

HNO Detection by Nanosized B₁₂N₁₂ Cage: A DFT/TDDFT Study

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The interaction of a nitrosyl hydride (HNO) molecule with B₁₂N₁₂ nanocage was explored by means of density functional calculations. It was found that HNO prefers to be adsorbed on a boron atom of the cage with adsorption energy of -0.65 eV. This adsorption process significantly shifts the HOMO-LUMO gap (E_g) of the cage to lower energies, thereby reducing E_g of the cage from 6.84 to 2.45 eV. Time-dependent density functional theory (TDDFT) calculations show a high intensity peak in 381.38 nm in the most stable complexes of HNO with B₁₂N₁₂. The change in electronic properties of the B₁₂N₁₂ nanocage on HNO adsorption is significant enough to consider it a potential sensor for HNO detection.

Keywords: B₁₂N₁₂ nanocage, HNO sensing, DFT, DOS

INTRODUCTION

After discovery of C₆₀ in 1985[1], scientists paid attention to other fullerene-like materials such as (BN)_n cages with n = 12, 24, 28 and 32 [2-5]. Among boron nitride nanocages, B₁₂N₁₂ is the most stable structure with T_h point group [2]. B₁₂N₁₂ nanocluster has been synthesized by Oku *et al.* in 2004 by using laser desorption time-of-flight mass spectrometry method [6,7]. Experimental results showed that the synthesized cage consists of 8 hexagon and 6 tetragonal B-N rings, with two distinct bonds between B and N atoms. One of the bonds is between two six membered rings (6-MR) and another one locates between one six membered and one four membered rings (4-MR). B₁₂N₁₂ has been attracted attention of many researchers due to notable physical and chemical properties such as oxidation resistance, wide band gap, large surface to volume ratio, low dielectric constant and high temperature stability

[8,9]. Several quantum mechanical studies about adsorption of different molecular moieties on the exterior surface of B₁₂N₁₂ nanocage were reported recently [10-24].

Nitrosyl hydride (HNO) is a small molecule employed in industrial, atmospheric and bacterial processes [25]. It has a significant role in chemical and biological systems, medicine and pharmacological responses. In biology, it can be applied as a number of enzyme inhibitor such as aldehyde dehydrogenase [26]. HNO may play role of an inhibitor that prevent tumor growth [27]. HNO was detected by membrane inlet mass spectrometry [28] in aqueous solution, but this method has disadvantages in the complexity of the apparatus with a large size and high cost. In the current study, an attempt has been made to present B₁₂N₁₂ nanocage with its unique electronic properties as a promising sensor for detection of HNO. Main focuses have been placed on adsorption energies and the changes of electronic properties of B₁₂N₁₂ in the presence of HNO. The advantage of the present work is introducing a pristine nanostructure as a sensor, avoiding the necessity of doping, functionalizing, and in general manipulating of its structure.

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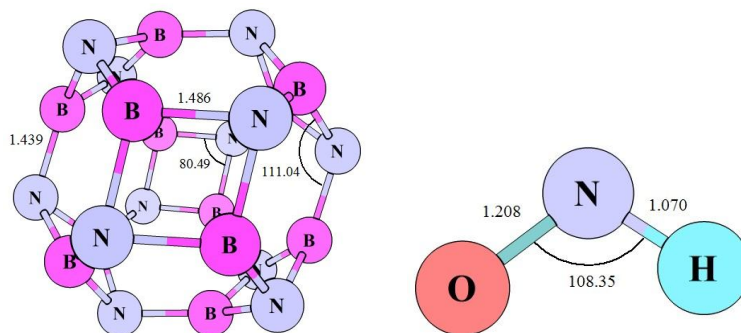


Fig. 1. The optimized geometry of pristine $B_{12}N_{12}$ and HNO molecule at B3LYP/6-31G (d) level.

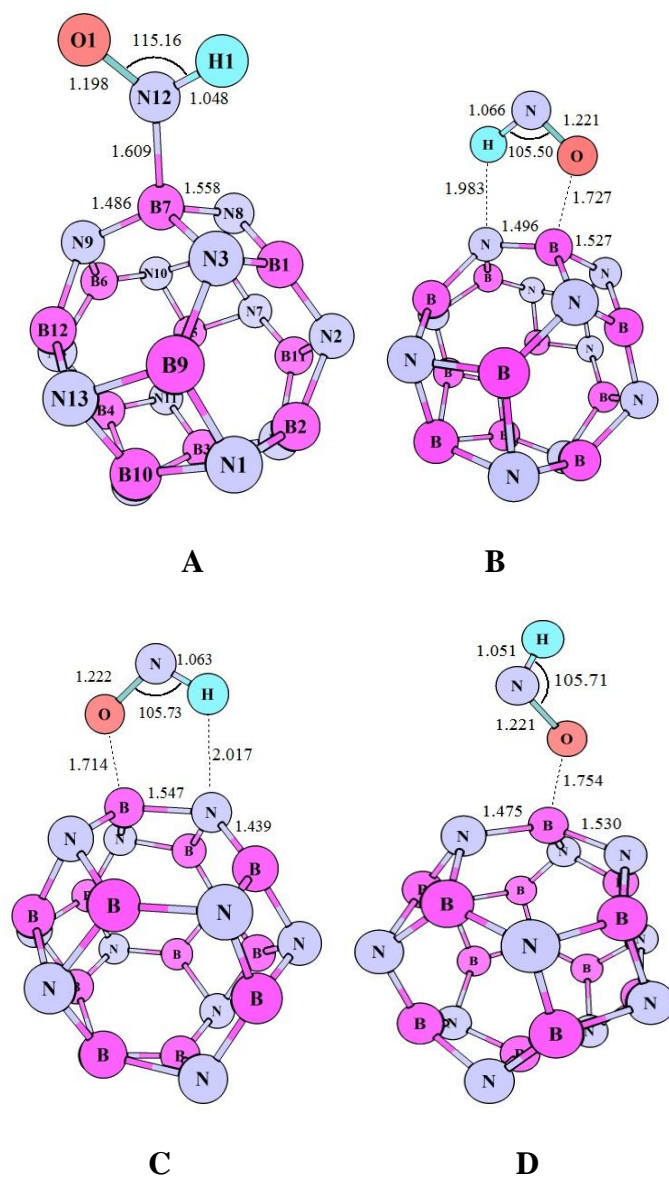


Fig. 2. Models for four stable complexes of HNO/ $B_{12}N_{12}$ (A, B, C, D).

COMPUTATIONAL METHODS

All the calculations were performed using Gaussian 09 package [29]. Geometry optimizations energy calculations and density of states (DOS) analysis were performed on the B₁₂N₁₂ nanocage and different HNO/B₁₂N₁₂ complexes using B3LYP [30,31] functional with 6-31G(d) basis set. To study the adsorption systems, the van der Waals interactions are recommended to be considered, while B3LYP method does not consider it. We have shown that it is not important in this system, so B3LYP is a reliable method in the present study (see supporting information). Vibrational frequencies were also calculated at the same level of theory to confirm all the stationary points corresponding to the local minima on the potential energy surface. Adsorption energy (E_{ad}) of the studied complexes is obtained in the usual way as

$$E_{ad} = E_{\text{complex}} - (E_{\text{HNO}} + E_{\text{B}_{12}\text{N}_{12}}) + E_{\text{BSSE}} \quad (1)$$

where E_{complex} corresponds to the energy of B₁₂N₁₂ in which HNO has been adsorbed on the cage, $E_{\text{B}_{12}\text{N}_{12}}$ is the energy of the isolated cage and E_{HNO} is the energy of a single HNO molecule. E_{BSSE} is the energy of the basis set superposition error calculated using the counterpoise method [32].

Natural bond orbitals (NBO) analysis [33] was performed to obtain charge transfer between B₁₂N₁₂ nanocage and HNO molecule. GaussSum program [34] was also used to present density of states (DOS) and partial density of states (PDOS) plots of pristine B₁₂N₁₂ and different complexes.

Thermodynamic parameters of adsorption (ΔH_{ad} and ΔG_{ad}) are obtained from the following equations;

$$\Delta H_{ad} = H_{\text{complex}} - (H_{\text{HNO}} + H_{\text{B}_{12}\text{N}_{12}}) \quad (2)$$

$$\Delta G_{ad} = \Delta H_{ad} - T\Delta S_{ad} = \Delta H_{ad} - T(S_{\text{complex}} - (S_{\text{HNO}} + S_{\text{B}_{12}\text{N}_{12}})) \quad (3)$$

where H is sum of electronic and the thermal enthalpy, G is sum of the electronic, the thermal Gibbs free energy and S is entropy at 298.14 K and 1 atmosphere. The UV-Vis spectra of complexes pairing HNO with B₁₂N₁₂ cage were simulated at TD-B3LYP/6-31G(d) level of theory [35].

RESULTS AND DISCUSSION

The optimized structures of HNO and pristine B₁₂N₁₂ at B3LYP/6-31G(d) computational level are shown in Fig. 1. In order to find the most stable site of HNO adsorption on B₁₂N₁₂, HNO molecule was located around the external surface of B₁₂N₁₂ with different orientations. We started our calculation with different structures by setting of HNO on the top of B and N atoms, center of hexagonal and tetragonal rings, and also the bridge site of B-N bonds. After full optimization without symmetry constrain, four favorable configurations (A, B, C, D) are obtained.

The optimized structure of different HNO/B₁₂N₁₂ complexes and corresponding binding distances are given in Fig. 2. The adsorption energies of the respective complexes are given in Table 1. In the most stable complex (A), HNO prefers to be adsorbed on a boron atom of the cage with B-N bond length of 1.61 Å and adsorption energy of -0.65 eV. The absorption process to form A complex is an exothermic reaction ($\Delta H_{ad} = -15.92$ kcal mol⁻¹), with the negative $\Delta G_{ad} = -6.25$ kcal mol⁻¹ value (Table 1). This means that association of HNO with B₁₂N₁₂ to form A complex is a spontaneous process at room temperature.

Three additional minima on the potential energy surface of the studied clusters have been located. The principal intermolecular interaction within B and C complexes corresponds to cyclic structures with pair of B-O and N-H interactions. In B and C complexes HNO is adsorbed on the top of B-N bonds that are between two 6-MR rings, and a 6-MR and a 4-MR ring, respectively. The formation process of B and C complexes is exothermic with $\Delta H_{ad} = -10.48$ and -9.95 kcal mol⁻¹, respectively, and positive values of ΔG_{ad} . Finally, the D complex presents a B-O interaction with the smallest adsorption energy. More calculations in water media was performed for pristine and more stable complex A (Table 1). Complex A is more stable in water media than gas phase. Significant blue shift of NH stretching mode in the ranges of 86-324 cm⁻¹ are calculated for the studied complexes (Table 1), which is in consistence with previous reports in the literature [36-39].

To comprehend the effect of adsorption on the electronic properties of B₁₂N₁₂, results of calculated highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) for the studied complexes are

Table 1. Adsorption Energy (E_{ad}), Highest Occupied Molecular Orbital (HOMO), Lowest Unoccupied Molecular Orbital (LUMO), Energy Gap (E_g), and Variation (Blue Shift) of the NH Bond Stretching Frequencies ($\Delta\nu$) Computed for Pristine HNO/ $B_{12}N_{12}$ Complexes, and Charge Transfer from HNO to $B_{12}N_{12}$ (Q_t)

Structure	E_{ad} (eV)	HOMO (eV)	LUMO (eV)	E_g (eV)	ΔE_g (%) ^a	ΔH_{ad}	ΔG_{ad}	$\Delta\nu_{N-H}$ (cm^{-1})	$Q_t e $
Pristine	-	-7.71 (-7.70)	-0.86 (-0.79)	6.84 (6.90)	-	-	-	-	-
A	-0.65 (-0.77) ^b	-7.22 (-7.27)	-4.87 (-4.54)	2.35 (2.73)	-65.7 (-60.43)	-15.92	-6.25	324	0.262
B	-0.39	-7.33	-4.77	2.56	-62.57	-10.48	0.2	86	0.223
C	-0.37	-7.37	-4.79	2.58	-62.33	-9.95	0.7	119	0.221
D	-0.12	-7.15	-4.92	2.23	-67.43	-3.78	5.98	284	0.199

^aChange of E_g of $B_{12}N_{12}$ upon adsorption of HNO. ^bNumbers in parentheses calculated at water media.

Table 2. Selected Excitation Energies (ΔE), Wavelength (λ), Oscillator Strength (f_0) and Relative Orbital Contribution Calculated of A, B, C and D Configurations

Configuration	Excited state	ΔE (eV)	λ (nm)	f_0	Assignment
A	10	3.25	381.38	0.0245	HOMO-8 \rightarrow LUMO
B	10	3.42	362.80	0.0148	HOMO-8 \rightarrow LUMO
C	2	1.96	631.94	0.0150	HOMO \rightarrow LUMO
D	10	3.04	407.75	0.0214	HOMO-8 \rightarrow LUMO

presented (Table 1). It is shown that adsorption of HNO on the surface of cage leads to the significant deduction of energy difference between HOMO and LUMO (E_g) in the range of 60-68%. Figure 3 reveals that HOMO in $B_{12}N_{12}$ distributed around more electronegative atoms (N) and LUMO located on less electronegative atoms (B). Moreover, in the studied complexes, LUMO is placed around HNO molecule and HOMO is located on N atoms of the cage. It is revealed from NBO analysis that in the most stable configuration (A), 0.26 e charge is transferred from

HNO to the cage (Table 2). In fact, $B_{12}N_{12}$ molecule will gain charge from HNO after adsorption and this charge leads to the change in electronic properties of the cage. Nice linear correlation with correlation coefficient $R^2 = 0.97$ is established between stabilization energy of the studied complexes and values of charge transferred from HNO to $B_{12}N_{12}$ (Fig. 4).

To justify above results, density of states (DOS) for $B_{12}N_{12}$ and HNO/ $B_{12}N_{12}$ complexes are plotted in Fig. 5. In $B_{12}N_{12}$, E_g is 6.84 eV which has been significantly

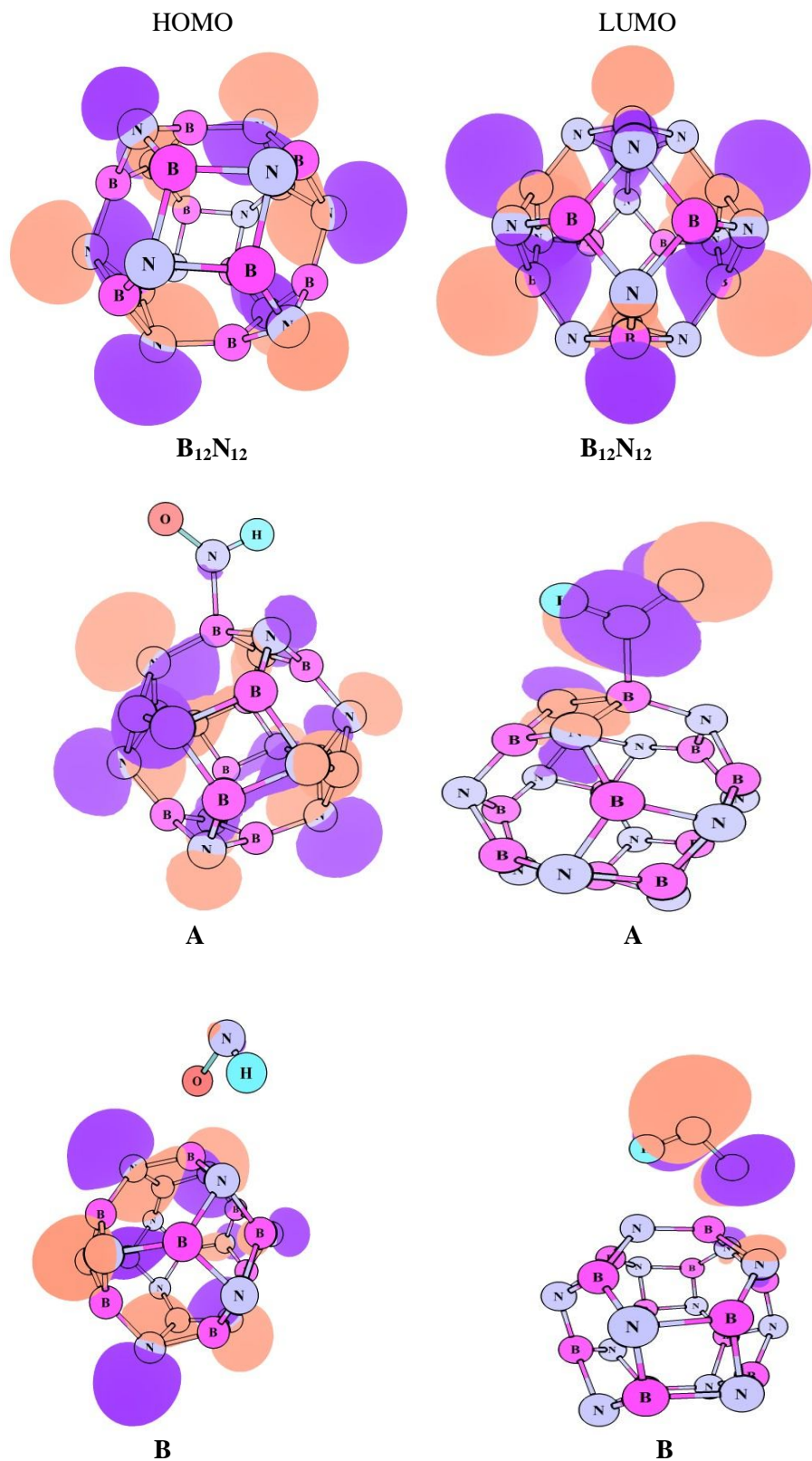


Fig. 3. Plots of the HOMO and LUMO for B₁₂N₁₂ pristine and four stable complexes of HNO/B₁₂N₁₂ (A, B, C, D).

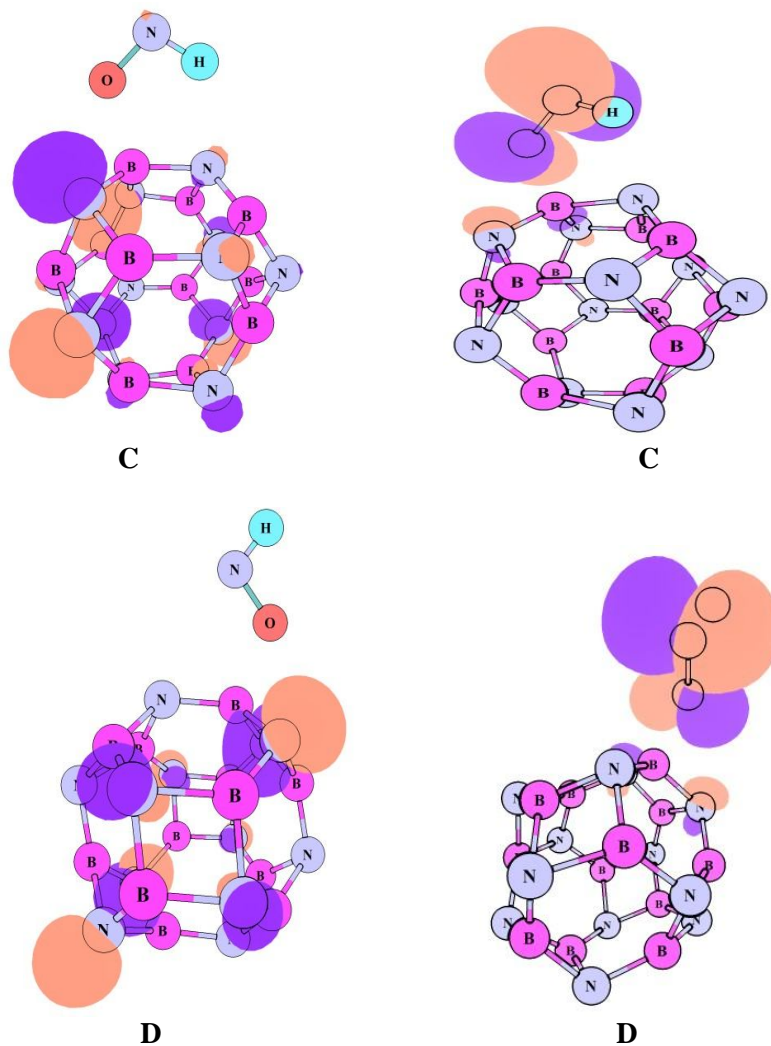


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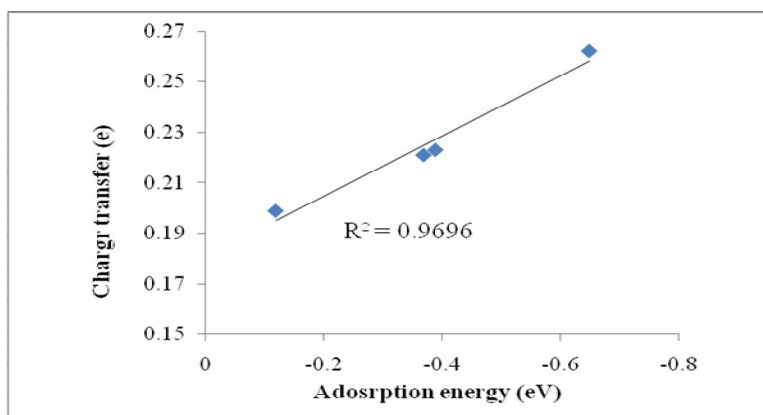


Fig. 4. Linear correlation between adsorption energy and charge transfer from HNO to B₁₂N₁₂ in HNO/B₁₂N₁₂ complexes.

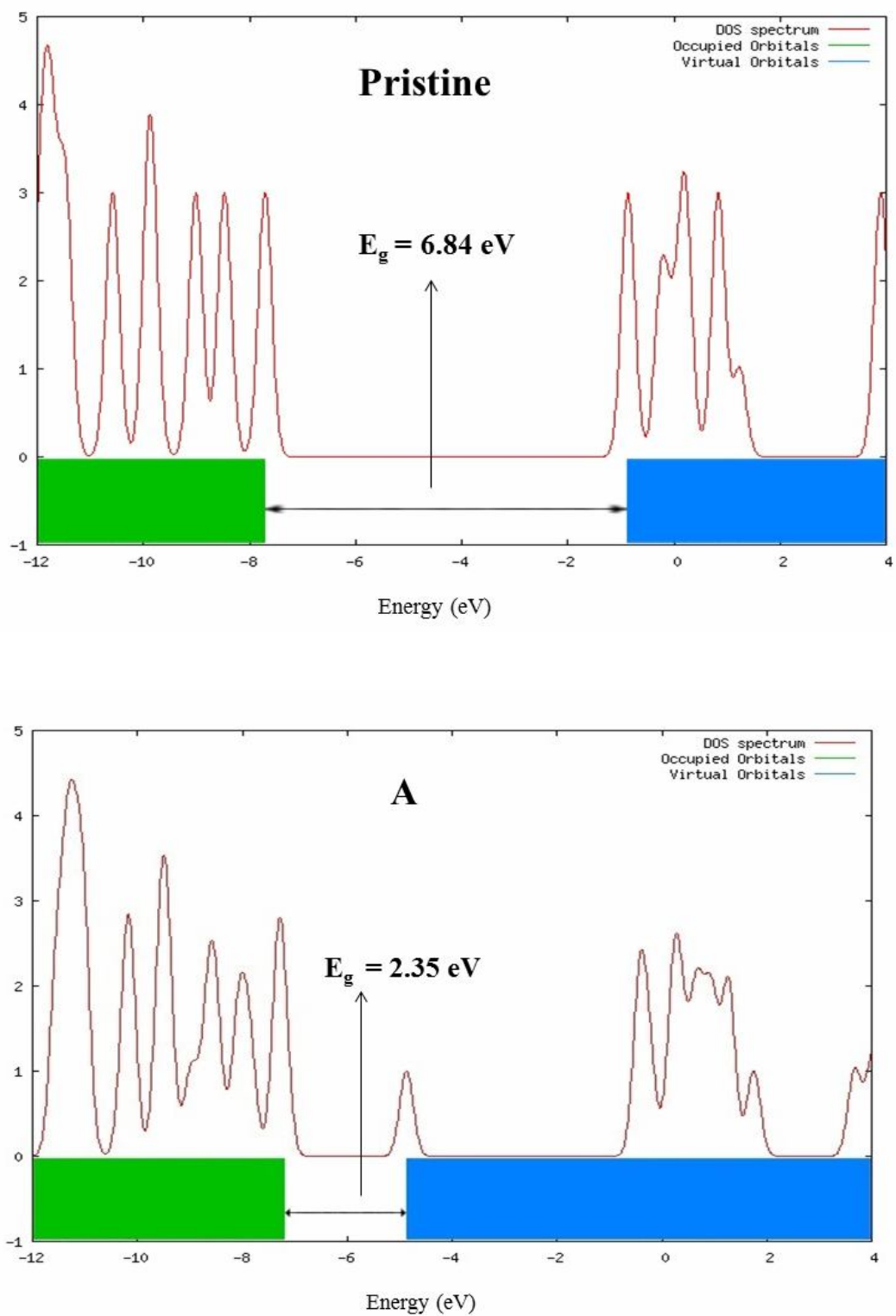


Fig. 5. Density of states (DOS) plots for four stable complexes of HNO/B₁₂N₁₂ (A, B, C, D) and partial density of states (PDOS) of A configuration.

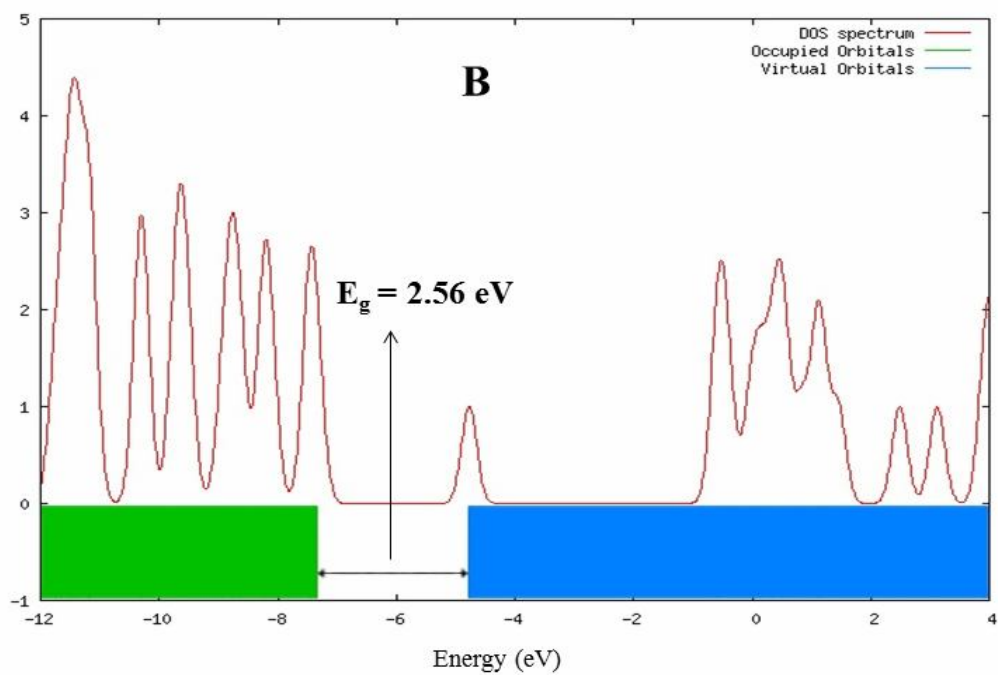
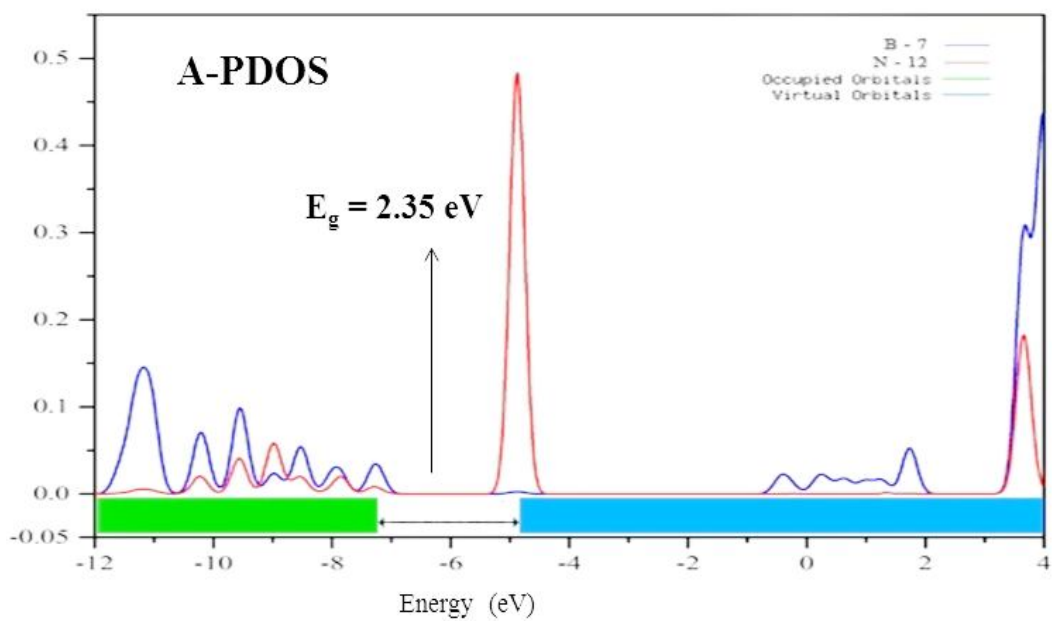


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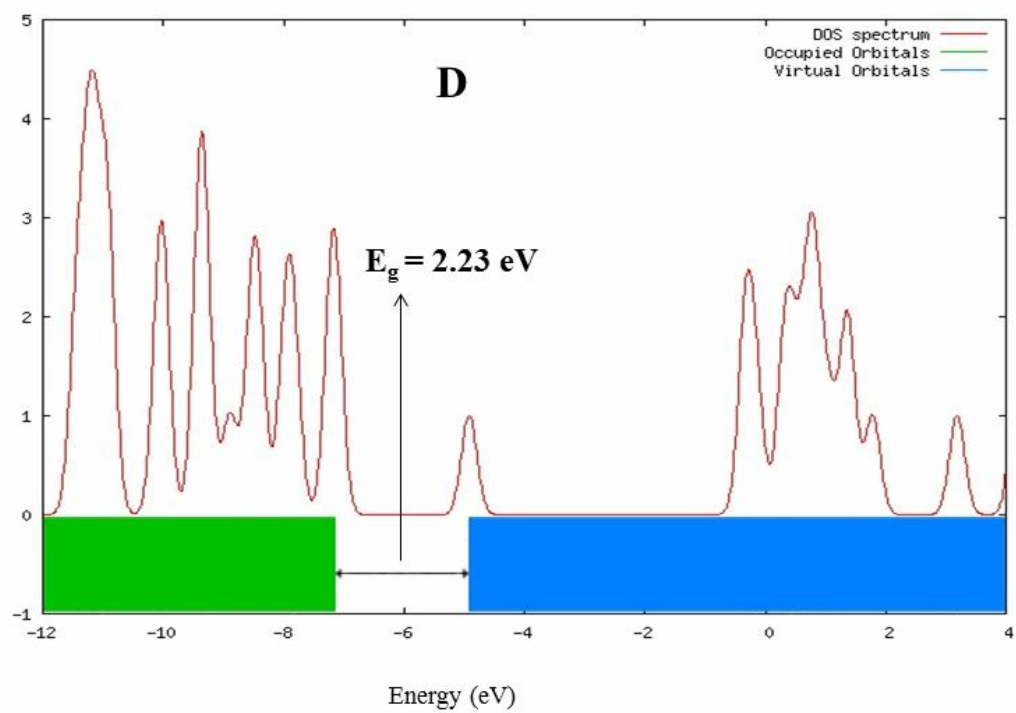
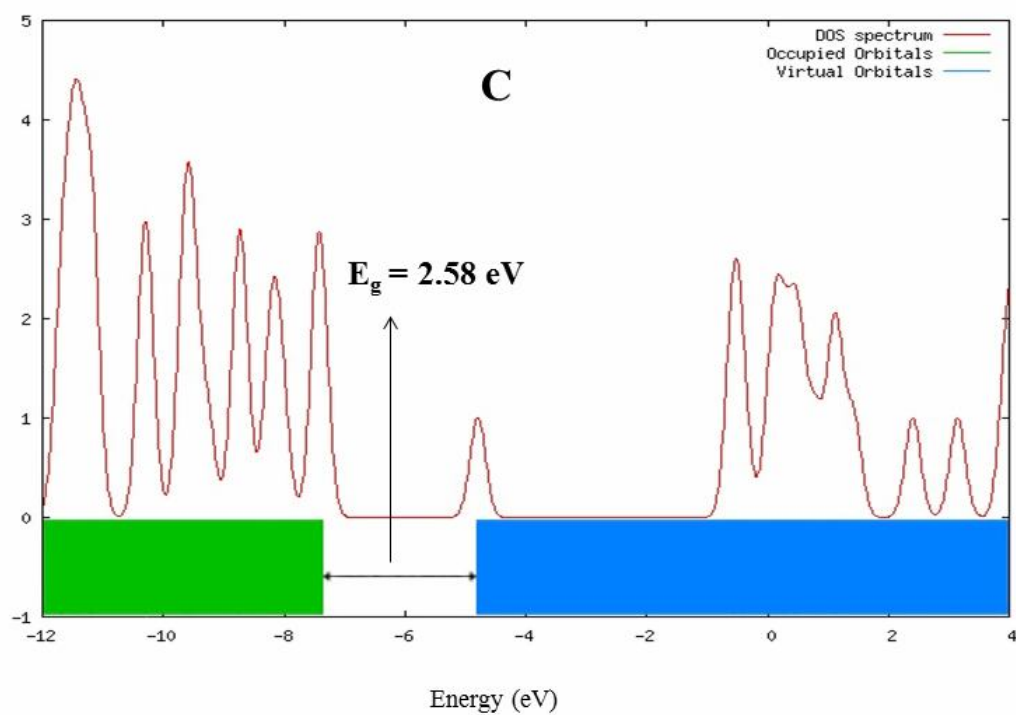


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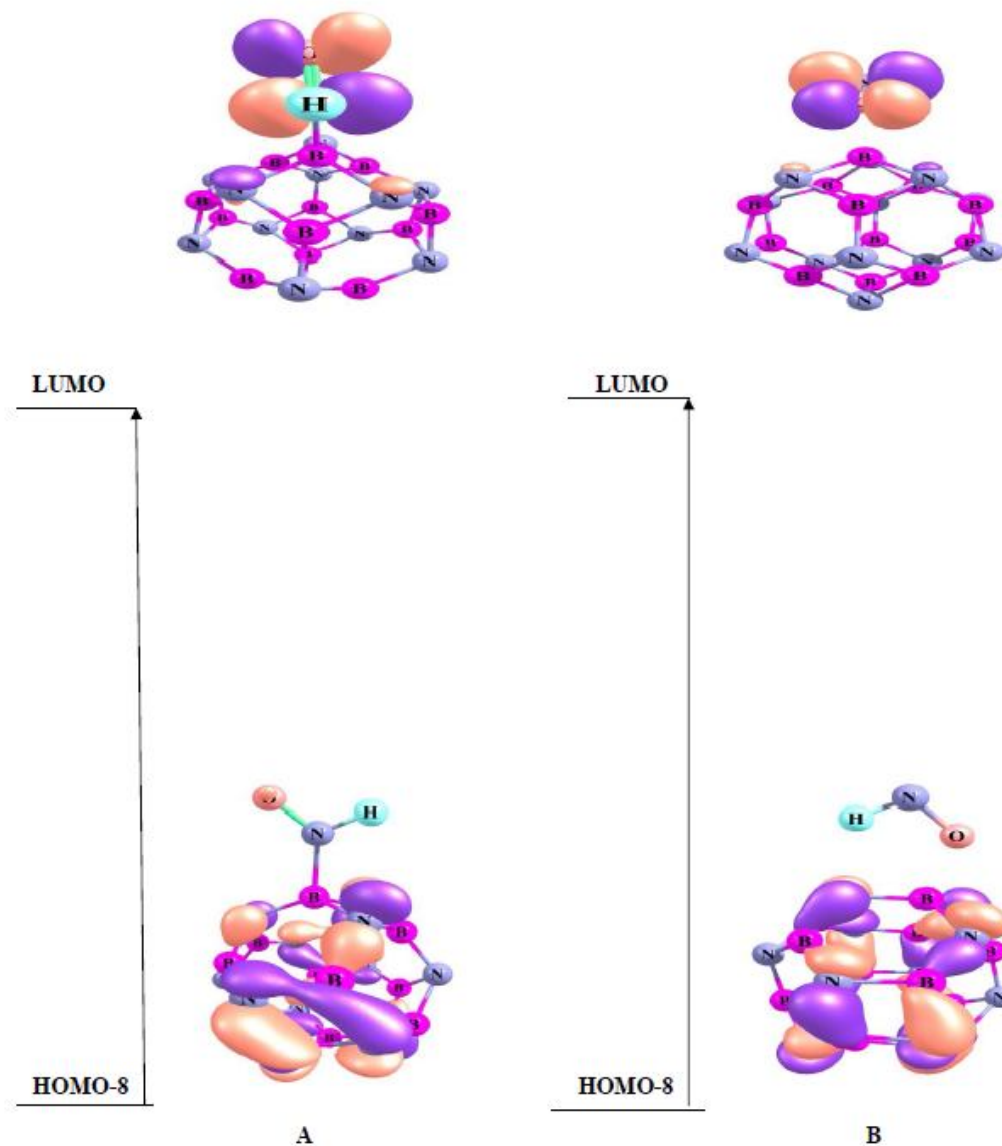


Fig. 6. Crucial transition states of four stable complexes of HNO/B₁₂N₁₂ (A, B, C, D) with the largest component coefficient marked.

decreased in all complexes due to low energy level as the newly formed LUMO reclining between the original LUMO and HOMO of B₁₂N₁₂. For the most stable complex, A, partial density of state (PDOS) calculation has been performed to identify those atoms involved in interaction with each other (Fig. 5). It is clarified from PDOS analysis that there is interaction between B7 of B₁₂N₁₂ with N12 of HNO in A complex. For this reason, the band gap of A is decreased by 66%; so this nanocage is sensitive enough for

sensing HNO molecule.

In the next step, we have used a TD-B3LYP/6-31G(d) calculation to determine the crucial excited states with the largest oscillator strength for the interaction of HNO molecule with B₁₂N₁₂ nanocage (Fig. 6). Selected excitation energies (ΔE), wavelength (λ), oscillator strength (f_0) and relative orbital contribution calculated for A, B, C and D complexes are presented in Table. 2. It is shown in Fig. 6 that electron cloud of LUMO is dominant over the HNO

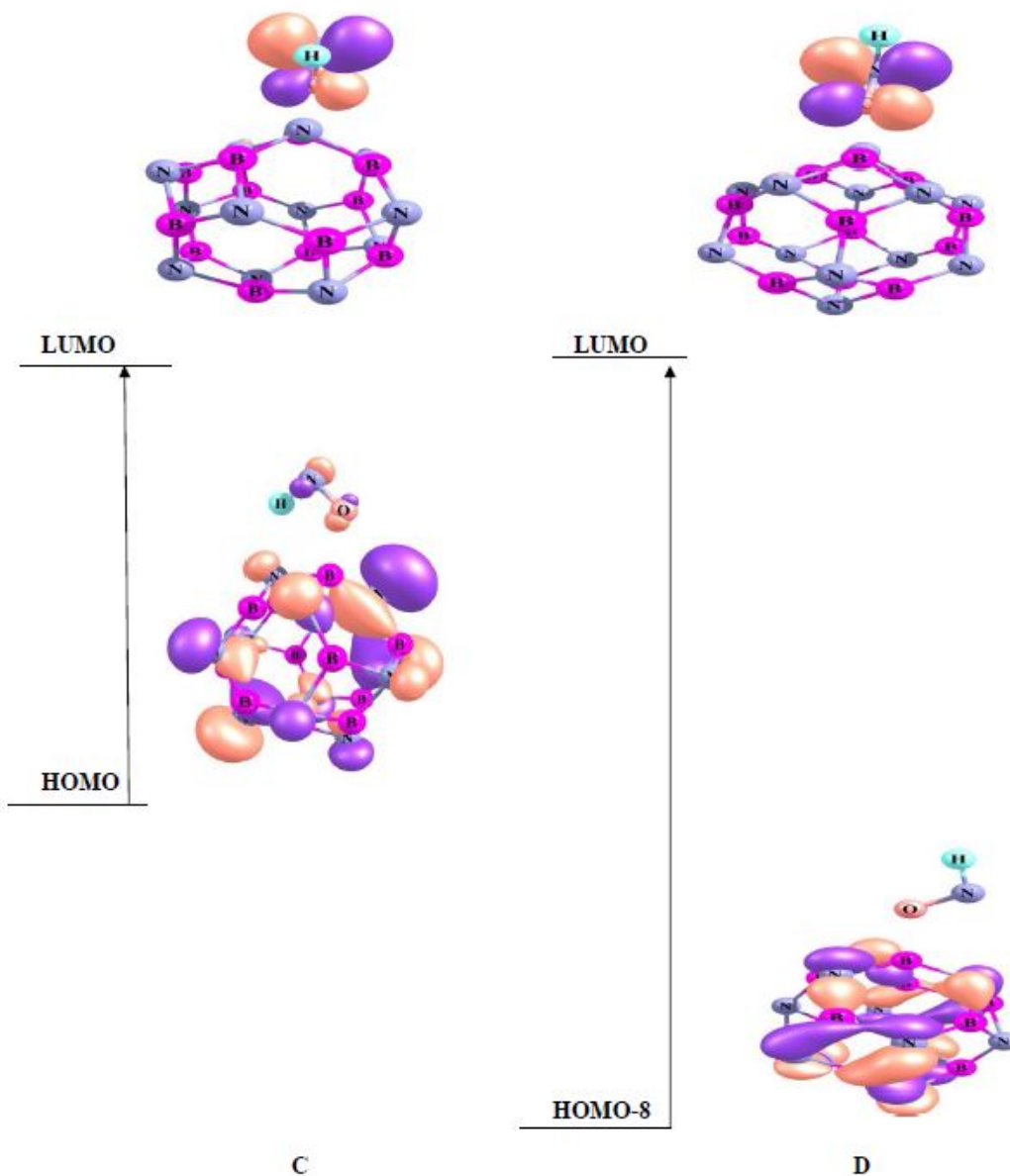


Fig. 6. Continued.

molecule, while electron clouds in HOMO and HOMO-8 orbital have been spread over the B₁₂N₁₂ nanocage. Furthermore, UV-Vis spectra of HNO/B₁₂N₁₂ complexes are depicted in Fig. 7. The major absorption peak of HNO/B₁₂N₁₂ complexes is at 381.38 nm which is accordance to tenth excited state of A complex with excitation energy of 3.25 eV for transition from HOMO-8 to LUMO. For the B complex, an adsorption peak at 362.8 nm corresponding to tenth excited state for transition from

HOMO-8 to LUMO with excitation energy of 3.42 eV is observed. The peak of C complex is appeared at 631.94 nm with excitation energy of 1.96 eV which is matched to excited state 2 for transition of HOMO to LUMO. For the D complex, an adsorption peak at 407.75 nm with the excitation energy of 3.04 eV concerning to the tenth excited state for transition from HOMO-8 to LUMO is observed. These observations imply to interaction between nitrosyl hydride and nanocage and charge transfer from HNO to

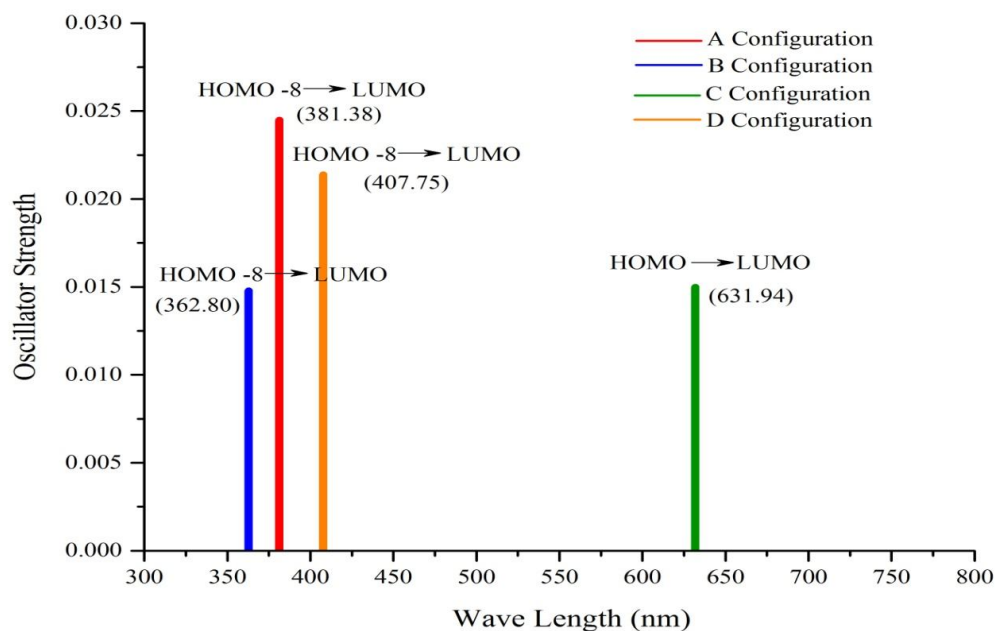


Fig. 7. UV-Vis spectra of the HNO/B₁₂N₁₂ configurations (A, B, C, D) with the largest component coefficient marked.

B₁₂N₁₂.

CONCLUSIONS

In this study, adsorption of HNO molecule on the exterior surface of B₁₂N₁₂ is presented by DFT calculation for the first time. Our results reveal that HNO prefers to be adsorbed on a boron atom of the cage with adsorption energy of -0.65 eV. Significant changes in electronic properties of the B₁₂N₁₂ nanocage on HNO adsorption leads to this conclusion that B₁₂N₁₂ is a potential new sensor for sensing HNO molecule.

SUPPORTING INFORMATION

Affirmation reliability of B3LYP method for study of title complexes.

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