based works are very much applicable for investigating the features of all material and biomaterial related systems.[28-36] The main advantage of employing such techniques is their insightful description of electronic and structural properties of matters at the lowest atomic scale avoiding any other interferer providing useful information prior to experiments.

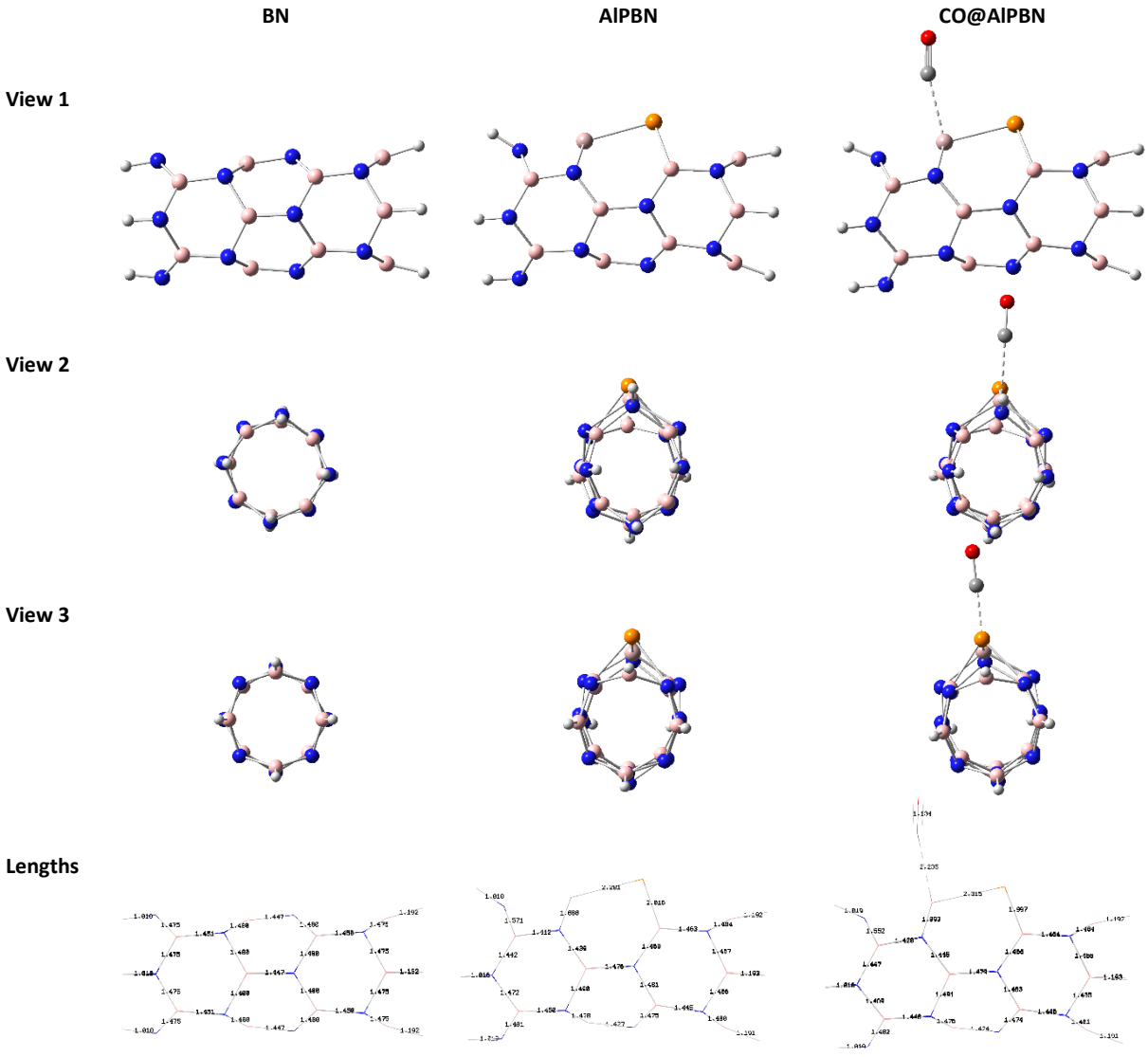


**Fig. 1:** Models systems. View 1: side view, View 2: N-end view, View 3: B-end view. Bond lengths are all in Å.

**METHODOLOGY.** Within this work, quantum chemical computations were performed based on density functional theory (DFT) approach employing the B3LYP exchange-correlation functional and the 6-31G* standard basis set as implemented in the Gaussian program.[37] A representative model of (4,0) BN nanotube was chosen to create AlP-doped model system (AlPBN) (Fig. 1). Avoiding dangling effects, the tubular tips were saturated by hydrogen atoms.[38, 39] This structure was fully optimized to be prepared for CO capturing, in which the next optimization was performed for the complex of nanotube and gas counterparts. By doing such optimizations, the model of captured CO by AlP-doped BN nanotube (CO@AlPBN) was obtained for further investigations. In addition to the optimized geometers and bond lengths, other molecule parameters and properties including capturing energy (CE), dipole moment (DM), molecular orbitals energy levels (HOMO and LUMO), and energy gap (EG) were evaluated for the investigated models. Distribution patterns of HOMO and LUMO and electrostatic potential (ESP) surfaces (Fig. 2) were evaluated for better interpretation of electronic properties especially at the tubular surface. To make sense the changes of systems for detection purposes, ultra-violet (UV) spectra of the models (Fig. 3) were evaluated based on time-dependent (TD) DFT calculations. All the results of this work were summarized in Table 1 and Figs. 1-3, which would be discussed in details by the following text.

**Table 1:** Molecular properties.*

| Property | BN | AlPBN | CO@AlPBN |
|---|---|---|---|
| **CE kcal/mol** | N/A | N/A | -7.074 |
| **HOMO eV** | -6.561 | -6.205 | -5.928 |
| **LUMO eV** | -3.460 | -3.111 | -3.008 |
| **EG eV** | 3.101 | 3.094 | 2.920 |
| **DM Debye** | 3.899 | 7.565 | 8.454 |

*See Figs. 1 and 2 for details.

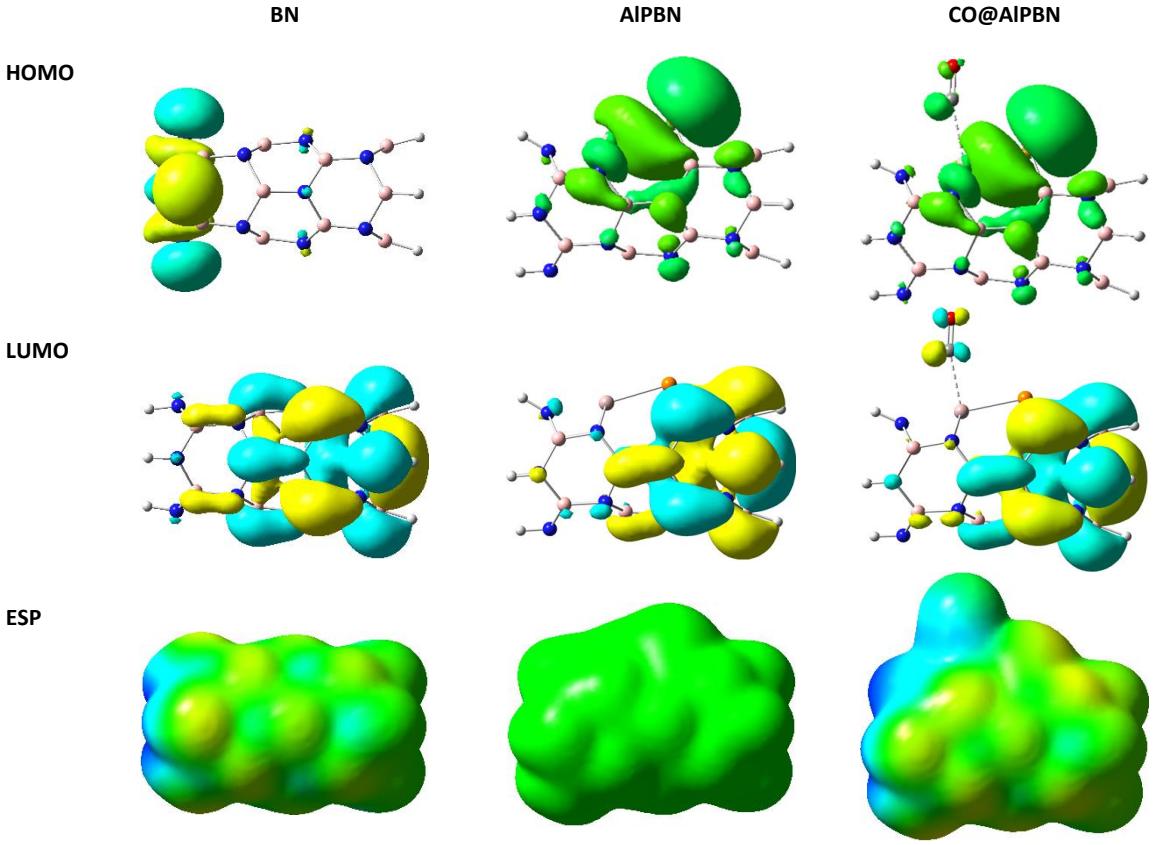


**Fig. 2:** Molecular orbitals (HOMO and LUMO) distribution patterns and electrostatic potential (ESP) surfaces.

**RESULTS & DISCUSSION.** The CO capturing by AlPBN nanotube (CO@AlPBN) was investigated in this work employing DFT calculations. First all singular model structures were optimized to obtain the minimized energy geometries, which are very much important factors for describing chemical systems at the lowest atomic or molecular scale. After optimizing the singular models of BN and AlPBN, they were used to compare the characteristic features impure nanostructure versus the original pure one. To obtain

this purpose, optimized structures were presented in Fig. 1 to exhibit the visual changes of such doping action. Comparing the models in different views could show the effects of AlP-dopant on the geometries of the pure BN nanotube. The bond length of AlP is longer than BP; therefore, implanting such new bond in the BN structure could change the chemical structure features. Carful examining the obtained bond lengths of two impure and pure models could provide helpful information for the effects of AlP-dopant on the geometries of pure BN nanotube. HOMO and LUMO distribution patterns and ESP surfaces (Fig. 2) could also approve the effects of such atomic replacements on the electronic properties of BN nanotube. Regarding the representation of molecular orbitals, the significant change was seen for the HOMO distribution patterns making the AlPBN more appropriate for the purpose of CO capturing. In the pure BN, such HOMO level was not suitable for contributing to interactions whereas it was prepared for the function in the AlPBN model. Analyses of content of Table 1 could declare that the energy of each of HOMO and LUMO levels were changed from pure to impure model, in which the value of EG was changed slightly. This achievement is very much important regarding the expected role of dopants not to change completely the resulted structure as could be seen by the obtained UV spectrum (Fig. 3). The models of pure and impure BN nanotubes of this work could be recognized by UV spectrum regarding the intensity of the obtained peaks at ~300 nm. Based on values of DM of Table 1, the electronic distribution of AlPBN was ready for interacting with CO gas more than the pure BN nanotube. Analyses of the AlPBN and BN models revealed that the dopant system could provide a better tubular surface for the CO gas capturing.

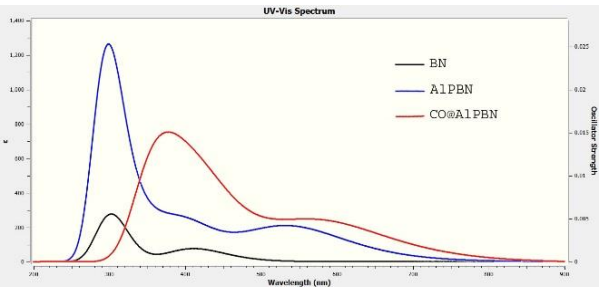


**Fig. 3:** UV spectra.

In the next step, the CO gas was captured at the AlPBN surface and the CO@AlPBN model was created during the two-molecular optimization process. As a result, the CO was relaxed perpendicularly at the tubular system towards Al atom of the AlP doped site with the interacting length of 2.205 Å. The obtained exact value for CE was 7.074 kcal/mol showing somehow a strong interaction. Based on such capturing function, the lengths of other bonds at the AlP-doped region were also changed. CO is a small molecule but its effects on the AlPBN model were significant. Analyses of content of Table 1 could revel information about the molecular orbitals representations, in which all three levels of HOMO, LUMO and EG were changed in the CO@AlPBN model in comparison with each of BN and AlPBN models. The obtained UV spectrum also approved such changes by shifting the maximum absorption to longer wavelengths ~400 nm. Each of distribution patterns and ESP also indicated the CO@AlPBN model could be recognized based on such electronic properties in the time of capturing function. As a result, the investigated AlPBN model was seen as a useful surface to capture CO gas and its detection could be done by recording the electronic changes as seen visually by the UV spectrum. Indeed, capability of detection of a gas-captured system is also very much important in addition to the initial ability of the surface to capture the gas only.

**CONCLUSION.** The CO gas capturing with AlPBN nanotube was investigated in this work employing computer-based DFT calculations. The obtained results indicated some achievements to be declared here as concluding remarks of this work. AlP-doped BN nanotube could be created by atomic replacement of pure BN nanotube. The electronic properties could indicate AlPBN better than pure BN for contributing to possible interactions with other substances as could be explored here for the CO gas capturing. HOMO and LUMO distribution patterns and ESP surfaces could show the significance of such doped system for interacting with CO gas. The CO@AlPBN model was created during capturing CO gas at the surface of AlPBN nanotube. The length and energy of such capturing function were both reasonable and acceptable. Detection of the CO@AlPBN model was done by recording the UV spectrum, in which significant changes were seen for the CO captured model in comparison with the raw surfaces. In sensor or

detector applications, this feature of correct and early detection could be an advantage for each working for the gas capturing function. And finally, the AlPBN model could be considered for further investigations for the CO capturing purposes.

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