REMUNOM
ISSN 2178-6925

Received: 13/03/2026 - **Accepted:** 10/05/2026
Vol: 13.09
DOI: 10.66104/zrwxm372
Pages: 1-17

SELECTIVE N_2O GAS SENSING PERFORMANCE OF Y-MODIFIED $B_{12}N_{12}$ NANOCAGE: A DFT APPROACH

DESEMPENHO SELETIVO NA DETECÇÃO DO GÁS N_2O POR NANOGAIOLA $B_{12}N_{12}$ MODIFICADA COM Y: UMA ABORDAGEM DFT

Wellington da Conceição Lobato do Nascimento
PhD student in Chemistry – Federal University of Maranhão – UFMA, Brazil
Email: wellington.conceicao@discente.ufma.br

Natanael de Sousa Sousa
PhD in Chemistry – Federal University of Maranhão – UFMA, Brazil
Email: 83.natan@gmail.com

Francivaldo Santos da Silva
PhD student in Chemistry – Federal University of Maranhão – UFMA, Brazil
Email: francivaldoss@gmail.com

Felipe Anderson Silva de Aquino
Master's degree in Materials Engineering - Federal Institute of Maranhão – IFMA, Brazil
Email: aquinofelipe444@gmail.com

Adeilton Pereira Maciel
Department of Chemistry - Federal University of Rio Grande of Norte – UFRN, Brazil
Email: adeilton.maciel@ufrn.br

Graphical Abstract

REMUNOM
ISSN 2178-6925

Received: 13/03/2026 - **Accepted:** 10/05/2026
Vol: 13.09
DOI: 10.66104/zrwxm372
Pages: 1-17

Abstract

The emission of nitrous oxide (N_2O) represents a serious environmental challenge due to its contribution to ozone layer depletion. In this work, density functional theory calculations with dispersion correction (DFT-D3), employing the B3LYP functional and the LanL2DZ basis set, were carried out to investigate the adsorption of N_2O on pristine and yttrium-modified $B_{12}N_{12}$ nanocages. Geometric, electronic, and energetic parameters were analyzed, as well as the electronic sensitivity of the systems toward gas adsorption. The Y@b_{66} nanocage exhibited the largest variation in the energy gap (ΔE_{gap} = 38.7%), indicating high sensitivity to N_2O. Energetic results reveal that N_2O is physically adsorbed on pristine $B_{12}N_{12}$ (E_{ads} = -0.16 eV), whereas it interacts moderately with the Y@b_{66} nanocage (E_{ads} = -1.07 eV), showing an appropriate recovery time (τ = 120.54 s). In addition, the Y@b_{66} system demonstrated good selectivity toward N_2O in the presence of interfering gases (H_2, CH_4, and CO). These findings indicate that the Y@b_{66} nanocage is a promising material for application as a selective N_2O gas sensor.

Keywords: $B_{12}N_{12}$ nanocage, adsorption, N_2O, sensor.

Resumo

A emissão de óxido nitroso (N_2O) representa um sério desafio ambiental devido à sua contribuição para a destruição da camada de ozônio. Neste trabalho, cálculos baseados na Teoria do Funcional da Densidade com correção de dispersão (DFT-D3), utilizando o funcional B3LYP e o conjunto de base LanL2DZ, foram realizados para investigar a adsorção de N_2O em nanogaiolas de $B_{12}N_{12}$ puras e modificadas com ítrio (Y). Foram analisados os parâmetros geométricos, eletrônicos e energéticos, bem como a sensibilidade eletrônica dos sistemas à adsorção do gás. A nanogaiola Y@b_{66} apresentou a maior variação do gap de energia (ΔE_{gap} = 38,7%), indicando elevada sensibilidade ao N_2O. Os resultados energéticos revelam que o N_2O se adsorve fisicamente na $B_{12}N_{12}$ pura (E_{ads} = -0,16 eV), enquanto interage de forma moderada com a nanogaiola Y@b_{66} (E_{ads} = -1,07 eV), exibindo um tempo de recuperação adequado (τ = 120,54 s). Além disso, o sistema Y@b_{66} demonstrou boa seletividade em relação a gases interferentes (H_2, CH_4 e CO). Esses resultados indicam que a nanogaiola Y@b_{66} é um material promissor para aplicação como sensor seletivo de N_2O.

Palavras-chave: Nanogaiola $B_{12}N_{12}$, adsorção, N_2O, sensor.

1. Introduction

The mission of scientists to find materials capable of detecting or eliminating harmful gases present in the atmosphere has not been an easy task. In recent decades, studies have intensified for the development of chemical sensors capable of rapid and efficient detection of these gases [1,2]. Nanometric materials have been investigated as an alternative for application as sensors, due to their small size, good precision and excellent reactivity properties. Among these materials, we have boron nitride $(BN)_n$ nanocages, which have gained prominence

REMUNOM
ISSN 2178-6925

Received: 13/03/2026 - **Accepted:** 10/05/2026
Vol: 13.09
DOI: 10.66104/zrwxm372
Pages: 1-17

due to their excellent properties, such as oxidation resistance, high sensitivity and low recovery time [3].

Even with their excellent properties, some gases, such as $COCl_2$, H_2S, NO tend not to be spontaneously adsorbed on the surface of the $B_{12}N_{12}$ nanocage [4]. In this context, recent studies have investigated the structural modification of this nanomaterial using transition metals; in order to overcome this limitation, as well as improve their adsorption properties [5, 6]. Among the second-row transition metals, yttrium (Y) has gained prominence in studies as a modifier of nanomaterials for application as a sensor of atmospheric gases [7, 8]. Agwamba et al. [9] investigated the adsorption of metal-doped silicon nanocages ($Si_{59}X$; X = Nb, Mo, Y, Zr) as N-Nitrosodimethylamine (NDMA) gas nanosensors using correlation-exchange functional (PBE) and Lanl2DZ basis set. The results reported that doping with transition metals (Nb, Mo, Y, Zr) in the Si_{60} fullerene nanostructure significantly improved the interaction with NDMA. Other molecular descriptors also indicated positive results, confirming the suitability of the surfaces for NDMA detection.

The objective of this study was to explore, using DFT calculations, the adsorption behavior of N_2O gas on Y-modified $B_{12}N_{12}$ nanocages, along with the interfering gases H_2, CH_4, and CO, to assess the potential of this material as an environmental sensor for toxic gases.

2. Computational Methodology

DFT calculations were performed using the ORCA 5.0 program [10]. The pure and Y-modified $B_{12}N_{12}$ nanocages were optimized using the B3LYP-D3 [11] functional and the Lanl2DZ basis set. The B3LYP functional-Grimme D3 dispersion correction/LANL2DZ basis set level of theory was adopted in this study due to its suitable balance between computational cost and reliability for investigating geometric parameters, adsorption energies, and electronic properties of B–N-based nanocage systems. The B3LYP functional has been widely applied in similar adsorption studies, while the D3 dispersion correction improves the description of long-range van der Waals interactions that are relevant in adsorption processes. For the yttrium atom, the LANL2DZ basis set was selected because it incorporates

REMUNOM
ISSN 2178-6925

Received: 13/03/2026 - **Accepted:** 10/05/2026
Vol: 13.09
DOI: 10.66104/zrwxm372
Pages: 1-17

effective core potentials (ECPs), enabling an efficient treatment of heavier atoms while maintaining methodological consistency across all investigated systems. This computational approach has also been frequently reported in previous studies involving transition-metal-modified nanomaterials. Frequency analysis was performed to confirm the global minima of the optimized structures. The modification of $B_{12}N_{12}$ with Y resulted in five optimized structures [12]: doped ($YB_{11}N_{12}$ and $B_{12}N_{11}Y$, with substitution of a boron atom and a nitrogen atom for a Y atom in the nanocage, respectively); decorated (Y@b_{64} and Y@b_{66}, with a Y atom positioned above the atomic bond between the tetragonal and hexagonal rings and above the atomic bond between two hexagonal rings, respectively) and the encapsulated structure (Y@$B_{12}N_{12}$, in which a Y atom is positioned inside the $B_{12}N_{12}$ nanocage). In the present work, the isolated nanocages (pristine and Y-modified) and the closed-shell gas molecules (N_2O, H_2, CH_4, and CO) were treated in their singlet ground states, which is the expected configuration for these species. For the adsorbed systems, the calculations were also predominantly performed assuming a singlet state. Additionally, spin-polarized calculations were considered for the Y@b_{66} system, as indicated by the reference to the α-spin state in the manuscript, using an unrestricted formalism to allow for possible spin-density redistributions induced by adsorption. The obtained results did not reveal significant electronic changes that would justify the need for a systematic exploration of other spin multiplicities. Therefore, the adopted methodological strategy represents an appropriate balance between theoretical rigor and computational feasibility and is sufficient to consistently describe the adsorption phenomena discussed in this study.

The structures were calculated as neutral, and their stability was investigated through the cohesive energy (E_{coh}), which was calculated according to the following equation [13]:

$$E_{coh} = \frac{1}{N}(E_{nanocage} - xE_B - yE_N - zE_{TM}), \quad (1)$$

where Enanocage is the total energy of the nanocage (either pure or yttrium-modified); E_B, E_N and E_Y are the energies of the B, N, and Y atoms, respectively; x,

REMUNOM
ISSN 2178-6925

Received: 13/03/2026 - **Accepted:** 10/05/2026
Vol: 13.09
DOI: 10.66104/zrwxm372
Pages: 1-17

y, and z represent the quantities of each atom (B, N, and Y, respectively) in the structure; and N is the total number of atoms in the nanocage.

Given the energy gap (E_{gap}), defined as the difference between the LUMO (E_{LUMO}) and HOMO (E_{HOMO}) energies, we determine the value of electronic sensitivity (ΔE_{gap}) for the interaction between the N_2O molecule and the pure or Y-modified $B_{12}N_{12}$ nanocages according to equation 2, below:

$$\Delta Egap = \left[\frac{(E_{gap(nanocage-N2O)} - E_{gap(nanocage)})}{E_{gap(nanocage)}}\right] \times 100\%, \quad (2)$$

where $E_{gap(nanocage-N2O)}$ is the energy gap for the interaction of N_2O with pure and modified $B_{12}N_{12}$ nanocages, and $E_{gap(nanocage)}$ is the energy gap for pure or Y-modified $B_{12}N_{12}$.

The E_{ads} value for the interaction between N_2O and $B_{12}N_{12}$ or Y-$B_{12}N_{12}$ was calculated according to equation 3:

$$E_{ads} = E_{(nanocage-N2O)} - (E_{(nanocage)} + E_{(N2O)}) + E_{BSSE} \quad (3)$$

where $E_{(nanocage-N2O)}$ is the energy of the $B_{12}N_{12}$ or Y-$B_{12}N_{12}$ nanocage bound to N_2O, $E_{(nanocage)}$ is the energy of the pure $B_{12}N_{12}$ or Y-modified $B_{12}N_{12}$ nanocages, $E_{(N2O)}$ is the energy of the N_2O molecule, and E_{BSSE} is the basis set superposition error (BSSE) [13].

The recovery time (τ), which is exponentially related to the system E_{ads}, can be calculated by equation 4 [14]:

$$\tau = v_0^{-1} e^{-E_{ads}/k_B T} \quad (4)$$

where v_0 is the attempt frequency (10^{12} v_0 s^{-1}), k_B is the Boltzmann constant (8.62 x 10^{-5} eV K^{-1}), and T is the thermodynamic temperature (K).

The yttrium-modified nanocage that showed the best result for N_2O detection was subjected to interaction with other gases considered interferents (H_2, CH_4 and CO) to investigate its selectivity for N_2O adsorption in comparison with these gases. The selectivity was evaluated by calculating the sensor response (S) and the selectivity coefficient (κ) using the following equations 5 and 6 [15]:

REMUNOM
ISSN 2178-6925

Received: 13/03/2026 - **Accepted:** 10/05/2026
Vol: 13.09
DOI: 10.66104/zrwxm372
Pages: 1-17

$$S = \frac{|R_{gas} - R_{pure}|}{R_{pure}} = \frac{\left|\frac{1}{\sigma_{gas}} - \frac{1}{\sigma_{pure}}\right|}{\frac{1}{\sigma_{pure}}} = \frac{|\sigma_{pure} - \sigma_{gas}|}{\sigma_{gas}}, \quad (5)$$

$$\kappa_{N2O-int} = \frac{S_{N2O}}{S_{int}}, \quad (6)$$

where σ_{gas} represents the conductivity of the gas adsorbed on the surface of the nanocage, σ_{pure} is the conductance of the isolated nanocage (equation 5). In equation 6, S_{N2O} and S_{int} indicate sensitivity to N_2O gas and to interferents gases, respectively, and $\kappa_{N2O-int}$ represents the sensitivity ratio to N_2O against an interfering gas.

3. Results and Discussion

The optimized structures of $B_{12}N_{12}$ and Y-modified nanocages are shown in Fig. 1 a), and their electronic properties are presented in Table 1. The interaction of N_2O gas is presented in Fig. 1 b). The results show that for $B_{12}N_{12}$ nanocages, the B-N bond lengths of 1.485 and 1.437 Å are in agreement with previous studies [16, 17].

As seen in Fig. 1 a), the modification with Y atom causes a local deformation in the nanocages and this may be due to their large atomic radius. After the optimization of the geometry of the modified cages, it is observed that there was an increase in the bond length; in the case of the encapsulated structure, the metal projected to the center of the nanocage. Fig. 1 b) shows that N_2O presents a nonlinear geometry when interacting with Y in the decorated nanocages, binding through the N atom and not through O as occurs in other analyzed systems.

REMUNOM
ISSN 2178-6925

Received: 13/03/2026 - **Accepted:** 10/05/2026
Vol: 13.09
DOI: 10.66104/zrwxm372
Pages: 1-17

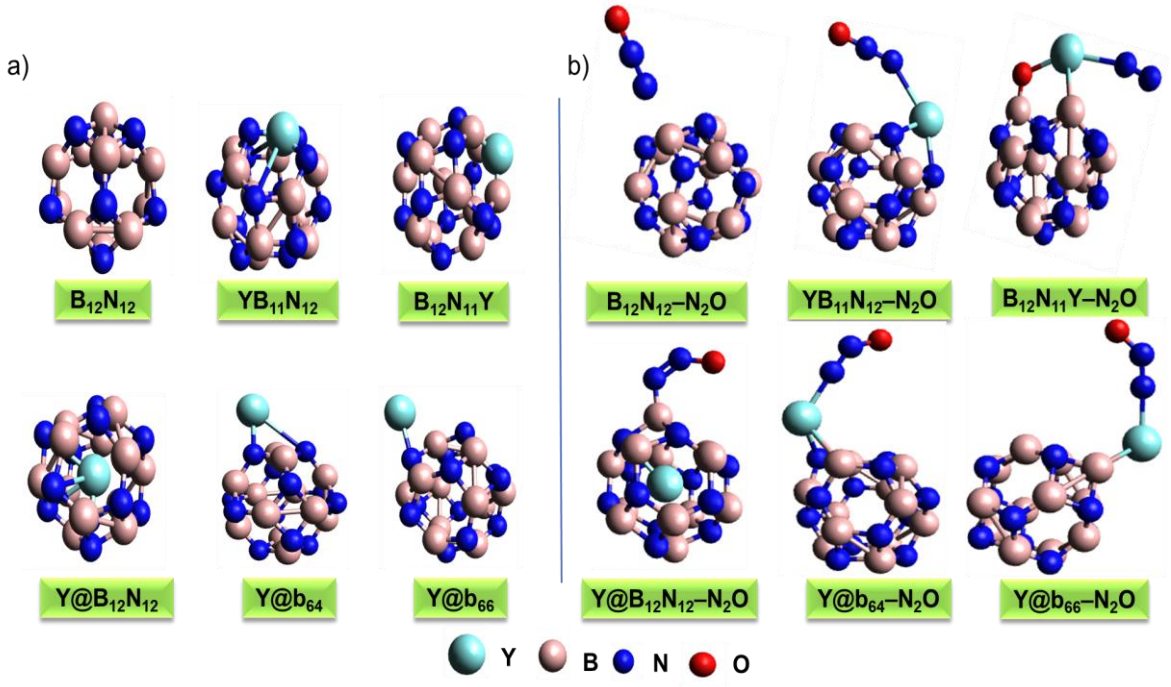


Figure 1. Optimized structures of pristine and Y-modified $B_{12}N_{12}$ nanocages (a), and adsorption configurations of the N_2O molecule on isolated and Y-modified $B_{12}N_{12}$ nanocages (b).

Table 1 shows the cohesion energy (E_{coh},), dipole moment (DM) and charge transfer (Q) for the pure and Y-modified $B_{12}N_{12}$ structures. The $B_{12}N_{12}$ nanocage showed a dipole moment equal to zero [18]. The highest dipole moment value was for $B_{11}N_{12}Y$ DM = 10.18 Debye, while the lowest was for $Y@B_{12}N_{12}$ DM = 1.63 Debye, indicating a lower charge partition in the encapsulated cage (-0.37 |e|). The largest charge shift from Y to the cage is seen in the $Y@b_{64}$ system (+0.45 |e|), where the metal replaces a B atom in $B_{12}N_{12}$. The E_{coh} analysis provides information about the affinity of the nanocage with the metal, exploring in detail the stability of the cage/metal systems. The results show that the lower E_{coh} values (less negative) for the modified nanocages prove that all structures are less stable than pure $B_{12}N_{12}$ [12]. In addition, $YB_{11}N_{12}$ stands out as the most unstable among the studied nanocages, with E_{coh} = -6.81 eV.

The parameters of the isolated and modified systems for N_2O gas adsorption: HOMO energy (E_H / eV), LUMO energy (E_L / eV), HOMO-LUMO gap (E_{gap} / eV), sensitivity (ΔE_{gap} / %) are shown in Table 2. It is noted that the energies

REMUNOM
ISSN 2178-6925

Received: 13/03/2026 - **Accepted:** 10/05/2026
Vol: 13.09
DOI: 10.66104/zrwxm372
Pages: 1-17

of the HOMO and LUMO orbitals of $B_{12}N_{12}$ underwent changes after the interaction with N_2O, this change directly reflected in the variation of E_{gap}.

Table 1 - Calculated cohesive energy (E_{coh}), dipole moment (DM), and yttrium atomic charges (Q) for the isolated systems.

System	E_{coh} / eV	DM / Debye	Q / |e|
$B_{12}N_{12}$	- 6.82	0.00	-
$YB_{11}N_{12}$	- 6.81	10.18	+0.63
$B_{12}N_{11}Y$	- 6.49	9.71	+0.05
$Y@b_{64}$	- 6.64	6.93	+0.45
$Y@b_{66}$	- 6.63	7.21	+0.33
$Y@B_{12}N_{12}$	- 6.27	1.63	-0.37

The bandgap of $B_{12}N_{12}$ decreased from 5.93 eV to 5.18 eV after adsorption, indicating weak interaction with N_2O gas. The sensitivity of a system is determined by the change in the bandgap before and after gas adsorption (see Equation 2) [19, 20]. In this context, modifying the nanocage with yttrium increases its sensitivity to the gas [21]. For the pure $B_{12}N_{12}$ system, the sensitivity to N_2O adsorption was (ΔE_{gap} = 12.54 %). These data are confirmed by the low adsorption energy obtained for the system (E_{ads} = -0.16 eV), characterizing a physisorption (E_{ads} > -0.3 eV) [22] with Van der Waals-type interaction. Among the metal-modified cages, $B_{12}N_{11}Y$ showed the lowest sensitivity (ΔE_{gap} = 7.42%) with adsorption energy (E_{ads} = -0.55 eV). In the case of the $Y@b_{66}$ (α - spin up) system, the energy was (E_{ads} = -1.07 eV), a value considered moderate for a chemisorption process.

REMUNOM
ISSN 2178-6925

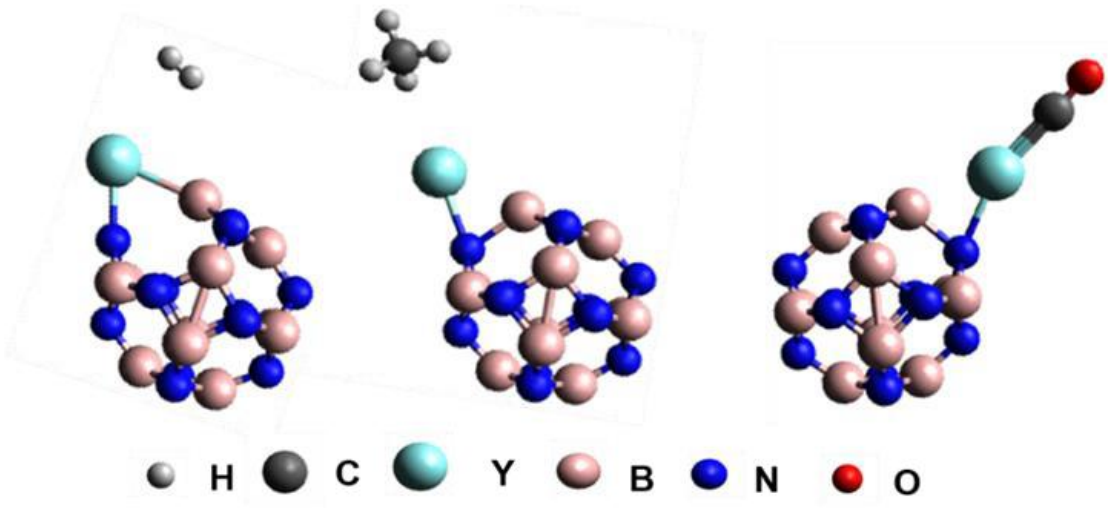
Received: 13/03/2026 - **Accepted:** 10/05/2026
Vol: 13.09
DOI: 10.66104/zrwxm372
Pages: 1-17

Table 2 – Calculated parameters for the isolated nanocages and their interaction with N_2O, including HOMO energy (E_H), LUMO energy (E_L), energy gap (E_{gap}), electronic sensitivity (ΔE_{gap}), and adsorption energy (E_{ads}).

System	S	Isolated			With N_2O adsorbed				
		E_H (eV)	E_L (eV)	E_{gap} (eV)	E_H (eV)	E_L (eV)	E_{gap} (eV)	ΔE_{gap} (%)	E_{ads} (eV)
$B_{12}N_{12}$		-7.77	-1.84	5.93	-7.61	-2.43	5.18	12.54	-0.16
$YB_{11}N_{12}$	α	-6.71	-2.78	3.93	-6.60	-3.33	3.27	16.87	-0.46
$B_{12}N_{11}Y$	α	-5.48	-2.79	2.69	-5.65	-3.16	2.49	7.42	-0.55
$Y@b_{64}$	α	-4.53	-2.19	2.34	-5.99	-2.91	3.08	31.44	-0.63
	β	-5.70	-2.63	3.07	-5.99	-3.35	2.64	14.12	
$Y@b_{66}$	α	-4.57	-2.20	2.37	-6.16	-2.87	3.29	38.70	-1.07
	β	-5.33	-2.72	2.61	-6.47	-3.32	3.15	20.53	
$Y@B_{12}N_{12}$	α	-4.88	-2.89	1.99	-4.87	-3.33	1.54	22.21	-0.49
	β	-5.00	-2.85	2.15	-5.19	-3.34	1.85	14.19	

α – spin up – (alpha); β – spin down – (beta)

Furthermore, it showed good sensitivity (ΔE_{gap} = 38.70%) with satisfactory recovery time at a temperature of 298 K (τ = 120.54 s), making it suitable as a material for application as a sensor. To assess the selectivity of the $Y@b_{66}$ nanocage for N_2O gas detection, the adsorption of other gases, including H_2, CH_4, and CO, was examined using the same calculation methods. The optimized structures are presented in Fig. 2.



REMUNOM
ISSN 2178-6925

Received: 13/03/2026 - **Accepted:** 10/05/2026
Vol: 13.09
DOI: 10.66104/zrwxm372
Pages: 1-17

Figure 2. Optimized adsorption configurations of interfering gases (H_2, CH_4, and CO) on the Y@b_{66} nanocage.

Table 3 presents the results for HOMO-LUMO (E_{gap}), distance (d), adsorption energy (E_{ads}) and sensitivity (ΔE_{gap}) for the adsorption of H_2, CH_4 and CO gases (considered interfering gases) on the surface of the Y@b_{66} nanocage. The selection of interfering gases (H_2, CH_4, and CO) was based on their practical relevance and frequent presence in environments where N_2O detection may occur. These gases commonly coexist with N_2O in industrial, environmental, and atmospheric contexts and may interfere with its detection. Additionally, their distinct physicochemical properties, such as polarity, molecular size, and reactivity, allow for a broader evaluation of the sensor's selectivity under realistic conditions.

The FMO data show that the nanocage is more sensitive to nitrous oxide compared to the other gases studied (ΔE_{gap} = 38.70%), indicating that N_2O is preferentially detected by the Y@b_{66} system. Regarding the adsorption distances of the interfering gases on the nanocage, it is noted that CH_4 has the largest interaction distance (d = 3.44 Å), while the smallest was observed for N_2O gas (d = 2.16 Å). The adsorption energies indicate that H_2, CH_4 and CO gases undergo physical adsorption on the surface of the Y@b_{66} cage [23]. For nitrous oxide gas adsorption, the resulting adsorption energy (E_{ads} = -1.07 eV) characterizes a chemisorption process. Regarding the recovery time of the interfering gases, the values obtained were high, making them unfavorable for adsorption on the Y@b_{66} surface. In contrast, the recovery time for the interaction between the nanocage and N_2O gas (τ = 120.54 s) is considered satisfactory at room temperature (however, this result should be considered only as a preliminary theoretical estimate, and experimental validation is required to confirm the practical recovery performance of the proposed material). The preference of the Y@b_{66} nanocage for N_2O results from a combination of electronic and structural factors. The yttrium atom creates a highly polarized electrophilic site, favoring interaction with N_2O, which exhibits an asymmetric electronic distribution. Adsorption occurs mainly through σ-donation from N_2O to the metal center, with possible π-back-donation, enhancing charge transfer and characterizing a moderate chemisorption process.

REMUNOM
ISSN 2178-6925

Received: 13/03/2026 - **Accepted:** 10/05/2026
Vol: 13.09
DOI: 10.66104/zrwxm372
Pages: 1-17

To analyze the interaction of Y@b_{66} with N_2O and interfering gases, the sensitivity (S) and selectivity (κ) were calculated using the same methodology as in previous studies.

Table 3 – Values of gap HOMO-LUMO (E_{gap}), cage/gas distance (d), adsorption energy (E_{ads}), electronic sensitivity (ΔE_{gap}), recovery time (τ), and also the sensitivity (S) and selectivity coefficient (κ) calculated for the interaction of H_2, CH_4 and CO gases with the Y@b_{66} cage.

System	E_{gap} (eV)	d (Å)	E_{ads} (eV)	ΔE_{gap} (%)	τ	S	κ
Y@b_{66} – N_2O	3.29	2.16	-1.07	38.70	120.54 s	5.93×10^{7}	____
Y@b_{66} – H_2	2.30	3.01	-0.19	3.04	1.13×10^{12} s	2.90	2.05×10^{7}
Y@b_{66} – CH_4	2.38	3.44	-0.04	0.34	1.24×10^{19} s	0.22	2.69×10^{8}
Y@b_{66} – CO	1.79	2.09	-0.60	24.54	5.15×10^{5} s	7.95×10^{4}	7.46×10^{2}

These parameters assess the system's effectiveness in gas detection and its ability to distinguish a specific gas in the atmosphere. Overall, the results indicate that the Y@b_{66} nanocage exhibits higher sensitivity to N_2O compared to other gases and can effectively differentiate it from interfering gases, showing the highest selectivity coefficient for the N_2O/CH_4 pair. These findings suggest that the Y@b_{66} nanocage holds potential as a sensor with strong sensitivity and selectivity for N_2O detection.

Table 4 presents the performance of different materials for N_2O gas adsorption, based on previously reported studies in the literature [24–27], along with the results obtained for the Y@b_{66} nanocage. It is observed that Y@b_{66} exhibits higher sensitivity toward N_2O (ΔE_{gap} = 38.70%) compared to the other analyzed systems.

The results obtained for the $B_{12}N_{12}$ nanocage indicate an adsorption energy typical of a physisorption process (E_{ads} = -0.22 eV), evidencing a weak interaction between the cage surface and the N_2O molecule, which suggests limited efficiency for sensing applications. In contrast, structural modification with the yttrium metal promotes significant changes in the electronic and reactive properties of the system, favoring a stronger interaction with the gas.

REMUNOM
ISSN 2178-6925

Received: 13/03/2026 - **Accepted:** 10/05/2026
Vol: 13.09
DOI: 10.66104/zrwxm372
Pages: 1-17

In fact, the Y@b_{66} nanocage exhibits a pronounced sensitivity (ΔE_{gap} = 38.70%), along with a more negative adsorption energy (E_{ads} = -1.07 eV), characteristic of a chemisorption process. This behavior indicates the formation of stronger chemical interactions, resulting in greater charge transfer and, consequently, a more significant electronic response of the material.

Table 4 - Comparison of the detection performance between Y@b_{66} and previously reported materials in the literature.

Sensor	Functional	E_{ads} / eV	ΔE_{gap} / (%)	References
$B_{12}N_{12}$	B3LYP	-0.22	34.95	[24]
B_{35}	B3LYP	-0.13	0.20	[25]
$Be_{12}O_{12}$	B3LYP-D3	-0.42	20.99	[26]
$Mg_{12}O_{12}$	B3LYP-D3	-0.53	1.44	[26]
Al-doped graphene	B3LYP	-0.23	15.91	[27]
$Zn_{12}O_{12}$	B3LYP	-0.70	19.80	[28]
B-SnS_2	PBE	-2.20	26.32	[29]
Mo-WSe_2	PBE	-2.85	16.37	[30]
Y@b_{66}	B3LYP-D3	-1.07	38.70	This work

Furthermore, the larger variation in the energy gap suggests superior performance in sensing applications, since small structural changes induced by gas adsorption generate detectable responses. Therefore, it can be concluded that the Y@b_{66} nanocage stands out as a promising material for the development of highly sensitive and selective sensors, with strong potential for the rapid and efficient detection of N_2O gas.

4. Conclusions

REMUNOM
ISSN 2178-6925

Received: 13/03/2026 - **Accepted:** 10/05/2026
Vol: 13.09
DOI: 10.66104/zrwxm372
Pages: 1-17

In summary, Y-modified nanocages exhibited improved theoretical performance compared to pristine $B_{12}N_{12}$ for N_2O adsorption. Among the investigated systems, the Y@b_{66} nanocage presented the most favorable adsorption energy, electronic sensitivity, and selectivity toward N_2O molecules among the analyzed structures. These computational findings suggest that Y@b_{66} may represent a promising theoretical candidate for future studies involving selective N_2O sensing applications. Nevertheless, the present results are based exclusively on theoretical calculations, and further experimental investigations are still required to evaluate synthesis feasibility, long-term stability, environmental effects, and practical sensor performance under real operating conditions before any definitive technological application can be established.

Data Availability Statement

The data that support the findings of this study are available from the corresponding author upon reasonable request.

Conflicts of Interest

The authors declare no conflicts of interest.

Funding

This study was supported by FAPEMA - Foundation for Research and Scientific and Technological Development of Maranhão, project number BD-05177/23.

Acknowledgments

This work has been supported by the following Brazilian research agencies: National Council for Scientific and Technological Development (CNPq), 304205/2018-4, National Council for the Improvement of Higher Education (CAPES), Finance Code 001, Maranhão Research and Scientific and Technological

REMUNOM
ISSN 2178-6925

Received: 13/03/2026 - **Accepted:** 10/05/2026
Vol: 13.09
DOI: 10.66104/zrwxm372
Pages: 1-17

Development Support Foundation (FAPEMA). The first author received fellowships from FAPEMA BD-05177/23.

References

[1] Yoosefian M (2017) Powerful greenhouse gas nitrous oxide adsorption onto intrinsic and Pd doped Single walled carbon nanotube, Appl. Surf. Sci. 392:225–230.

[2] Rad AS (2015) First principles study of Al-doped graphene as nanostructureadsorbent for NO_2 and N_2O: DFT calculations, Appl. Surf. Sci. 357:1217–1224.

[3] Ding S, Gu W (2022) Evaluate the potential utilization of $B_{24}N_{24}$ fullerene in the recognition of COS, H_2S, SO_2, and CS_2 gases (environmental pollution), J. Mol. Liq. 345:117041.

[4] Silva ALP, Sousa NS, Varela JJG (2023) Theoretical studies with $B_{12}N_{12}$ as a toxic gas sensor: a review, J. Nanopart. Research 25:22.

[5] Qadir KW, Mohammadi MD, Ridha NJ, Abdullah HY (2024) Determining the binding mechanism of $B_{12}N_{12}$(Zn) with CH_4, CO, CO_2, H_2O, N_2, NH_3, NO, NO_2, O_2, and SO_2 gases, Microp. Mesop. Mater. 379:113289.

[6] Sousa NS, Nascimento WCL, Silva ALP, Varela JJG (2024) DFT study of TM (Sc-Zn) modified $B_{12}N_{12}$ nanocage as sensor for N_2O gas selective detection. Sens Actuat A 378:115841.

[7] Nascimento WCL, Sousa NS, Silva ALP, Maciel AP (2026) Yttrium-Modified $B_{12}N_{12}$ Nanocages for High-Performance H_2 Sensing: Insights from DFT Calculations on Sensitivity, Selectivity, and Recovery, ACS Omega 11:6421-6433.

REMUNOM
ISSN 2178-6925

Received: 13/03/2026 - **Accepted:** 10/05/2026
Vol: 13.09
DOI: 10.66104/zrwxm372
Pages: 1-17

[8] Esrafili MD, Sadeghi SY (2022) decorated all-boron B_{38} nanocluster for reversible molecular hydrogen storage: A first-principles investigation, Int. J. Hydrog. Energy 47:11611–11621.

[9] Agwamba EC, Mathias GE, Louis H, Ikenyirimba O, Unimuke TO, Ahuekwe et al. Single (2023) metal-doped silicon ($Si_{59}X$; X = Nb, Mo, Y, Zr) nanostructured as nanosensors for N-Nitrosodimethylamine (NDMA) pollutant: Intuition from computational study, Mater. Today Commun. 35:106173.

[10] Neese F (2022) Software update: The ORCA program system–Version 5.0. WIREs, Comput. Mol. Sci. 12:e1606.

[11] Grimme S (2011) Density functional theory with London dispersion corrections. WIREs, Comput. Mol. Sci. 1:211–228.

[12] Silva ALP, Varela JJG (2023) Density Functional Theory Study of Cu-Modified $B_{12}N_{12}$ Nanocage as a Chemical Sensor for Carbon Monoxide Gas, Inorg Chem. 62:1926–1934.

[13] Silva ALP, Varela JJG (2024) $MB_{11}N_{12}$ (M = Fe–Zn) Nanocages for Cyanogen Chloride Detection: A DFT Study. J. Inorg. Organom. Polym. Mat. 34:302–312.

[14] Koettgen J, Zacherle T, Grieshammer S, Martin M (2017) Ab initio calculation of the attempt frequency of oxygen diffusion in pure and samarium doped ceria. Phys. Chem. Chem. Phys. 19:9957-9973.

[15] Cui H, Jia P, Peng X, Li P (2020) Adsorption and sensing of CO and C_2H_2 by S-defected SnS_2 monolayer for DGA in transformer oil: A DFT study. Mater. Chem. Phys. 249:123006.

[16] Rad AS, and Ayub K (2017) O_3 and SO_2 sensing concept on extended surface of $B_{12}N_{12}$ nanocages modified by Nickel decoration: A comprehensive DFT study Solid State Sci. 69:22–30.

[17] Ma S, Li D, Rao X, Xia X, Su Y, Lu Y (2020) Pd-doped h-BN monolayer: a promising gas scavenger for SF_6 insulation devices. Adsorption 26:619-626.

REMUNOM
ISSN 2178-6925

Received: 13/03/2026 - **Accepted:** 10/05/2026
Vol: 13.09
DOI: 10.66104/zrwxm372
Pages: 1-17

[18] Escobedo-Morales A, Tepech-Carrillo L, Bautista-Hernández A, Camacho-García JH, Cortes-Arriagada D, Chigo-Anota, E. (2019) Effect of Chemical Order in the Structural Stability and Physicochemical Properties of $B_{12}N_{12}$ Fullerenes. Sci. Rep. 9:16521.

[19] Baei MT (2013) Si-Doped $B_{12}N_{12}$ Nanocage as an Adsorbent for Dissociation of N_2O to N_2 Molécule. Heteroatom Chem. 24:476-481.

[20] Sousa NS, Silva ALP, Nascimento WCL, Martins J dos Santos, Bezerra CWB (2025). Theoretical Study of Ni-Modified $B_{12}N_{12}$ Nanocages: Insights into CO Capture Potential. Microporous and Mesoporous Materials, 113823.

[21] Nascimento WCL, Sousa NS, Martins J dos S, Maciel AP (2024) Estudo a Nível DFT do $B_{12}N_{12}$ Puro e Modificado com Y para Adsorção do Gás Hidrogênio. Anais do Congresso Brasileiro de Química - CBQ 63º edição.

[22] Hadipour NL, Peyghan AA, Soleymanabadi H (2015) Theoretical Study on the Al-Doped ZnO Nanoclusters for CO Chemical Sensors. J. Phys. Chem. C 119:6398–6404.

[23] Choir AA, Amelia SR, Martoprawiro MA, Kusumawati Y, Ivansyah AL (2024) Insight into the adsorption properties of CO_2 and H_2 gas on the $B_{12}Y_{12}$ (Y - N, P, As, Sb) nanocages from host-guest interaction perspective. Int. J. Hydrog. Energy 53:780–791.

[24] Baei MT, Ghasemi AS, Lemeski ET, Soltani A, Gholami N (2016) BN Nanotube Serving as a Gas Chemical Sensor for N_2O by Parallel Electric Field. J. Clust. Sci. 27:1081–1096.

[25] Hossain MdA, Hossain MdR, Hossain MdK, Khandaker JI, Ahmed F, Ferdous T, Hossain Md A (2020) An ab initio study of the boron nanocluster for application as atmospheric gas (NO, NO_2, N_2O, NH_3) sensor. Chem. Phys. Lett. 754:137701.

[26] Sajid H, Siddique SA, Ahmed E, Arshad M, Gilani MA, Rauf A, Imran M, Mahmood T (2022) DFT outcome for comparative analysis of $Be_{12}O_{12}$, $Mg_{12}O_{12}$ and

REMUNOM
ISSN 2178-6925

Received: 13/03/2026 - **Accepted:** 10/05/2026
Vol: 13.09
DOI: 10.66104/zrwxm372
Pages: 1-17

$Ca_{12}O_{12}$ nanocages toward sensing of N_2O, NO_2, NO, H_2S, HCN and SO_3 gases, Comput. Theor. Chem. 1211:113694.

[27] Rad AS (2015) First principles study of Al-doped graphene as nanostructure adsorbent for NO_2 and N_2O: DFT calculations, Appl. Surf. Sci. 357:1217–1224.

[28] Beheshtian J, Peyghan AA, Bagheri Z (2012) Adsorption and dissociation of Cl_2 molecule on ZnO nanocluster. Appl. Surf. Sci. 258:8171–8176.

[29] Hang A, Dong A, Gui Y (2022) Gas-sensing properties of B/N-modified SnS_2 monolayer to greenhouse gases (NH_3, Cl_2, and C_2H_2). Mat. 15(15):5152–5152.

[30] Cheng S, Chen J, Zeng W, Zhou Q (2023) The adsorption and sensing mechanism of toxic gases HCN, NO_2, NH_3 and Cl_2 on Mo, Ag-modified WSe_2 monolayer: insights from the first-principles computations. Mater. Today Commun. 35:105906.