

Biosensing of CO and NO by Transition Metal Doped BN-based Nanocage: A Computational Study

Fatemeh Mollaamin ^{1,*} , Majid Monajjemi ² 

¹ Department of Biomedical Engineering, Faculty of Engineering and Architecture, Kastamonu University, Kastamonu, Turkey

² Department of Biology, Faculty of Science, Kastamonu University, Kastamonu, Turkey

* Correspondence: fmollaamin@kastamonu.edu.tr;

Received: 30.12.2025; Accepted: 16.05.2026; Published: 30.09.2026

Abstract: Adsorption of toxic gases, CO or NO molecules, using transition metals of Cr, Co, Cu, Zn, which have been implanted on the boron nitride nanocage (B_5N_{10}), has been studied by computational chemistry. Based on NQR analysis, X-doped on B_5N_{10} has shown the lowest fluctuation in electric potential and the highest negative atomic charge including 0.2331 (copper), 0.3112 (cobalt), 0.5883 (chromium), 0.6853 (zinc) coulomb for CO adsorption and 0.2962 (cobalt), 0.3710 (copper), 0.5970 (chromium), 0.7768 (zinc) coulomb for NO adsorption have presented the most tendency for being the electron acceptors. Moreover, the parameters of the NMR method have indicated that the yield of electron acceptance for doping atoms on the X- B_4N_{10} through gas molecules adsorption can be ordered as: Cu > Co >> Cr > Zn for CO adsorption and Co $\approx$ Cr > Cu > Zn for NO adsorption. The Gibbs free energy has shown that the maximum efficiency of Cr, Co, Cu, and Zn atoms doping of B_5N_{10} for gas molecules adsorption depends on the covalent bond between CO or NO molecules and X- B_4N_{10} as a potent sensor for air pollution removal. Therefore, for a given number of carbon or nitrogen donor sites in CO or NO, the stabilities of complexes owing to doping atoms of Cr, Co, Cu, and Zn can be considered as: CO@Cu- B_4N_{10} >> CO@Co- B_4N_{10} > CO@Cr- B_4N_{10} > CO@Zn- B_4N_{10} . Therefore, the TM-doped B_5N_{10} can be used as CO and NO gas sensor manufacturing, and it may be a potential material for nanodevice applications.

Keywords: CO; NO; gas sensor; transition metal; pollution; nanomaterials; B_5N_{10} ; DFT.

© 2026 by the authors. This article is an open-access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (<https://creativecommons.org/licenses/by/4.0/>), which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited. The authors retain copyright of their work, and no permission is required from the authors or the publisher to reuse or distribute this article, as long as proper attribution is given to the original source.

1. Introduction

The privileged attributes of boron nitrides, especially their structural and electronic properties, have made them appropriate for pollutant adsorption and semiconducting applications [1,2]. Boron nitride nanomaterials usually exhibit semiconducting behavior, which is considered a proper alternative to carbon nanotubes. The properties of boron and nitrogen atoms, which are the first neighbors of carbon in the periodic table, make boron nitride an interesting subject of numerous studies [3,4].

In recent years, different investigations on the adsorption of chemical contaminants and the application of various boron nitride nanostructures as adsorbents for water purification have been studied [5,6].

Various physical shapes of boron nitride (BN)-based nano adsorbents such as nanoparticles, fullerenes, nanotubes, nanofibers, nanoribbons, nanosheets, nanomeshes,

nanoflowers, and hollow spheres have been broadly considered possible adsorbents owing to their exceptional characteristics such as large surface area, structural variability, great chemical/mechanical strength, abundant structural defects, high reactive sites, and functional groups [7].

The interactions between carbon monoxide gas and boron nitride nanocage were investigated using two DFT functionals (B3LYP and B97D), and 6-31G(d) basis set. The computational results indicated the capability of B₁₂N₁₂ as a sensor for potential applications in the detection of CO under an external electric field [8].

Ammar et al. have studied the effect of transition metals of magnesium and iron doping the boron nitride nano-cage (B₁₂N₁₂) for the adsorption of CO, NO, and NH₃ gases through the electrical and optical properties using DFT-D3 and TD-DFT calculations at B3lyp/6-311+g(d) level of theory. They found that binding energy, ionization potential, electron affinity, chemical hardness, and softness are estimated to emphasize the stability of the doped MnB₁₁N₁₂ and FeB₁₁N₁₂ [9].

Particularly, this research work aims to assess the influences of doping atoms of Cr, Co, Cu, Zn on B₅N₁₀ for increasing gas detection through measurement of some parameters containing charge transfer, electric potential, electromagnetic and thermodynamic properties, surface area, functional group, and to examine the removal of selected toxic gas molecules of carbon monoxide during the adsorption process. These discoveries are supposed to open new nanosensors in applications for selective sensing of carbon monoxide and nitric monoxide in future detection implementations.

2. Materials and Methods

2.1. CO and NO molecules adsorption on X–B₄N₁₀.

This research article aims to remove toxic gas molecules, including CO or NO, from air through an eco-friendly approach by using (Cr, Co, Cu, Zn)-doped B₅N₁₀. Boron nitride nanocage has been designed by doping atoms of chromium, cobalt, copper, and zinc, which can increase the gas-sensing potential of the BN nanocage. The status of CO or NO adsorption on the X–B₄N₁₀ surface, towards the formation of complexes containing CO/NO @Cr–B₄N₁₀, CO/NO @Co–B₄N₁₀, CO/NO @Cu–B₄N₁₀, and CO/NO @Zn–B₄N₁₀ by computational chemistry has been declared. The charge distribution of the mentioned complexes is calculated using Bader charge analysis [10]. The trapping of CO molecules by X–B₄N₁₀ (X = Cr, Co, Cu, Zn) was successfully incorporated due to binding formation consisting of C/N→Cr, C/N→Co, C/N→Cu, C/N→Zn.

2.2. Density functional theory background.

Considering the electronic density within the KS image directs us to a remarkable reduction in quantum computing. Thus, the KS methodology lightens the route for pursuing systems that cannot be discussed by conventional ab initio methodologies. Kohn and Sham" introduces the solution which brings up the mono-electronic orbitals to account for the kinetic energy in a simple and relatively exact way, by finding a residual modification that might be computed apart. So, one starts with a reference model of M with non-interacting electrons related to the external potential v_s and with Hamiltonian [11–13]:

$$\hat{H}_s = -\sum_i^M \frac{1}{2} \bar{V}_i^2 + \sum_i^M v_s(\vec{r}_i) = \sum_i^M \hat{h}_s; \quad \hat{h}_s = -\frac{1}{2} \bar{V}_i^2 + v_s(\vec{r}_i) \quad (1)$$

By representing the single-particle orbitals ψ_i all electronic densities physically acceptable for the system of "non-interacting" electrons are written in equation (2):

$$\rho(\vec{r}) = \sum_i^M |\psi_i(\vec{r})|^2 \quad (2)$$

Finally, the total energy could be measured by the KS method due to equation (3):

$$E[\rho] = \sum_i^M n_i \langle \psi_i | -\frac{1}{2} \nabla^2 + v_{ext}(\vec{r}) + \frac{1}{2} \int \frac{\rho(\vec{r}')}{|\vec{r}-\vec{r}'|} d\vec{r}' | \psi_i \rangle + E_{xc}[\rho] + \frac{1}{2} \sum_{\alpha}^N \sum_{\beta}^N \frac{Z_{\alpha} Z_{\beta}}{|\vec{R}_{\alpha} - \vec{R}_{\beta}|} \quad (3)$$

In this article, the rigid PES using DFT calculations has been computed using Gaussian 16 revision C.01 software [14]. The input Z-matrix for adsorption of CO molecules in air by X-B₄N₁₀ has been designed with GaussView 6.1 [15] using 6-311+G (d,p), EPR-3, and LANL2DZ basis sets with multiplicity of +1 and convergence on RMS density matrix=1.00D-08 and convergence on MAX density matrix=1.00D-06. In this study, the interaction between gas molecules and X-B₄N₁₀ was modeled and analyzed. As revealed by DFT-based analysis, the potency of X-B₄N₁₀ for grabbing CO molecules was determined mainly by the electronegativity of the functional groups, as well as the interaction between X-B₄N₁₀ and the CO molecules.

3. Results and Discussion

One of the most dominant gas pollutants in the air is carbon monoxide. The results have estimated the yield of boron nitride nanocages doped with Cr, Co, Cu, and Zn for gas detection. In fact, it can be remarked that the chemisorptive nature of the bond between the gas molecules and the boron and nitrogen elements is attributed to the equilibrium distribution of doping atoms, B₅N₁₀, and a monolayer attribute.

3.1. PDOS and electronic evaluation.

The electronic structure of CO adsorption using X (X= Cr, Co, Cu, Zn)-doped B₅N₁₀ has been illustrated using CAM-B3LYP-D3/6-311+G (d,p), LANL2DZ level of theory.

Figure 1 (a-h) shows the projected density of states (PDOS) of CO/NO @ X - B₄N₁₀ through gas-molecule adsorption. The existence of the energy states (*p*-orbital) of C, N, O, and (*d*-orbital) of Cr, Co, Cu, Zn within the gap of X - B₄N₁₀ induces the reactivity of the system. It is clear from the figure that after trapping with gas molecules, there is a significant contribution of *d*-orbital in the unoccupied level. Therefore, the curve of partial PDOS describes that the *p* states of N atoms in gas molecules and *d*-orbital in Cr, Co, Cu, Zn transition metals in X-B₄N₁₀ overlap due to the conduction band (Figure 1a-h). A distinguished adsorption trait might be seen in CO/NO @X-B₄N₁₀ because of the potent interaction between the *p* states of the carbon atom in gas molecules and the *d* states of Cr, Co, Cu, Zn in X-B₄N₁₀ complexes.

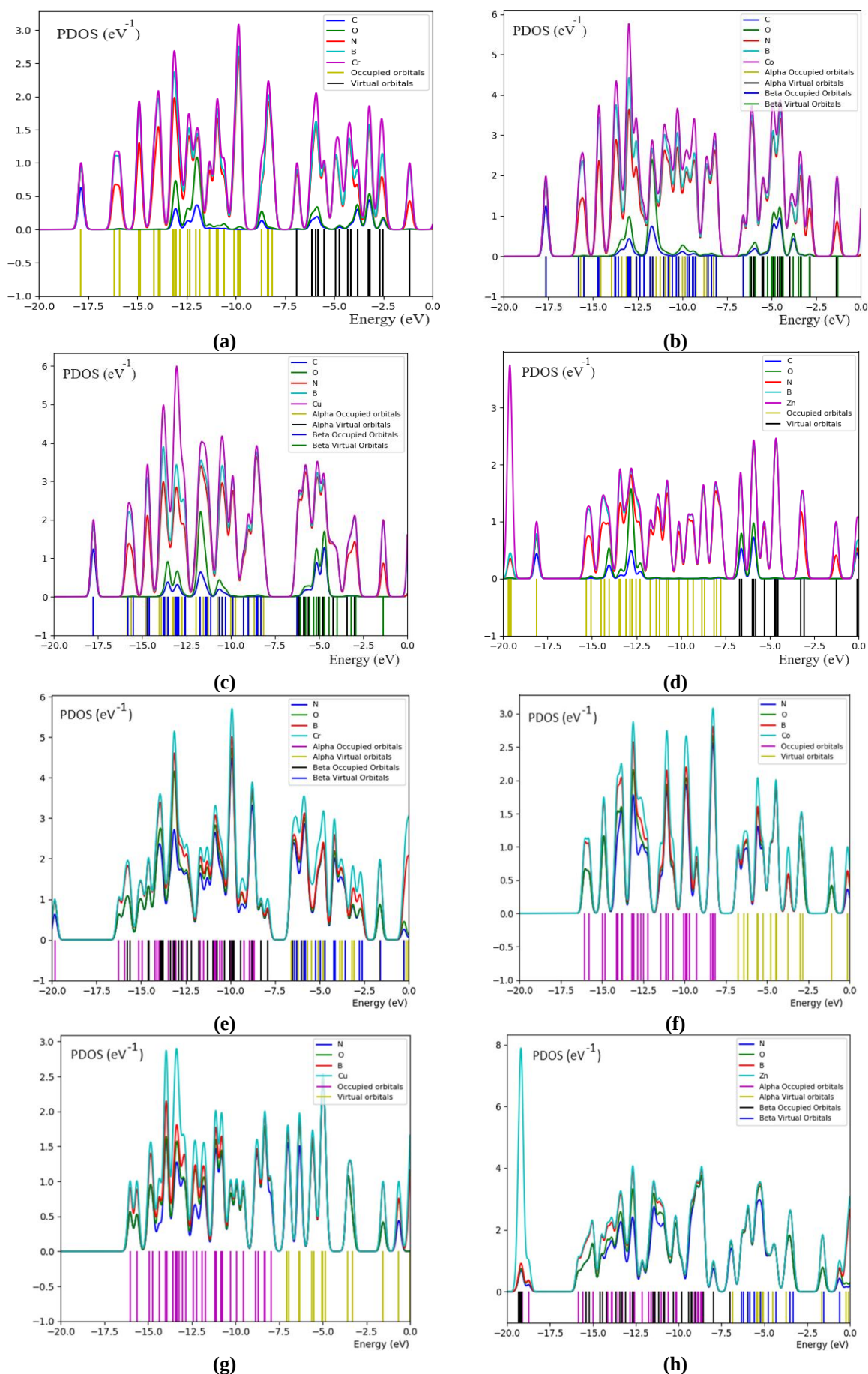


Figure 1. PDOS of gas molecules of CO or NO adsorbed on $X-B_4N_{10}$, including (a) $CO@Cr-B_4N_{10}$; (b) $CO@Co-B_4N_{10}$; (c) $CO@Cu-B_4N_{10}$; (d) $CO@Zn-B_4N_{10}$; (e) $NO@Cr-B_4N_{10}$; (f) $NO@Co-B_4N_{10}$; (g) $NO@Cu-B_4N_{10}$; (h) $NO@Zn-B_4N_{10}$ complexes by CAM-B3LYP-D3/6-311+G (d,p), LANL2DZ.

Figure 1(a–h) shows that $\text{CO@Cr-B}_4\text{N}_{10}$, $\text{CO@Co-B}_4\text{N}_{10}$, $\text{CO@Cu-B}_4\text{N}_{10}$, $\text{CO@Zn-B}_4\text{N}_{10}$, $\text{NO@Cr-B}_4\text{N}_{10}$, $\text{NO@Co-B}_4\text{N}_{10}$, $\text{NO@Cu-B}_4\text{N}_{10}$, and $\text{NO@Zn-B}_4\text{N}_{10}$ complexes through gas molecules adsorption, respectively, have the most contribution at the middle of the conduction band between -5 to -15 eV, while contribution of boron and nitrogen states are enlarged and similar together, and adsorbing of CO or NO depicts interfacial electronic of the B_4N_{10} for selection of this gas. CO @ Cr- B_4N_{10} complex (Figure 1a) has exhibited two sharp peaks around -10 eV for V and Cr atoms, respectively. Furthermore, CO@ Co- B_4N_{10} (Figure 1 b) and Cu@ Cu- B_4N_{10} (Figure 1c) have exhibited a strong peak around -12.5 eV in the graphs for Co and Cu atoms, respectively. However, the Zn graph in CO@ Zn- B_4N_{10} (Figure 1d) with a sharp peak around -20 eV attracts our attention. Therefore, the order of adsorption strength by doping atoms of Cr, Co, Cu, Zn on X- B_4N_{10} based on the PDOS might be shifted as: $\text{Zn-B}_4\text{N}_{10} > \text{Cu-B}_4\text{N}_{10} \sim \text{Co-B}_4\text{N}_{10} > \text{Cr-B}_4\text{N}_{10}$.

Moreover, the NO@ Cr- B_4N_{10} complex (Figure 1e) exhibited two sharp peaks around -10 and -14.5 eV for Cr atoms, respectively. NO@ Co- B_4N_{10} (Figure 1f) exhibited four strong peaks around -8 , -10 , -11.5 , and -14.5 eV in the graphs for the Co atom. Furthermore, the Cu graph shows two sharp, closely spaced peaks around -14 and -14.5 eV in NO@ Cu- B_4N_{10} (Figure 1g). However, the Zn graph in NO@ Zn- B_4N_{10} (Figure 1h), with a sharp peak around -19.5 eV, attracts our attention. Therefore, the order of potency of gas adsorption by doping atoms of Cr, Co, Cu, Zn on X- B_4N_{10} based on the PDOS might be shifted as: $\text{Cu-B}_4\text{N}_{10} > \text{Co-B}_4\text{N}_{10} > \text{Cr-B}_4\text{N}_{10} > \text{Zn-B}_4\text{N}_{10}$.

3.2. Insight into nuclear quadrupole resonance.

As the electric field gradient (EFG) at the citation of the nucleus in CO or NO is allocated by the valence electrons twisted in the attachment with close nuclei of X- B_4N_{10} (X=Cr, Co, Cu, Zn) through trapping of gas molecules (Figure 2), the nuclear quadrupole resonance (NQR) frequency at which transitions occur is particular for CO/NO @X- B_4N_{10} complexes (Table1).

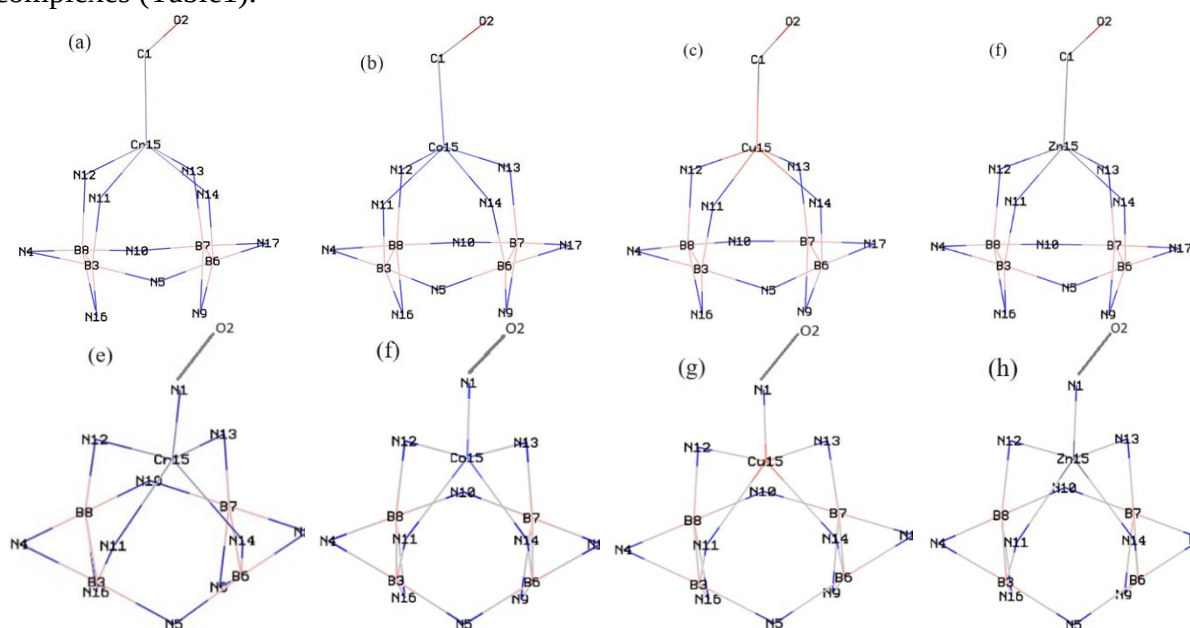


Figure 2. Optimized structures of CO adsorbed on the surface of X- B_4N_{10} (X= Cr, Co, Cu, Zn) towards formation of (a) $\text{CO@Cr-B}_4\text{N}_{10}$; (b) $\text{CO@Co-B}_4\text{N}_{10}$; (c) $\text{CO@Cu-B}_4\text{N}_{10}$; (d) $\text{CO@Zn-B}_4\text{N}_{10}$; (e) $\text{NO@Cr-B}_4\text{N}_{10}$; (f) $\text{NO@Co-B}_4\text{N}_{10}$; (g) $\text{NO@Cu-B}_4\text{N}_{10}$; (h) $\text{NO@Zn-B}_4\text{N}_{10}$ complexes.

The NQR method is related to the multipole expansion in Cartesian coordinates as in equation (4) [16,17]:

$$V(r) = V(0) + \left[\left(\frac{\partial V}{\partial x_i} \right) \Big|_0 \cdot x_i \right] + \frac{1}{2} \left[\left(\frac{\partial^2 V}{\partial x_i \partial x_j} \right) \Big|_0 \cdot x_i x_j \right] + \quad (4)$$

After that, a simplification of equation (4), there are only the second derivatives related to the identical variable for the potential energy [16,17]:

$$U = -\frac{1}{2} \int_{\mathcal{D}} d^3 r \rho_r \left[\left(\frac{\partial^2 V}{\partial x_i^2} \right) \Big|_0 \cdot x_i^2 \right] = -\frac{1}{2} \int_{\mathcal{D}} d^3 r \rho_r \left[\left(\frac{\partial E_i}{\partial x_i} \right) \Big|_0 \cdot x_i^2 \right] = -\frac{1}{2} \left(\frac{\partial E_i}{\partial x_i} \right) \Big|_0 \cdot \int_{\mathcal{D}} d^3 r [\rho(r) \cdot x_i^2] \quad (5)$$

There are two parameters that must be obtained from NQR experiments: the quadrupole coupling constant, χ , and the asymmetry parameter of the EFG tensor, η :

$$\chi = \frac{e^2 Q q_{zz}}{h} \quad (6)$$

$$\eta = \frac{q_{xx} - q_{yy}}{q_{zz}} \quad (7)$$

where q_{ii} are the components of the EFG tensor at the quadrupole nucleus, determined in the EFG principal axes system, Q is the nuclear quadrupole moment, e is the proton charge, and h is Planck's constant [18,19].

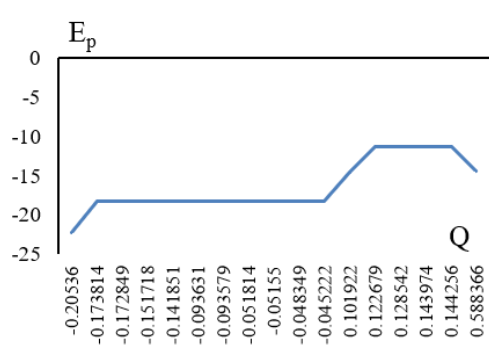
In this research work, the electric potential, defined as the work energy required to carry the electric charge from one position to another position in the presence of the electric field, has been evaluated for CO/NO @Cr-B₄N₁₀, CO/NO @Co-B₄N₁₀, CO/NO @Cu-B₄N₁₀, and CO/NO @Zn-B₄N₁₀ complexes (Table 1).

Table 1. The electric potential (E_p /a.u.) and Bader charge (Q /coulomb) through NQR calculations for CO/NO@Cr-B₄N₁₀, CO/NO@Co-B₄N₁₀, CO/NO@Cu-B₄N₁₀, and CO/NO@Zn-B₄N₁₀ complexes using CAM-B3LYP-D3/EPR-3, LANL2DZ calculations.

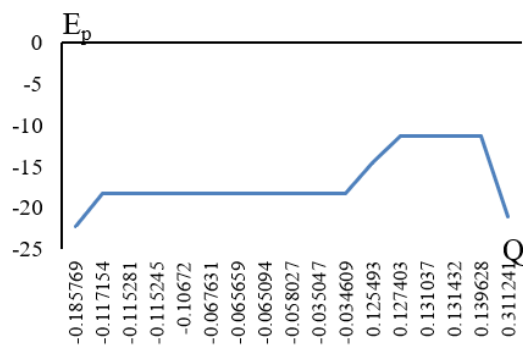
CO@Cr-B ₄ N ₁₀			CO@Co-B ₄ N ₁₀			CO@Cu-B ₄ N ₁₀			CO@Zn-B ₄ N ₁₀		
Atom	Q	E _p	Atom	Q	E _p	Atom	Q	E _p	Atom	Q	E _p
C1	0.1019	-14.5703	C1	0.1255	-14.5643	C1	0.1820	-14.5522	C1	0.2162	-14.5178
O2	-0.2053	-22.2094	O2	-0.1857	-22.2102	O2	-0.1756	-22.2044	O2	-0.1318	-22.1584
B3	0.1285	-11.271	B3	0.1396	-11.2851	B3	0.1277	-11.2865	B3	0.0982	-11.2942
N4	-0.0515	-18.2755	N4	-0.0346	-18.2779	N4	-0.0300	-18.2904	N4	-0.0316	-18.2923
N5	-0.0936	-18.2746	N5	-0.0651	-18.2712	N5	-0.0630	-18.266	N5	-0.0690	-18.2603
B6	0.1442	-11.2733	B6	0.1314	-11.2867	B6	0.1262	-11.284	B6	0.1036	-11.2942
B7	0.1227	-11.2688	B7	0.1274	-11.2867	B7	0.1261	-11.2843	B7	0.0992	-11.2939
B8	0.1439	-11.2743	B8	0.1310	-11.284	B8	0.1203	-11.2865	B8	0.1032	-11.294
N9	-0.0452	-18.2605	N9	-0.0676	-18.2828	N9	-0.0670	-18.2879	N9	-0.0513	-18.2827
N10	-0.0936	-18.2754	N10	-0.0656	-18.2731	N10	-0.0635	-18.2662	N10	-0.0679	-18.2598
N11	-0.1418	-18.2607	N11	-0.1153	-18.275	N11	-0.1046	-18.2728	N11	-0.2191	-18.2894
N12	-0.1738	-18.2605	N12	-0.1171	-18.2739	N12	-0.1140	-18.272	N12	-0.2207	-18.2896
N13	-0.1517	-18.2623	N13	-0.1067	-18.2718	N13	-0.0960	-18.2696	N13	-0.2109	-18.2884
N14	-0.1728	-18.2598	N14	-0.1152	-18.2705	N14	-0.1140	-18.2688	N14	-0.2225	-18.2899
Cr15	0.5883	-14.3983	Co15	0.3112	-21.031	Cu15	0.2331	-26.0904	Zn15	0.6853	-16.151
N16	-0.0518	-18.2647	N16	-0.0580	-18.2849	N16	-0.0597	-18.2861	N16	-0.0504	-18.2829
N17	-0.0483	-18.2739	N17	-0.0350	-18.2876	N17	-0.0280	-18.288	N17	-0.0304	-18.292
NO@Cr-B ₄ N ₁₀			NO@Co-B ₄ N ₁₀			NO@Cu-B ₄ N ₁₀			NO@Zn-B ₄ N ₁₀		

Atom	Q	E _p	Atom	Q	E _p	Atom	Q	E _p	Atom	Q	E _p
N1	-0.1006	-18.2437	N1	0.0813	-18.1696	N1	0.0377	-18.1784	N1	-0.0503	-18.2247
O2	-0.0957	-22.2099	O2	-0.1111	-22.1930	O2	-0.0847	-22.1827	O2	-0.0987	-22.1976
B3	0.1151	-11.2746	B3	0.1511	-11.2799	B3	0.1439	-11.2831	B3	0.1150	-11.2782
N4	-0.0326	-18.2739	N4	-0.0547	-18.2763	N4	-0.0320	-18.2747	N4	-0.0185	-18.2727
N5	-0.0825	-18.2753	N5	-0.0626	-18.2520	N5	-0.0657	-18.2511	N5	-0.0436	-18.2528
B6	0.1111	-11.2739	B6	0.1449	-11.2800	B6	0.1362	-11.2829	B6	0.1141	-11.2787
B7	0.1199	-11.2748	B7	0.1460	-11.2798	B7	0.1301	-11.2822	B7	0.1127	-11.2786
B8	0.1163	-11.2758	B8	0.1462	-11.2809	B8	0.1247	-11.2809	B8	0.1128	-11.2786
N9	-0.0326	-18.2658	N9	-0.0739	-18.2786	N9	-0.0631	-18.273	N9	-0.0645	-18.2693
N10	-0.0994	-18.2819	N10	-0.0678	-18.2558	N10	-0.0536	-18.2432	N10	-0.0414	-18.25
N11	-0.1406	-18.2638	N11	-0.1124	-18.2576	N11	-0.1440	-18.2666	N11	-0.2080	-18.2814
N12	-0.1407	-18.2624	N12	-0.125	-18.2642	N12	-0.1344	-18.2611	N12	-0.2116	-18.2823
N13	-0.1347	-18.2608	N13	-0.1081	-18.257	N13	-0.1352	-18.2648	N13	-0.2026	-18.2819
N14	-0.1442	-18.2639	N14	-0.1174	-18.2619	N14	-0.1410	-18.2634	N14	-0.2102	-18.2826
Cr15	0.5970	-14.3934	Co15	0.2962	-21.0329	Cu15	0.3710	-26.0693	Zn15	0.7768	-16.175
N16	-0.0291	-18.2635	N16	-0.0817	-18.2785	N16	-0.0604	-18.273	N16	-0.0642	-18.2689
N17	-0.0265	-18.2683	N17	-0.0510	-18.2718	N17	-0.0294	-18.2757	N17	-0.0174	-18.2724

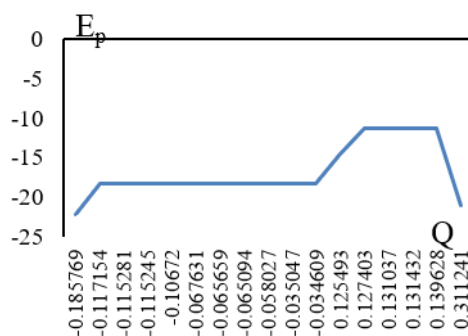
In Table 1, the Bader charge and electronic potential properties of Cr, Co, Cu, Zn, and B, N in X–B₄N₁₀ and C, O of CO molecules trapped on doped-boron nitride nanocages have been investigated. The amounts indicate that as the negative charge of different atoms, the electric potential resulting from NQR calculations increases. Moreover, the doping atoms of Cr(15), Co(15), Cu(15), Zn(15) on B₅N₁₀ have shown the most potential for accepting the electron from the electron donor of C(1) and O (2) in CO adsorbed on the X–B₄N₁₀ (Table 1).



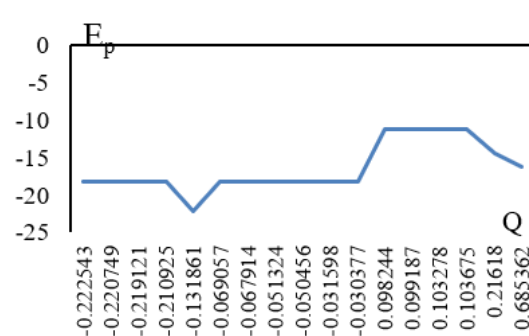
(a)



(b)



(c)



(d)

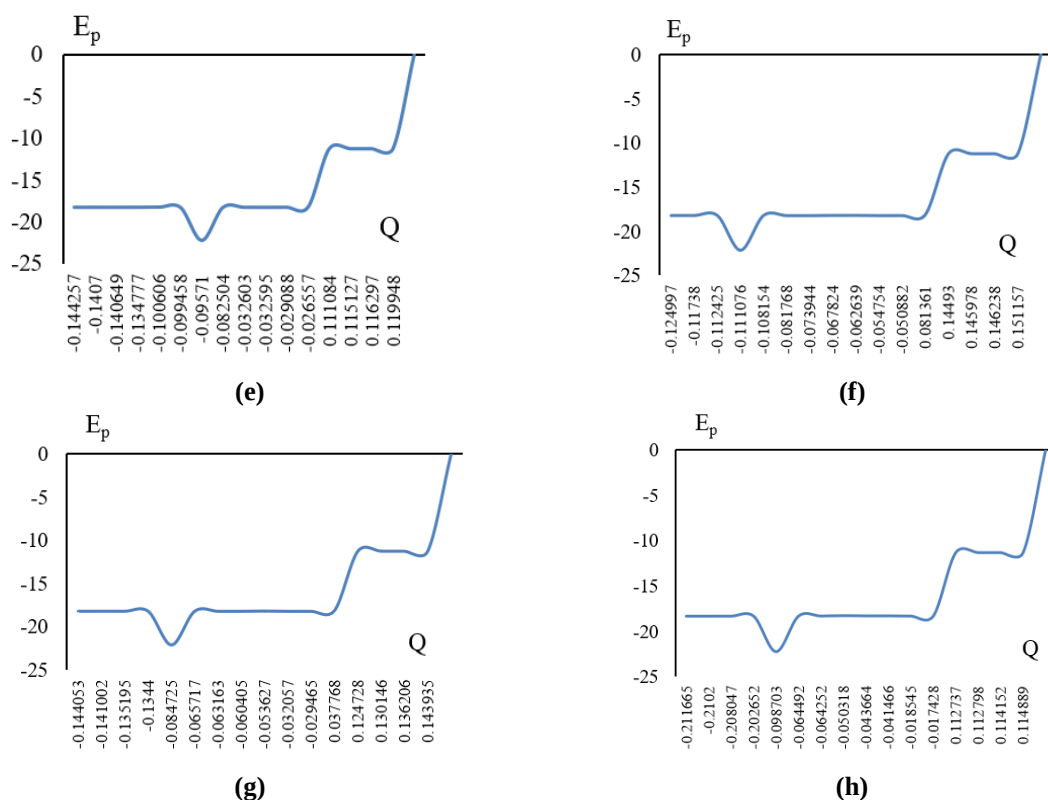


Figure 3. Electric potential (a.u.) versus Bader charge (coulomb) through NQR calculation for **(a)** CO @ Cr-B₄N₁₀; **(b)** CO @ Co-B₄N₁₀; **(c)** CO @ Cu-B₄N₁₀; **(d)** CO @ Zn-B₄N₁₀; **(e)** NO @ Cr-B₄N₁₀; **(f)** NO @ Co-B₄N₁₀; **(g)** NO @ Cu-B₄N₁₀; **(h)** NO @ Zn-B₄N₁₀ complexes by CAM-B3LYP-D3/EPR-3, LANL2DZ.

In addition, the Bader charge and electronic potential properties of Cr, Co, Cu, Zn, and B, N in X-B₄N₁₀ and N, O of NO molecules trapped on doped-boron nitride nanocages have been investigated. The amounts indicate that, as the negative charge of different atoms increases, the electric potential resulting from NQR calculations increases. Moreover, the doping atoms of Cr(15), Co(15), Cu(15), Zn(15) on the B₅N₁₀ have shown the most potential for accepting the electron from the electron donor of N(1) and O(2) in NO adsorbed on the X-B₄N₁₀ (Table 1).

Furthermore, in Figure 3 (a–h), it has been sketched the electric potential of nuclear quadrupole resonance for some atoms of Cr, Co, Cu, Zn / B, N in X-B₄N₁₀ and C, N, O of gas molecules (CO and NO) trapped on doped-boron nitride nanocages has been sketched, which has been calculated by CAM-B3LYP-D3/EPR-3, LANL2DZ. Adsorption of CO on the Cr-B₄N₁₀, Co-B₄N₁₀, and Cu-B₄N₁₀ in Figure 3 (a), (b), and (c), respectively, has illustrated the highest sensing of $R^2 = 0.9666$ and $R^2 = 0.9679$ (both Co-B₄N₁₀ and Cu-B₄N₁₀). However, Figure 3 (d) shows that CO @ Zn-B₄N₁₀ has a lower potential than other nanocage surfaces for CO removal from air ($R^2 = 0.687$). Adsorption of NO on the Cr-B₄N₁₀ and Co-B₄N₁₀ in Figure 3 (e) and (f), respectively, has illustrated the highest sensing of $R^2 = 0.9332$ and $R^2 = 0.9218$. In addition, Figures 3 (g) and (h) show that NO @ Cu-B₄N₁₀, and NO @ Zn-B₄N₁₀, respectively, have a good detection of NO removal from air with correlation coefficients of $R^2 = 0.9477$ and $R^2 = 0.9533$.

It is evident that the curve of X-B₄N₁₀ is affected by CO or NO molecules. The fluctuating peaks for electric potential have been observed around CO or NO trapping on the X-B₄N₁₀, which demonstrate the electron-accepting properties of carbon, nitrogen, and oxygen versus the chromium, cobalt, copper, and zinc doped on the B₄N₁₀ (Figure 3a–h). Besides, it can be considered that transition metals, such as ferromagnetic semiconductors in the

functionalized B₅N₁₀, might have more impressive sensitivity for accepting the electrons from CO or NO by Cr, Co, Cu, Zn in the process of the adsorption mechanism.

Table 1 shows that Cu-doped B₅N₁₀ and Co-doped B₅N₁₀ have high fluctuations between Bader charge versus electric potential extracted from NQR parameters and negative atomic charge, including 0.2331 and 0.3112 coulomb in Cu @Co–B₄N₁₀ and CO @Co–B₄N₁₀, respectively, which can be appropriate options with the highest tendency for electron acceptance in the adsorption current (Table 1). In addition, the adsorbents of chromium with 0.5883 and zinc with 0.6853 coulomb, respectively, have presented the greatest tendency to be electron acceptors. In fact, the uptake of gas molecules has been known to be associated with X–B₄N₁₀, indicating that the adsorbed CO molecules in the X–doped nanocage can be internalized through a different pathway from the pristine nanocage. Cobalt-doped B₅N₁₀ has the lowest fluctuation between Bader charge and electric potential extracted from NQR parameters and the highest negative atomic charge, including 0.2962 coulomb in NO@Co–B₄N₁₀, which can be an appropriate option with the highest tendency for electron acceptance in the adsorption current (Table 1). In addition, the adsorbents of copper with 0.3710 coulomb, chromium with 0.5970 coulomb, and zinc with 0.7768 coulomb, respectively, have presented the greatest tendency for being the electron acceptors during NO adsorption. In fact, the uptake of gas molecules has been known to be associated with X–B₄N₁₀, indicating that the adsorbed NO molecules in the X–doped nanocage can be internalized through a different pathway from the pristine nanocage.

3.3. Nuclear magnetic resonance.

NMR spectra of X–B₄N₁₀ (X= Cr, Co, Cu, Zn) as a potent sensor for adsorbing toxic gas molecules of CO or NO can unravel the efficiency of X–B₄N₁₀ for detecting and removing these hazardous gases in air as an eco-friendly approach.

From the DFT calculations, it has been attained the chemical shielding (CS) tensors in the principal axes system have been obtained to estimate the isotropic chemical shielding (CSI) and anisotropic chemical shielding (CSA) [20,21]:

$$\sigma_{iso} = (\sigma_{11} + \sigma_{22} + \sigma_{33})/3 \quad (8)$$

$$\sigma_{aniso} = \sigma_{33} - (\sigma_{22} + \sigma_{11})/2 \quad (9)$$

The NMR data of isotropic (σ_{iso}) and anisotropic shielding tensors (σ_{aniso}) of gas molecules trapped in the X–B₄N₁₀ towards formation of CO/NO@Cr–B₄N₁₀, CO/NO @Co–B₄N₁₀, CO/NO@Cu–B₄N₁₀, and CO/NO@Zn–B₄N₁₀ complexes have been computed by the Gaussian 16 revision C.01 program package [14] and are shown in Table 2.

Table 2. Data of NMR shielding tensors for selected atoms of CO/NO @Cr–B₄N₁₀, CO/NO @Co–B₄N₁₀, CO/NO @Cu–B₄N₁₀, and CO/NO@Zn–B₄N₁₀ complexes using CAM–B3LYP–D3/6–311+G (d,p), LANL2DZ calculation.

CO@Cr–B ₄ N ₁₀			CO@Co–B ₄ N ₁₀			CO@Cu–B ₄ N ₁₀			CO@Zn–B ₄ N ₁₀		
Atom	σ_{iso}	σ_{aniso}	Atom	σ_{iso}	σ_{aniso}	Atom	σ_{iso}	σ_{aniso}	Atom	σ_{iso}	σ_{aniso}
C1	292.1782	694.1805	C1	236.7354	564.5258	C1	203.5355	617.4635	C1	257.7474	592.4371
O2	633.1859	3188.7465	O2	734.6573	1565.6378	O2	726.2906	1300.8011	O2	843.7191	1329.2058
B3	39.2967	99.6046	B3	68.9199	67.7533	B3	72.2837	77.4514	B3	97.6044	107.2476
N4	1870.0279	2661.9993	N4	364.1386	807.7547	N4	595.1884	1409.1634	N4	2231.2755	5778.7287
N5	131.5764	2171.5379	N5	328.3577	1013.4882	N5	545.3801	617.9658	N5	476.9844	9155.3197
B6	52.5392	46.2836	B6	57.9880	75.7327	B6	63.8370	79.6242	B6	87.7693	106.0778

CO@Cr-B ₄ N ₁₀			CO@Co-B ₄ N ₁₀			CO@Cu-B ₄ N ₁₀			CO@Zn-B ₄ N ₁₀		
Atom	σ_{iso}	σ_{aniso}	Atom	σ_{iso}	σ_{aniso}	Atom	σ_{iso}	σ_{aniso}	Atom	σ_{iso}	σ_{aniso}
B7	38.0691	111.9754	B7	58.2838	70.2613	B7	63.7860	78.3922	B7	92.6279	113.0517
B8	54.2128	45.9159	B8	70.0946	74.7531	B8	72.6591	78.0618	B8	89.0662	96.9983
N9	378.9198	1752.4055	N9	344.3997	658.6215	N9	338.7207	254.9285	N9	2048.7010	8332.6107
N10	928.6784	2162.4106	N10	384.4197	935.6162	N10	540.1666	624.4985	N10	379.2790	8951.7586
N11	813.3494	2124.0132	N11	911.7619	703.4108	N11	454.4266	357.8068	N11	785.1710	1756.5284
N12	70.9784	2292.9194	N12	792.8207	735.7745	N12	473.0107	371.9460	N12	513.8596	1121.0887
N13	1115.8864	2122.6552	N13	781.2989	680.5794	N13	523.3912	680.3183	N13	1255.5158	1825.1782
N14	147.3939	1954.1015	N14	736.7560	539.9430	N14	532.5175	679.2489	N14	791.7575	1017.0261
Cr15	12676.2274	4962.3842	Co15	12319.7965	4125.6887	Cu15	2243.5444	806.4926	Zn15	335.1748	1057.4872
N16	14.0527	1720.0787	N16	391.9645	522.6333	N16	246.6325	550.8873	N16	2106.9316	8278.3243
N17	1283.8952	4581.8198	N17	359.8620	1190.9198	N17	428.7270	601.6366	N17	2872.1260	5426.2698
NO@Cr-B ₄ N ₁₀			NO@Co-B ₄ N ₁₀			NO@Cu-B ₄ N ₁₀			NO@Zn-B ₄ N ₁₀		
Atom	σ_{iso}	σ_{aniso}	Atom	σ_{iso}	σ_{aniso}	Atom	σ_{iso}	σ_{aniso}	Atom	σ_{iso}	σ_{aniso}
N1	657.46	449.15	N1	6235.13	21991.86	N1	63293.00	94223.48	N1	1551.16	1716.94
O2	638.05	829.81	O2	13191.61	46595.00	O2	88823.60	132087.84	O2	1866.55	1659.43
B3	73.15	59.20	B3	315.80	857.56	B3	31.0022	237.228	B3	59.21	86.06
N4	864.67	935.73	N4	11531.79	25317.62	N4	3081.29	26445.87	N4	867.69	1132.70
N5	663.8211	1162.01	N5	18262.38	59345.21	N5	2474.98	20423.95	N5	80.45	310.76
B6	73.63	64.90	B6	371.00	784.1426	B6	39.79	210.98	B6	59.63	89.72
B7	70.66	58.23	B7	322.72	820.1116	B7	66.86	321.73	B7	58.66	84.79
B8	67.77	55.83	B8	351.29	762.9027	B8	1.84	182.22	B8	58.32	90.12
N9	194.59	867.75	N9	2775.17	43699.70	N9	1189.16	18670.09	N9	270.49	738.94
N10	637.10	1350.34	N10	16350.09	52405.72	N10	2089.78	23940.52	N10	113.63	385.12
N11	739.01	891.46	N11	2593.17	5918.10	N11	1208.41	5659.78	N11	913.16	606.23
N12	648.83	703.63	N12	3290.23	6195.62	N12	4479.93	27757.65	N12	967.93	781.41
N13	686.99	715.76	N13	653.93	6410.61	N13	2635.56	6052.16	N13	871.75	595.94
N14	708.80	622.45	N14	1621.05	5288.46	N14	6411.38	25786.03	N14	916.85	656.01
Cr15	7806.68	2373.72	Co15	49289.45	84963.85	Cu15	16157.16	44143.15	Zn15	5.2	431.41
N16	309.99	704.31	N16	6136.67	43276.78	N16	3203.10	17623.09	N16	273.41	716.23
N17	1013.79	1526.37	N17	14002.19	27833.11	N17	8941.76	21869.78	N17	877.54	1156.93

NMR data have reported notable amounts of CO or NO adsorbed on the X-B₄N₁₀ (Table 2). The increase in the chemical shift anisotropies spans for C (1), O (2) atoms of CO and N (1), O (2) atoms of NO adsorption on the X-B₄N₁₀. It is notable that doping of Cr, Co, Cu, and Zn on B₄N₁₀ might promote the strength of the nanocage. In fact, the adsorption of CO can present spin polarization on the X-B₄N₁₀, which indicates that these nano-surfaces may be employed as a magnetic scavenging surface as a gas detector. The parameters of isotropic and anisotropic shielding change with the occupancy of electrons, resulting in trapped gas molecules in the atom-doped boron nitride nanocage.

Table 2 indicates the similar orientation of shielding for boron and nitrogen; however, a remarkable deviation is observed for doping atoms of Cr (15), Co (15), Cu (15), Zn(15) through interaction with C (1), O (2) of CO and N (1), O (2) of NO during adsorption on the B₅N₁₀. Table 2 shows the gap chemical shielding between chromium, cobalt, copper, and zinc doping of X-B₄N₁₀ nanocage and CO/NO gas molecules. The yield of electron acceptors for doping atoms on the X-B₄N₁₀ through gas molecules adsorption can be ordered as: Cu> Co >>Cr > Zn for CO adsorption and Co≈Cr > Cu >Zn for NO adsorption, which supports the possibility of a covalent bond between chromium, cobalt, copper, zinc, and carbon monoxide for removing it from the air.

Therefore, the authors believe that the extracted results would be useful in the design of X-B₄N₁₀ complexes based on doped nanomaterials for increasing the adsorption of CO/NO

gas molecules, in addition to the structural studies using solid-state and solution NMR techniques.

3.4. Thermodynamic factors and IR spectroscopy.

The IR calculations have been done for the adsorption of CO or NO molecules by X-B₄N₁₀ during toxic gas sensing in air. Therefore, it has been simulated the several clusters containing CO@ Cr-B₄N₁₀ (Figure 4a), CO@Co-B₄N₁₀ (Figure 4b), CO@Cu-B₄N₁₀ (Figure 4c), CO @Zn-B₄N₁₀ (Figure 4d), NO@ Cr-B₄N₁₀ (Figure 4e), NO@Co-B₄N₁₀ (Figure 4f), NO@Cu-B₄N₁₀ (Figure 4g), and NO @Zn-B₄N₁₀ (Figure 4h) complexes using CAM-B3LYP-D3/6-311+G (d,p), LANL2DZ.

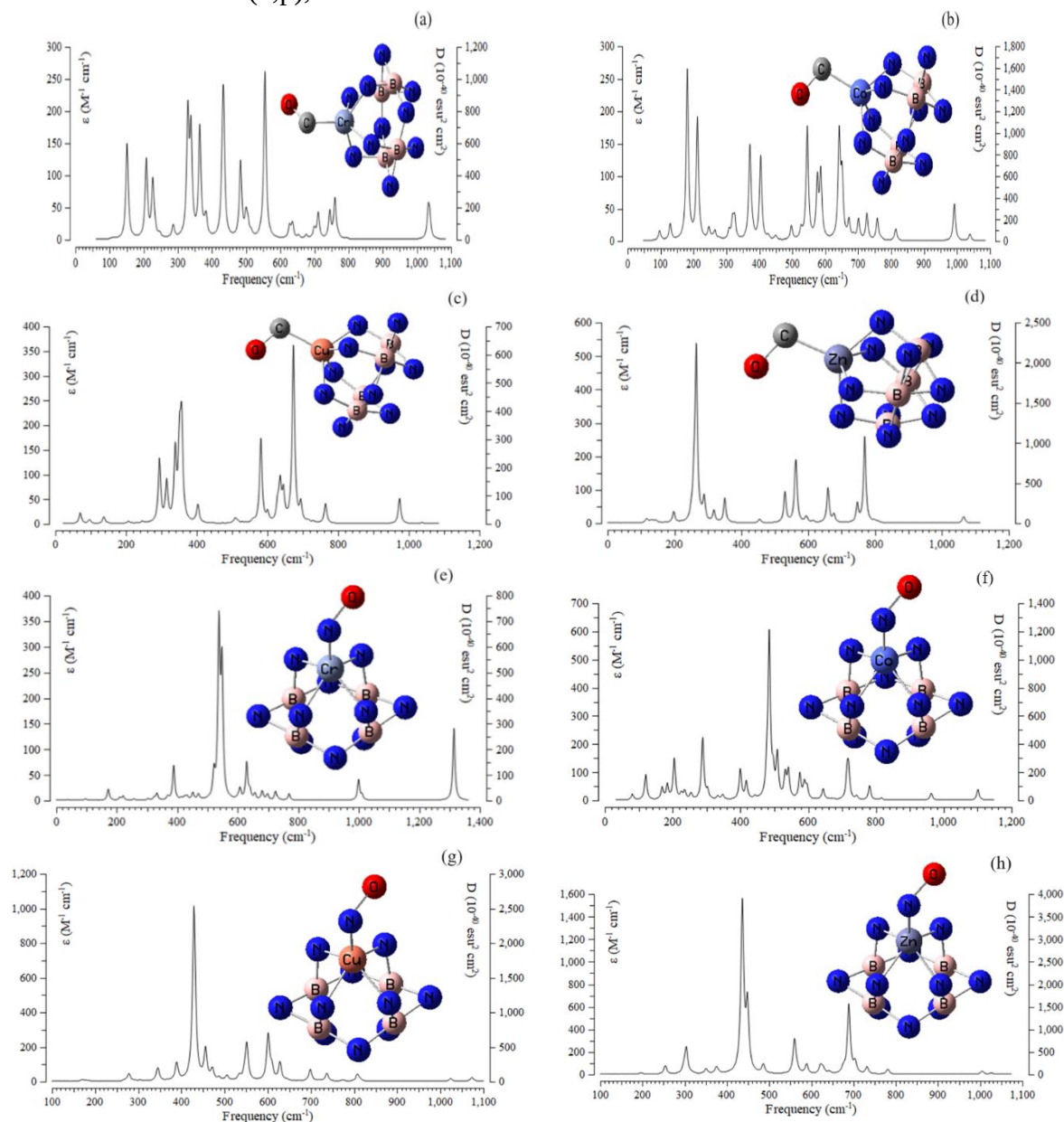


Figure 4. The frequency (cm^{-1}) changes through the IR spectra for (a) CO @ Cr-B₄N₁₀; (b) CO @ Co-B₄N₁₀; (c) CO@ Cu-B₄N₁₀; (d) CO@ Zn-B₄N₁₀; (e) NO @ Cr-B₄N₁₀; (f) NO @ Co-B₄N₁₀; (g) NO@ Cu-B₄N₁₀; (h) NO@ Zn-B₄N₁₀ complexes using CAM-B3LYP-D3/6-311+G (d,p), LANL2DZ.

The graph in Figure 4 (a) indicates the fluctuation of frequency between 100–1100 cm^{-1} for CO@ Cr-B₄N₁₀ with several sharp peaks around 328.93, 433.18, and 554.91 cm^{-1} . Figure 4 (b) shows the fluctuation of frequency between 100–1100 cm^{-1} for CO@ Co-B₄N₁₀ with sharp peaks around 180.91, 211.68, 370.94, 403.62, 545.15, and 642.16 cm^{-1} . Moreover, it has

been observed that the frequency range between 200–1100 for CO@ Cu–B₄N₁₀ shows sharp peaks around 357.09, 581.27, and 673.35 cm⁻¹ (Figure 4c). Besides, Figure 4 (d) exhibits the frequency between 200–1100 for CO@ Zn–B₄N₁₀ with sharp peaks around 264.84, 563.65, and 769.01cm⁻¹. Furthermore, Figure 4 (e) indicates the fluctuation of frequency between 100–1400 cm⁻¹ for NO@ Cr–B₄N₁₀ with several sharp peaks around 537.56, 547.52, and 1314.38 cm⁻¹. Figure 4 (f) shows the fluctuation of frequency between 100–1200 cm⁻¹ for NO@ Co–B₄N₁₀, with two sharp peaks around 485.02 and 508.81cm⁻¹. Moreover, it has been observed that the frequency range between 200–1100 for NO@ Cu–B₄N₁₀, with sharp peaks around 429.12 cm⁻¹ (Figure 4g). Besides, Figure 4 (h) shows the frequency range between 200–1100 for NO@Zn–B₄N₁₀ with two sharp peaks around 448.61 and 688.63 cm⁻¹.

The IR spectra of CO or NO adsorption on the X–B₄N₁₀ have indicated that the formation of the principal complex correlates with the electron potency of doped X (X= Cr, Co, Cu, Zn) on the B₅N₁₀. As has been seen, the doped nanocages of Cr–B₄N₁₀, Co–B₄N₁₀, Cu–B₄N₁₀, and Zn–B₄N₁₀ complexes have the most fluctuations and the highest tendency for adsorption of CO or NO around 450 cm⁻¹.

Thermodynamic specifications indicate that X–B₄N₁₀, due to the adsorption of CO or NO, might be more efficient sensors for detecting and removing the gas molecules from the polluted air (Table 3).

Table 3. The thermodynamic characters of CO/NO @Cr–B₄N₁₀, CO/NO @Co–B₄N₁₀, CO/NO @Cu–B₄N₁₀, and CO/NO @Zn–B₄N₁₀ complexes using CAM–B3LYP–D3/6–311+G (d,p), LANL2DZ calculation.

Compound	$\Delta E^\circ \times 10^{-3}$ (kcal/mol)	$\Delta H^\circ \times 10^{-3}$ (kcal/mol)	$\Delta G^\circ \times 10^{-3}$ (kcal/mol)	S° (cal/K.mol)	Dipole moment (Debye)
CO@Cr–B ₄ N ₁₀	-530.213	-530.213	-530.244	104.267	1.2359
CO@Co–B ₄ N ₁₀	-567.365	-567.365	-567.397	108.482	1.2664
CO@Cu–B ₄ N ₁₀	-599.390	-599.389	-599.422	109.196	1.5135
CO@Zn–B ₄ N ₁₀	-517.415	-517.415	-517.448	113.042	3.3803
NO@Cr–B ₄ N ₁₀	-540.960	-540.959	-540.993	111.987	0.7802
NO@Co–B ₄ N ₁₀	-577.471	-577.471	-577.503	109.405	0.5716
NO@Cu–B ₄ N ₁₀	-609.782	-609.781	-609.813	106.275	0.4199
NO@Zn–B ₄ N ₁₀	-527.877	-527.876	-527.907	103.769	0.5630

Thermodynamic parameters of CO or NO gas molecules adsorption on the X–B₄N₁₀ have been measured by the DFT approach. It has been indicated that for a given number of carbon donor sites in CO, the stabilities of complexes owing to doping atoms of Cr, Co, Cu, Zn can be considered as: CO@Cu–B₄N₁₀>> CO@Co–B₄N₁₀> CO@Cr–B₄N₁₀> CO@Zn–B₄N₁₀> (Table 3). Besides, for a given number of nitrogen donor sites in NO, the stabilities of complexes owing to doping atoms of Cr, Co, Cu, and Zn can be considered as: NO@Cu–B₄N₁₀>>NO@Co–B₄N₁₀>NO@Cr–B₄N₁₀> > NO@Zn–B₄N₁₀ (Table 3).

The thermodynamic information in Figure 5 can explain the high efficiency of Cr, Co, Cu, and Zn atoms doping of B₅N₁₀ for gas molecules adsorption through ΔG_R° which depends on the covalent bond between CO or NO gas molecules and X–B₄N₁₀ as a potent sensor for air pollution removal.

The adsorption process of CO or NO gas molecules on the X–B₄N₁₀ is affirmed by the ΔG_{ads}° quantities:

$$\Delta G_{ads}^\circ = \Delta G_{CO/NO @X-B_4N_{10}}^\circ - (\Delta G_{CO/NO}^\circ + \Delta G_{X-B_4N_{10}}^\circ); X = Cr, Co, Cu, Zn \quad (10)$$

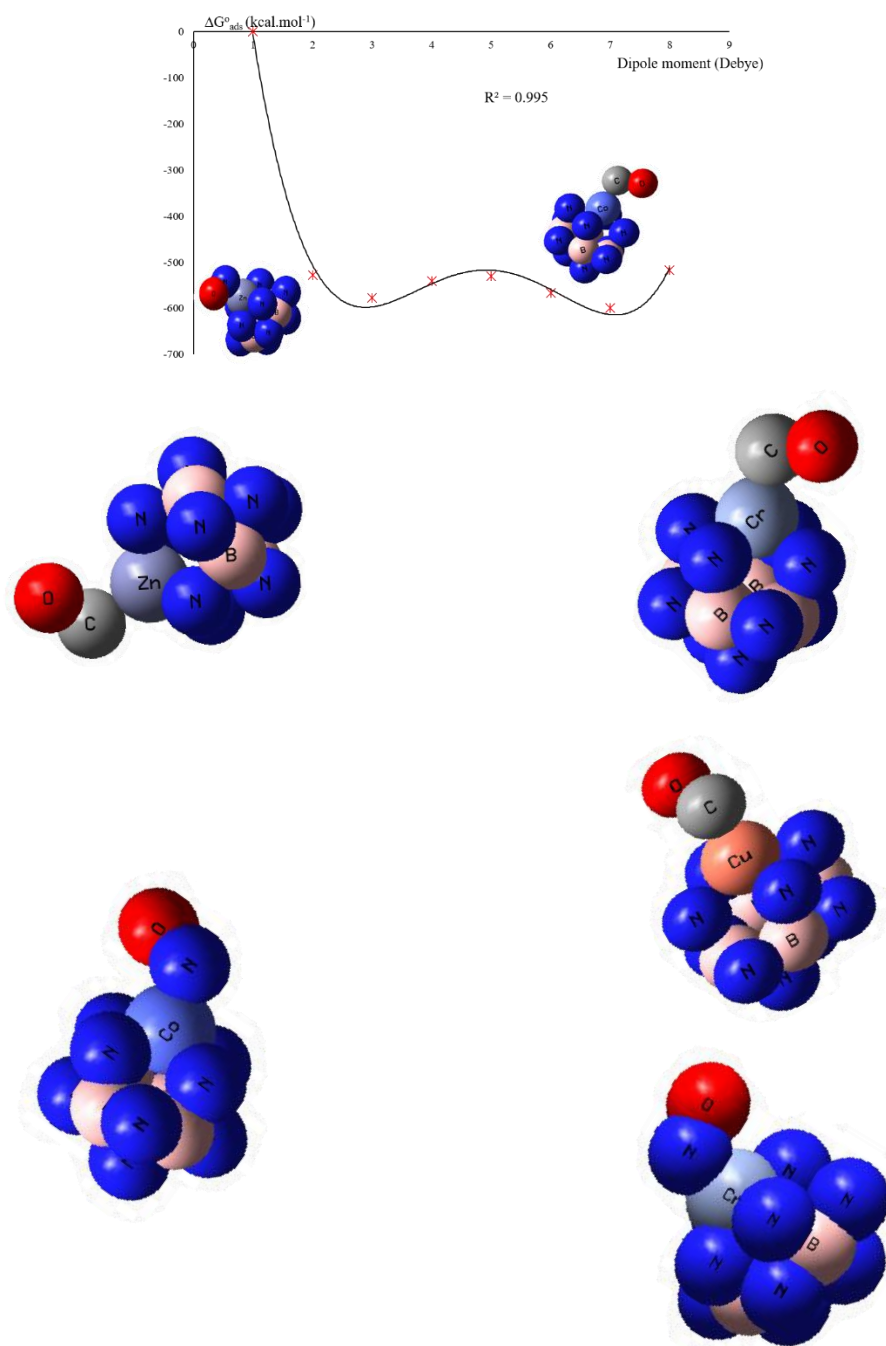


Figure 5. The Gibbs free energy ($\Delta G_{\text{ads}}^{\circ}$) versus dipole moment (Debye) for CO@Cr-B₄N₁₀, CO@Co-B₄N₁₀, CO@Cu-B₄N₁₀, CO@Zn-B₄N₁₀ and NO@Cr-B₄N₁₀, NO@Co-B₄N₁₀, NO@Cu-B₄N₁₀, NO@Zn-B₄N₁₀ complexes using CAM-B3LYP-D3/6-311+G (d,p), LANL2DZ calculation.

Figure 5 shows the key role of doped atoms of Cr, Co, Cu, and Zn during the interaction between the adsorbates of CO or NO gas molecules as electron donors and the adsorbents of Cr-B₄N₁₀, Co-B₄N₁₀, Cu-B₄N₁₀, and Zn-B₄N₁₀ as electron acceptors. Therefore, the selectivity of atom-doping on boron nitride nanocage (gas sensor) for gas molecules adsorption can be summarized as: Cu>>Co>Cr>Zn for CO or NO adsorption (Table 3 and Figure 5).

4. Conclusions

This research has investigated doping of Cr, Co, Cu, and Zn transition metals on the boron nitride nanocage (X-B₄N₁₀) for enhancing toxic gas sensing of these nanomaterials for air pollution removal. Therefore, CO or NO gas molecules separation involving X-B₄N₁₀ has

been experimented with based on electrostatic interactions between the gas molecules and X–B₄N₁₀. The electromagnetic and thermodynamic properties of X–B₄N₁₀ complexes were computed using the DFT method. The data have demonstrated that the chosen gas molecules adsorbed on X–B₄N₁₀ are rather stable, with the most stable adsorption site being in the center of the X–B₄N₁₀ system. The selectivity of atom-doping on boron nitride nanocage (gas sensor) for gas molecules adsorption can be expressed as: CO/NO@Cu–B₄N₁₀>> CO/NO@Co–B₄N₁₀> CO/NO@Cr–B₄N₁₀> CO/NO@Zn–B₄N₁₀>, respectively. This work proposes that transition metals, as ferromagnetic semiconductors, can be examined through doping of nanomaterials to enhance adsorption potency for designing pollution removal sensors.

Author Contributions

Conceptualization, F.M.; methodology, F.M.; software, F.M.; validation, F.M. and M.M.; formal analysis, F.M. and M.M.; investigation, F.M. and M.M.; resources, F.M. and M.M.; data curation, F.M.; writing—original draft preparation, F.M.; writing—review and editing, M.M.; visualization, F.M. and M.M.; supervision, F.M.; project administration, F.M. All authors have read and agreed to the published version of the manuscript.

Institutional Review Board Statement

Not applicable.

Informed Consent Statement

Not applicable.

Data Availability Statement

Not applicable.

Funding

This research received no funding.

Acknowledgments

In successfully completing this paper and its research, the authors are grateful to Kastamonu University.

Conflict of Interest

The authors declare no conflict of interest.

References

1. Alamro, A.; Balbaied, T. Boron Nitride Nanostructures (BNNs) Within Metal–Organic Frameworks (MOFs): Electrochemical Platform for Hydrogen Sensing and Storage. *Analytica* **2024**, *5*, 599–618, <https://doi.org/10.3390/analytica5040040>.
2. Liu, G.; Hao, C. Theoretical Calculations on Hexagonal-Boron-Nitride-(h-BN)-Supported Single-Atom Cu for the Reduction of Nitrate to Ammonia. *Molecules* **2025**, *30*, 4700, <https://doi.org/10.3390/molecules30244700>.

3. Mollaamin, F., Mohammadi, S., Khalaj, Z. *et al.* Computational Modelling of Boron Nitride Nanosheet for Detecting and Trapping of Water Contaminant. *Russ. J. Phys. Chem. B* **2024**, *18*, 67–82, <https://doi.org/10.1134/S1990793124010330>.
4. Huo, X.S.; Jeon, K.-W.; Fang, L.; de Graaf, K.; Espinosa, B.I.; Parker, S.D.T.; Piao, H.; Li, T.; Wang, X. Boron Nitride Supported Copper Single Atom Catalyst for Nitrate Reduction Reaction. *Catal. Today* **2025**, *459*, 115381, <https://doi.org/10.1016/j.cattod.2025.115381>.
5. Zhang, S.; Wang, Y.; Liu, F.; Ding, L.; Wang, S.; Wu, Y.; Li, L.; Sun, X.; Wu, Y. Molecular engineering of 3D porous boron nitride via dual-nitrogen synergy for enhanced tetracycline adsorption. *Ceram. Int.* **2025**, *52*, 7122–7131, <https://doi.org/10.1016/j.ceramint.2025.12.458>.
6. Mollaamin, F. Features of parametric point nuclear magnetic resonance of metals implantation on boron nitride nanotube by density functional theory/electron paramagnetic resonance. *J. Comput. Theor. Nanosci.* **2014**, *11*, 2393–2398, <https://doi.org/10.1166/jctn.2014.3653>.
7. Wadhwa, G.K.; Late, D.J.; Charhate, S.; Sankhyani, S.B. 1D and 2D Boron Nitride Nano Structures: A Critical Analysis for Emerging Applications in the Field of Nanocomposites. *ACS Omega* **2024**, *9*, 26737–26761, <https://doi.org/10.1021/acsomega.3c10217>.
8. Purnomo, M.J.; Febrita, Y.; Dinaryanto, O.; Gierlotka, W.; Yu, I.-S. The Stability Prediction and Epitaxial Growth of Boron Nitride Nanodots on Different Substrates. *Molecules* **2024**, *29*, 1313, <https://doi.org/10.3390/molecules29061313>.
9. Ammar, H.Y.; Badran, H.M.; Eid, Kh.M. TM-doped B₁₂N₁₂ nano-cage (TM = Mn, Fe) as a sensor for CO, NO, and NH₃ gases: A DFT and TD-DFT study. *Mater. Today Commun.* **2020**, *25*, 101681, <https://doi.org/10.1016/j.mtcomm.2020.101681>.
10. Mollaamin, F., Monajjemi, M. In Situ Ti-Embedded SiC as Chemiresistive Nanosensor for Safety Monitoring of CO, CO₂, NO, NO₂: Molecular Modelling by Conceptual Density Functional Theory. *Russ. J. Phys. Chem. B* **2024**, *18*, 49–66, <https://doi.org/10.1134/S1990793124010159>.
11. Kohn, W.; Sham, L.J. Self-Consistent Equations Including Exchange and Correlation Effects. *Phys. Rev.* **1965**, *140*, A1133–A1138, <https://doi.org/10.1103/PhysRev.140.A1133>.
12. Becke, A.D. Density-functional thermochemistry. III. The role of exact exchange. *J. Chem. Phys.* **1993**, *98*, 5648–5652, <https://doi.org/10.1063/1.464913>.
13. Lee, C.; Yang, W.; Parr, R.G. Development of the Colle–Salvetti correlation-energy formula into a functional of the electron density. *Phys Rev B.* **1988**, *37*, 785–789, <https://doi.org/10.1103/PhysRevB.37.785>.
14. Frisch, M.J.; Trucks, G.W.; Schlegel, H.B.; Scuseria, G.E.; Robb, M.A.; Cheeseman, J.R.; Scalmani, G.; Barone, V.; Petersson, G.A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A.V.; Bloino, J.; Janesko, B.G.; Gomperts, R.; Mennucci, B.; Hratchian, H.P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J.L.; Williams-Young, D.; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V.G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery, J.A., Jr.; Peralta, J.E.; Ogliaro, F.; Bearpark, M.J.; Heyd, J.J.; Brothers, E.N.; Kudin, K.N.; Staroverov, V.N.; Keith, T.A.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.P.; Burant, J.C.; Iyengar, S.S.; Tomasi, J.; Cossi, M.; Millam, J.M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J.W.; Martin, R.L.; Morokuma, K.; Farkas, O.; Foresman, J.B.; Fox, D.J. Gaussian 16, Revision C.01, Gaussian, Inc., Wallingford CT, **2016**.
15. Dennington, R.; Keith Todd, A.; Millam John, M. GaussView, Version 6.06.16. Semichem Inc., Shawnee Mission, KS, USA, **2016**.
16. Trontelj, Z.; Pirnat, J.; Jazbinšek, V.; Lužnik, J.; Srčič, S.; Lavrič, Z.; Beguš, S.; Apih, T.; Žagar, V.; Seliger, J. Nuclear Quadrupole Resonance (NQR)—A Useful Spectroscopic Tool in Pharmacy for the Study of Polymorphism. *Crystals* **2020**, *10*, 450, <https://doi.org/10.3390/cryst10060450>.
17. Monea, C.; Bizon, N. Nuclear Quadrupole Resonance Spectroscopy. In Signal Processing and Analysis Techniques for Nuclear Quadrupole Resonance Spectroscopy, Monea, C., Bizon, N., Eds.; Springer International Publishing: Cham, **2022**; pp. 17–31, https://doi.org/10.1007/978-3-030-87861-0_3.
18. Collins, R.L.; Travis, J.C. The Electric Field Gradient Tensor. In Proceedings of the Mössbauer Effect Methodology, Boston, MA, 1967; **1967**; pp. 123–161, https://doi.org/10.1007/978-1-4757-1547-7_7.
19. Shinoda, K.; Kobayashi, Y. An Intensity Tensor and Electric Field Gradient Tensor for Fe³⁺ at M1 Sites of Aegirine–Augite Using Single-Crystal Mössbauer Spectroscopy. *Minerals* **2023**, *13*, 1452, <https://doi.org/10.3390/min13111452>.

20. Gerothanassis, I.P.; Kupka, T. New Insights into Nuclear Magnetic Resonance (NMR) Spectroscopy. *Molecules* **2025**, *30*, 1500, <https://doi.org/10.3390/molecules30071500>.
21. Charisiadis, P.; Venianakis, T.; Papaemmanouil, C.D.; Primikyri, A.; Tzakos, A.G.; Siskos, M.G.; Gerothanassis, I.P. On the use of strong proton donors as a tool for overcoming line broadening in NMR: A comment. *Magn. Reson. Chem.* **2025**, *63*, 170–179, <https://doi.org/10.1002/mrc.5499>.

Publisher's Note & Disclaimer

The statements, opinions, and data presented in this publication are solely those of the individual author(s) and contributor(s) and do not necessarily reflect the views of the publisher and/or the editor(s). The publisher and/or the editor(s) disclaim any responsibility for the accuracy, completeness, or reliability of the content. Neither the publisher nor the editor(s) assume any legal liability for any errors, omissions, or consequences arising from the use of the information presented in this publication. Furthermore, the publisher and/or the editor(s) disclaim any liability for any injury, damage, or loss to persons or property that may result from the use of any ideas, methods, instructions, or products mentioned in the content. Readers are encouraged to independently verify any information before relying on it, and the publisher assumes no responsibility for any consequences arising from the use of materials contained in this publication.