Journal of Science Research and Reviews
PRINT ISSN: 1595-9074
E-ISSN: 1595-8329
DOI: https://doi.org/10.70882/josrar.2026.v3i5.284
Homepage: https://josrar.esrgngr.org
Original Research Article

Adsorption Properties of CO_2 on both Pristine and B-doped Coronene Quantum Dots: A Density Functional Theory Study

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KEYWORDS
Coronene quantum dots (CQDs),
Boron-doped Coronene quantum dots (B-CQDs),
Density functional theory,
CO_2 molecule,
Electronic properties.

ABSTRACT
The study of the interactions between nanomaterials and target molecules at the molecular level is a key factor in the design of new materials for high-performance applications of nanosensors. In this study, the adsorption properties of CO_2 molecules on the surface of pristine Coronene quantum dots (pCQDs) and Boron-doped Coronene (B-CQDs) clusters were estimated using density functional theory (DFT) calculations. The results show that CO_2 molecules are weakly adsorbed (physisorption) on the pristine Coronene surface, while they are strongly chemisorbed on the B-Coronene surface with a large adsorption energy. The recovery time for CO_2 on the pristine Coronene is very short, which makes the practical detection of this molecule almost impossible, regardless of any intrinsic electronic sensitivity. The substitution of a carbon atom in the Coronene framework with a Boron atom greatly enhances the adsorption properties. This change increases the chemical reactivity of the system favoring stronger interactions. The electrical conductivity of the B-Coronene cluster is greatly enhanced after the interaction with the CO_2 molecule, and the energy gap exhibits a drastic change. Therefore, the B-Coronene cluster is a very promising nanosensor candidate for CO_2 detection based on its high electrical sensitivity. Therefore, Boron dopants greatly promote the chemisorption of CO_2 and enhance the overall sensing performance of Coronene. Overall, boron-doped coronene clusters demonstrate significant potential for application in the design and development of highly sensitive and efficient CO_2 gas detection systems.

CITATION
Kzar, M. K. (2026). Adsorption Properties of CO_2 on both Pristine and B-doped Coronene Quantum Dots: A Density Functional Theory Study. *Journal of Science Research and Reviews*, *3*(5), 13-24. https://doi.org/10.70882/josrar.2026.v3i5.284

INTRODUCTION

The isolation of graphene raised great scientific interest due to its extraordinary properties and huge possibilities for industrial applications. Its high carrier mobility, high saturation velocity and long spin diffusion length make it a very promising material for next generation electronics and spintronic devices (Feng et al., 2018; Rabeya et al., 2022). However, the intrinsic zero bandgap of pristine graphene is a major hurdle for its wide technological integration (Feng et al., 2018; Yeh et al., 2018). A very efficient way to overcome this limitation is to take advantage of the finite-size effect: the patterning of the infinite graphene sheet in specific geometric fragments with hydrogen-passivated edges allows to engineer a tunable bandgap (Feng et al., 2018; Abdelati et al., 2021). The resulting planar hydrocarbons are classified based on their structural geometry, size and edge configurations. It is interesting to note that, when the sizes of these nanosized fragments are

less than 30 nm, they are officially named Graphene Quantum Dots (GQDs) (Abdelati et al., 2021; Rabeya et al., 2022). Among the polycyclic aromatic hydrocarbons (PAHs), coronene C_24H_{12}, denoted as Coro, has been the subject of intense scientific interest. Coronene has a well-defined planar structure and strongly delocalized pi-electrons, therefore it naturally forms a stacking structure and is an ideal model to investigate graphene nano-flakes (Martin, 1996; Fedorov, 2017; Yeh et al., 2018). The detailed knowledge of the stacking and electronic structure of Coronene in the neutral and ionic state is central, because they are strongly correlated to the conduction mechanisms of the graphene-based nanostructures (Martin, 1996; Fedorov, 2017; Yeh et al., 2018). Graphene has revolutionized the modern electronics and spintronics due to its exceptional carrier mobility, high saturation velocity and long spin diffusion length (Feng et al., 2018; Rabeya et al., 2022). But the intrinsic zero band gap of graphene limits its extensive industrial application (Feng et al., 2018; Yeh et al., 2018). Such a finite-size effect can be overcome only by cleaving the infinite graphene lattice into geometrically defined structures terminated with hydrogen, such as zero-dimensional Graphene Quantum Dots (GQDs) (Abdelati et al., 2021; Feng et al., 2018). This is a feasible solution to this problem (Abdelati et al., 2021). When the lateral size of these GQDs is reduced to below 10 nm, the quantum confinement effect results in a significant broadening of the band gap and a strong photoluminescence response (Abdelati et al., 2021; Feng et al., 2018; Rabeya et al., 2022).

In addition, chemical functionalization and doping of these structures with heteroatoms, mostly nitrogen (N) and Sulphur (S), enable precise tuning of their optoelectronic properties, which makes them highly attractive for advanced sensing and electrocatalysis (Feng et al., 2018; Feng et al., 2021; Khudhair et al., 2023). Apart from nano-electronics, pi-conjugated carbon materials and PAHs are widely used to design high-performance anode materials for Lithium-Ion Batteries (LIBs) (Nair et al., 2024; Prodhan & Ramasesha, 2025). The high specific surface area, great mechanical flexibility and excellent electrical conductivity of these systems contribute to the growing global need for efficient energy storage devices in portable electronics and electric vehicles (Nair et al., 2024). At the same time, these advanced carbon nanostructures hold great promise for environmental and biomedical monitoring, particularly for the detection of volatile organic compounds (VOCs) (Rabeya et al., 2022; Ajeel et al., 2019). Therefore, a key frontier rests in the design of highly sensitive GQD-based electrochemical and optical sensors, inspired by well-defined systems (e.g. Coronene), for environmental safety and non-invasive medical diagnostics (Ajeel et al., 2019; Rabeya et al., 2022; Zeng et al., 2025). Coronene was chosen as the main substrate for this study, as it offers better structural and electronic properties than other graphene quantum dots such as ovalene (Fedorov, 2017; Yeh et al., 2018). Its larger and well-defined architecture provides a highly predictable and efficient platform for technology applications and makes it a prominent member of the carbon-based nanomaterial family (Fedorov, 2017; Yeh et al., 2018). Coronene's intrinsic electrical conductivity, mechanical strength and chemical stability offer a strong scaffold for interaction with target analyses (Fedorov, 2017). However, the real potential of this structure is achieved by a strategic Boron-doping (B-doping) (Ajeel & Ben Ahmed, 2023; Khamees et al., 2024). The delocalized pi-electrons of Coronene provide a basic adsorption ability, but the substitution of carbon by electron-deficient Boron atoms systematically tunes the surface chemistry and creates localized Lewis's acid sites (Ajeel & Ben Ahmed, 2023; Khamees et al., 2024). Such a synergistic combination of the structural stability of Coronene and the electronic modulation of Boron improves the sensitivity of chemical signal transmission and optimizes the substrate for high-performance pollutant removal and rapid-sensing applications, especially for CO_2 capture (Khamees et al., 2024; Almansour et al., 2026). Based on these structural advantages and theoretical challenges, in the present work, we systematically investigate the effect of boron-doping (B-doping) on the geometric, electronic and adsorption properties of Coronene by using spin-polarized Density Functional Theory (DFT) calculations. When a carbon atom in the highly symmetric polyarene core is replaced by an electron-deficient boron atom, the localized charge density is drastically redistributed (Ajeel & Ben Ahmed, 2023; Khamees et al., 2024). This doping process opens the intrinsic zero band-gap of the carbon matrix and the surrounding region is converted into highly active, localized Lewis's acid sites (p-type semiconductor behavior) (Khamees et al., 2024). Therefore, these boron-induced electron-deficient regimes interact strongly with carbon dioxide by polarizing and binding with the robust quadrupole moment of the CO_2 molecule. The interaction causes a significant increase in the adsorption energy and charge transfer in comparison to pristine Coronene, without any irreversible chemical deformation (Almansour et al., 2026). Overall, this comprehensive molecular study provides essential atomistic insights towards the design of high-performance graphene quantum dots for efficient and selective strategic carbon capture technologies (Feng et al., 2018; Feng et al., 2021; Zeng et al., 2025).

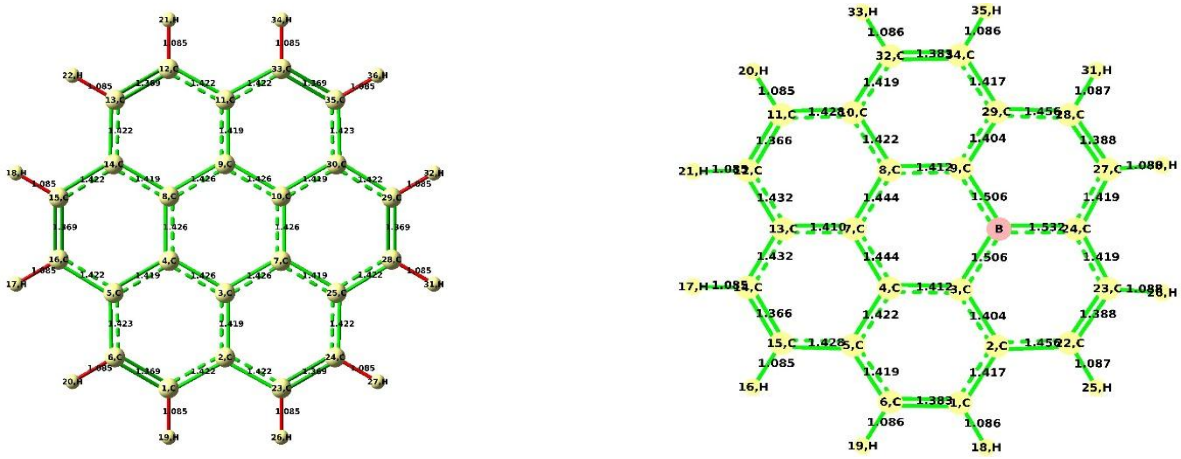


Figure 1: Optimized structure of pristine coronene quantum dot (CQDs) and B-doped CQDs composed of seven benzene rings ($C_{24}H_{12}$) and (B-$C_{23}H_{12}$), showing a hexagonal arrangement with hydrogen passivation at the edges

Coronene quantum dots (CQDs) are important zero-dimensional nanomaterials of graphene structures. The reduced dimensionality of these systems leads to quantum confinement effects, which opens a controllable energy band gap (E_g), making them excellent candidates for carbon-based nanotechnology (Abdelati et al., 2021; Feng et al., 2018). The unique electrical properties and structural stability of these CQDs have attracted significant interest in their application as physical transducers in gas sensors with higher sensitivity and selectivity than conventional diagnostic devices (Feng et al., 2018; Rabeya et al., 2022). Recently, the adsorption of environmental gases, in particular carbon dioxide CO_2 on the carbon-based nanostructures has been widely investigated by both theoretical and experimental approaches (Xiong et al., 2022; Almansour et al., 2026). The modification of electronic properties caused by the adsorption of target molecules on these surfaces is an important research area for the development of nano-scale sensors (Zeng et al., 2025; Almansour et al., 2026). Literature points out that the intrinsic reactivity of coronene structures can be greatly amplified by heteroatom substitution, e.g. doping with Boron, to overcome the limitations of pristine frameworks (Ajeel & Ben Ahmed, 2023; Khamees et al., 2024). Hence, the inclusion of a boron (B) dopant into the coronene lattice is presumed to significantly improve its surface reactivity and selectivity for particular environmental and hazardous gases, such as CO_2 and Formaldehyde (Ajeel & Ben Ahmed, 2023; Khamees et al., 2024). Topological defects or doping by heteroatoms can effectively tune the electronic properties of coronene (Feng et al., 2018; Rabeya et al., 2022; Khamees et al., 2024). Though gas molecules adsorb weakly on pristine coronene due to its very stable, planar conjugated structure, it is important to realise that this structural perfection limits its sensing performance (Fedorov, 2017; Yeh et al., 2018). Pristine coronene is insensitive to molecules like CO_2 and Formaldehyde, so the introduction of a Boron (B) dopant is considered to be highly preferable (Ajeel & Ben Ahmed, 2023; Khamees et al., 2024). Besides modifying the local electronic distribution, the B-doping also induces a slight structural distortion, which produces highly reactive active sites that greatly improve the sensitivity and selectivity of the sensing platform (Ajeel & Ben Ahmed, 2023; Khamees et al., 2024). The main objective of the present study is thus to systematically explore the potential of boron-doped coronene (B-coronene) as a promising sensing platform for the detection of environmental and hazardous gases namely CO2 and Formaldehyde. We carry out a detailed analysis of the structural stability, adsorption energetics, charge transfer mechanisms, and changes in the electronic properties (energy gap and Density of States (DOS)) upon gas adsorption using first-principles Density Functional Theory (DFT) calculations (Almansour et al., 2026; Khamees et al., 2024). The theoretical insight is expected to open up new routes for designing advanced carbon-based nanoscale sensors (Fedorov, 2017; Yeh et al., 2018; Rabeya et al., 2022; Zeng et al., 2025).

MATERIALS AND METHODS

Computational details

All the quantum chemical calculations were carried out with the Gaussian 09 (or 16) software package. The geometry optimizations and the electronic structure calculations were performed in the framework of the Density Functional Theory (DFT) using the hybrid exchange-correlation functional B3LYP and the basis set 6-31G (d, p) or 6-311G (d, p) (Kh & Abbas, 2019; Feng et al., 2018). This level of theory is well established and validated for the study of carbon-based nanostructures providing a good compromise between computational efficiency and accuracy (Feng et al., 2018; Yeh et al., 2018). Full optimization of the molecular structures of pristine coronene quantum dots (pCQDs) $C_{24}H_{12}$, boron doped coronene quantum dots (B-CQDs) and the adsorption

complexes with gas molecules CO_2 was carried out without any symmetry constraints (Symmetry=None). The obtained geometries were verified to be true local minima on the potential energy surface (NIMAG = 0) by performing the vibrational frequency calculations at the same level of theory. The optimized structures and their respective electronic properties were further analysed for the evaluation of the sensing potential of the B-doped coronene. For the purpose of investigating the electronic properties of the systems, we have performed the following calculations: Frontier molecular orbitals (HOMO-LUMO) for determining the energy gap and orbital distributions; Density of states (DOS) to assess the contributions of energy levels to the electronic transitions (Feng et al., 2018; Yeh et al., 2018); Molecular electrostatic potential (MEP) maps to visualize regions of electron richness or deficiency; and Global reactivity descriptors like electronegativity (χ), chemical potential (μ), chemical hardness (η), chemical softness (S) and electrophilicity (ω), all derived from conceptual DFT. The discrete energy levels were broadened to a continuous DOS profile by a Gaussian function with a standard deviation of 0.2 eV, which gives a clearer view of the electronic states distributed near the Fermi level. Moreover, the electronic charge distribution in pristine and B doped coronene has been studied by the Molecular Electrostatic Potential (MEP) analysis. To further investigate the effect of boron doping and gas adsorption on the electron density, partial atomic charges were calculated. The electrostatic potential maps presented here along with the charge transfer analysis provide a visual representation of the interaction mechanisms and charge redistribution that take place upon adsorption of CO_2 and Formaldehyde on the modified coronene surface. The global chemical reactivity indices were calculated with the energies of the frontier molecular orbitals (HOMO and LUMO). The indices are useful for the understanding of electronic properties, chemical stability and reactivity of the pristine and B-doped coronene systems. In addition, the electronic response of the modified surfaces upon gas adsorption was assessed for these parameters, underlining their potential applications in highly sensitive gas sensing devices (Kh & Abbas, 2019; Feng et al., 2018).

$$\mu = -\frac{E_{HOMO}+E_{LUMO}}{2} \quad (1)$$

$$\eta = \frac{E_{LUMO}-E_{HOMO}}{2} \quad (2)$$

$$S = \frac{1}{2\eta} \quad (3)$$

$$\omega = \frac{\mu 2}{2\eta} \quad (4)$$

$$E_g = E_{LUMO} - E_{HOMO} \quad (5)$$

$$E_{FL} = \frac{EHOMO+ELUMO}{2} \quad (6)$$

The calculation of B-codoped CQDs structural stability depends on the cohesive energy per atom (E_{coh}) value obtained through atom energy reduction from system-wide energy per atom:

$$E_{coh} = \frac{(Eatom-Etot)}{n} \quad (7)$$

where E_{tot} is the total energy of the quantum dot and *n* the number of atoms of the structure.

$$E_{ads(PCQDs)} = E_{CO2/PCQDs} - (E_{PCQDs} + E_{CO_2}) \quad (8)$$

$$E_{ads(B-CQDs)} = E_{CO_2/B-CQDs} - (E_{B-CQDs} + E_{CO_2}) \quad (9)$$

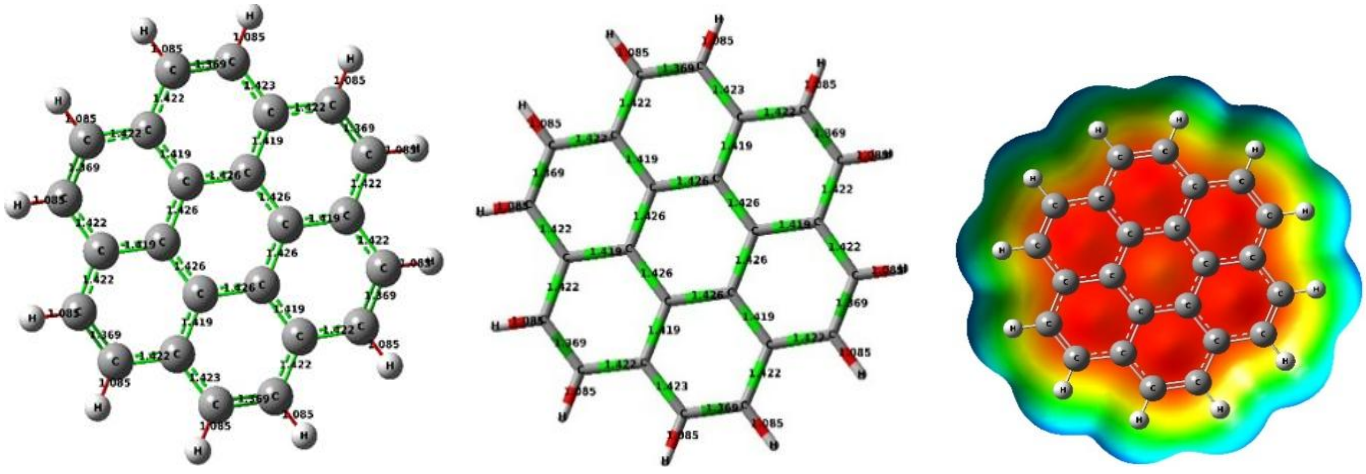
the complexed forms of the pristine and B-doped CQDs (coronene quantum dots) have relaxed energies denoted by $E_{CO2/PCQDs}$ and $E_{ads(B-CQDs)}$, respectively. E_{PCQDs} and E_{B-CQDs} are the total energy of the pristine CQDs and B-doped CQDs; and then E_{CO_2} is equivalent to the energy of an isolated CO_2 molecule. The initial structures were built with Chem-Draw ultra 16.0 and all of the calculations were carried out using the Gaussian 09 W electronic structure software. Gauss Sum program was used to get the DOS results.

RESULTS AND DISCUSSION

As shown in Fig. 1a, the pristine coronene ($C_{24}H_{12}$) exhibits a symmetric seven-benzene ring structure with an average C–C bond length of approximately 1.42 Å, which is consistent with the characteristic values for aromatic carbon systems (Martin, 1996; Fedorov, 2017) .To achieve an in-depth understanding of the alterations in the electronic behaviour of the system, it is imperative to perform an investigation of the electronic density of states (DOS) of the coronene both pre- and post-substitution of a carbon atom with a Boron (B) atom. Boron was chosen as a dopant since it is electron deficient and can serve as a p-type dopant, which is well established to enhance the chemical reactivity and electronic properties of carbon-based nanostructures (Ajeel & Ben Ahmed, 2023; Khamees et al., 2024). Known properties of boron are the introduction of localized electronic states near the Fermi level, improved charge transfer and band gap tuning. It is an effective and widely studied dopant for generating active sites with enhanced adsorption and sensing capabilities towards gas molecules including CO_2 and Formaldehyde, owing to its compatibility with carbon-based frameworks (Ajeel & Ben Ahmed, 2023; Khamees et al., 2024). The structural, electronic, and electrostatic properties of the pristine coronene system are shown in Fig. 1a. The ideal structure of coronene shown in Fig. 1b has a symmetric hexagonal arrangement of carbon atoms with hydrogen atoms at the edges for stability of the structure (Khamees et al., 2024; Martin, 1996; Fedorov, 2017)). The bond lengths in the coronene structure are shown in detail in Fig.1c, showing the uniformity and stability of the sp2-hybridized carbon network with an average C-C bond length of about 1.42 Å (Martin, 1996). The Molecular Electrostatic Potential (MEP) map is presented in Fig.1d, with the red portions indicating the electron rich areas and the blue portions indicating the electron poor areas, and this map exhibits the charge

distribution of the pristine surface (Martin, 1996; Yeh et al., 2018; Khamees et al., 2024).

The present study aims to examine the effect of introducing a single Boron (B) dopant on the electronic characteristics of the coronene system. As shown in Fig. 2, the substitution is performed by replacing a single carbon atom at a specific site within the coronene framework to form the B-doped coronene. The structural stability and the alterations in the electronic properties of the system modified with this Boron atom were thoroughly investigated (Khamees et al., 2024; Ajeel et al., 2024). Fig.2 displays the optimized structure and the corresponding electronic distribution after the doping process. Fig. 2 shows the optimized structures of the four different studied configurations, namely: the pristine coronene, the B-doped coronene, and the adsorption complexes with CO_2, along with their corresponding Density of States (DOS) spectra. The electronic band gaps (E_g) for each configuration were obtained from the energy difference between the HOMO and the LUMO orbitals (Feng et al., 2018; Yeh et al., 2018). The pristine coronene possesses a relatively large band gap of 4.021 eV, which is significantly altered upon the introduction of the Boron dopant to 3.892 eV, and further modified following the gas adsorption processes to -1.632 eV for CO_2. As depicted in Fig. 3a, the pristine coronene possesses an initial band gap of 4.021 eV (Ajeel & Ben Ahmed, 2023; Khamees et al., 2024). Upon introducing the Boron dopant, as shown in Fig. 3b, the B-doped configuration exhibits a significantly reduced band gap of 3.892 eV. This strong decrease with respect to the pristine structure suggests that the Boron substitution induces strong electronic interactions in the coronene framework (Ajeel & Ben Ahmed, 2023; Khamees et al., 2024). The lack of Boron atom results in localized mid-gap states near Fermi level, thus effectively narrowing the energy gap and promoting charge transfer that is very beneficial to improve the conductivity and reactivity of the sensing platform. Additional structural and electronic changes upon adsorption of gas molecules lead to a modulated band gap of 3.892 eV as demonstrated for the CO_2 adsorption complex in Fig. 3c (Almansour et al., 2026; Khamees et al., 2024). This variation is due to the increased orbital hybridization and electronic interaction between the adsorbed gas molecule and the Boron active site which introduces new states near the Fermi level, thus significantly changing the electronic structure (Almansour et al., 2026). These quantifiable band gap modifications upon interaction with gas indicate excellent charge transport modulations, confirming the high suitability of the B-doped coronene configurations for advanced highly sensitive gas sensing applications. The nature of these electronic changes is further elucidated by the Density of States (DOS) spectra (Feng et al., 2018; Yeh et al., 2018). The presence of new electronic states induced by the Boron dopant and subsequently by the adsorbed gas molecules is evidenced by a substantial redistribution of states in the occupied and unoccupied orbitals, especially around the Fermi level. Strong orbital interactions between the Boron active site and the target gas CO_2 induce a distinct shift of the density of states (DOS) that fundamentally alters the electronic transport behavior of the sensing system. It is worth noting the emergence and broadening of the DOS peaks in the adsorption configurations. They reflect the enhanced delocalization of charge carriers and the significant charge transfer between the gas molecules and the B-doped coronene surface (Khamees et al., 2024; Ajeel et al., 2024; Almansour et al., 2026). This is the underlying mechanism critical for the highly efficient gas sensing applications. These results demonstrate that the addition of a Boron dopant and its interaction with adsorbed gas molecules can be used to efficiently tune the energy band gap of the coronene system. The tunability of these electronic properties by Boron functionalization is a very promising approach for the design of carbon-based nanomaterials for high-performance gas sensing and environmental monitoring applications (Khamees et al., 2024; Ajeel et al., 2024; Almansour et al., 2026).



(a) (b) (c)

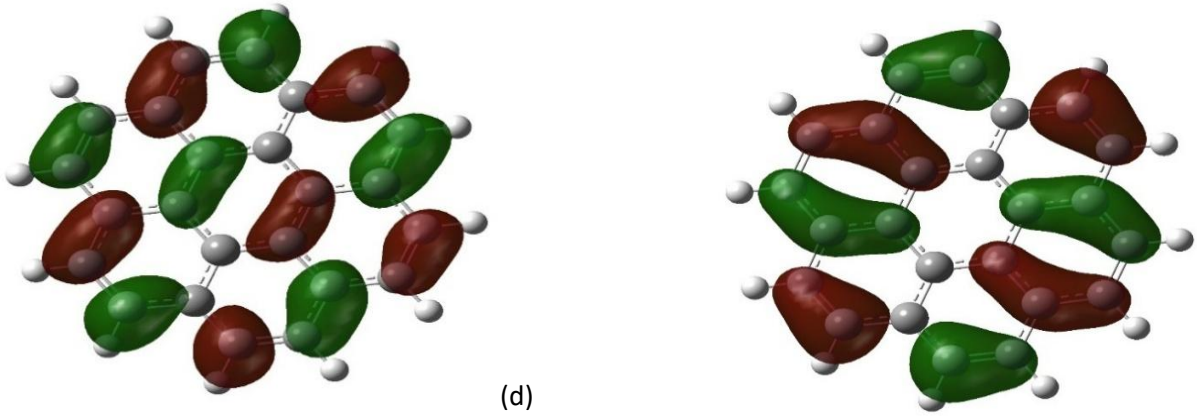


Figure 2: Atomic structure (a) the bond lengths (in Å unit), (b), Molecular electrostatic potential (MEP), (c) and the HOMO-LUMO plots (d) of pristine coronene quantum dot (CQDs)

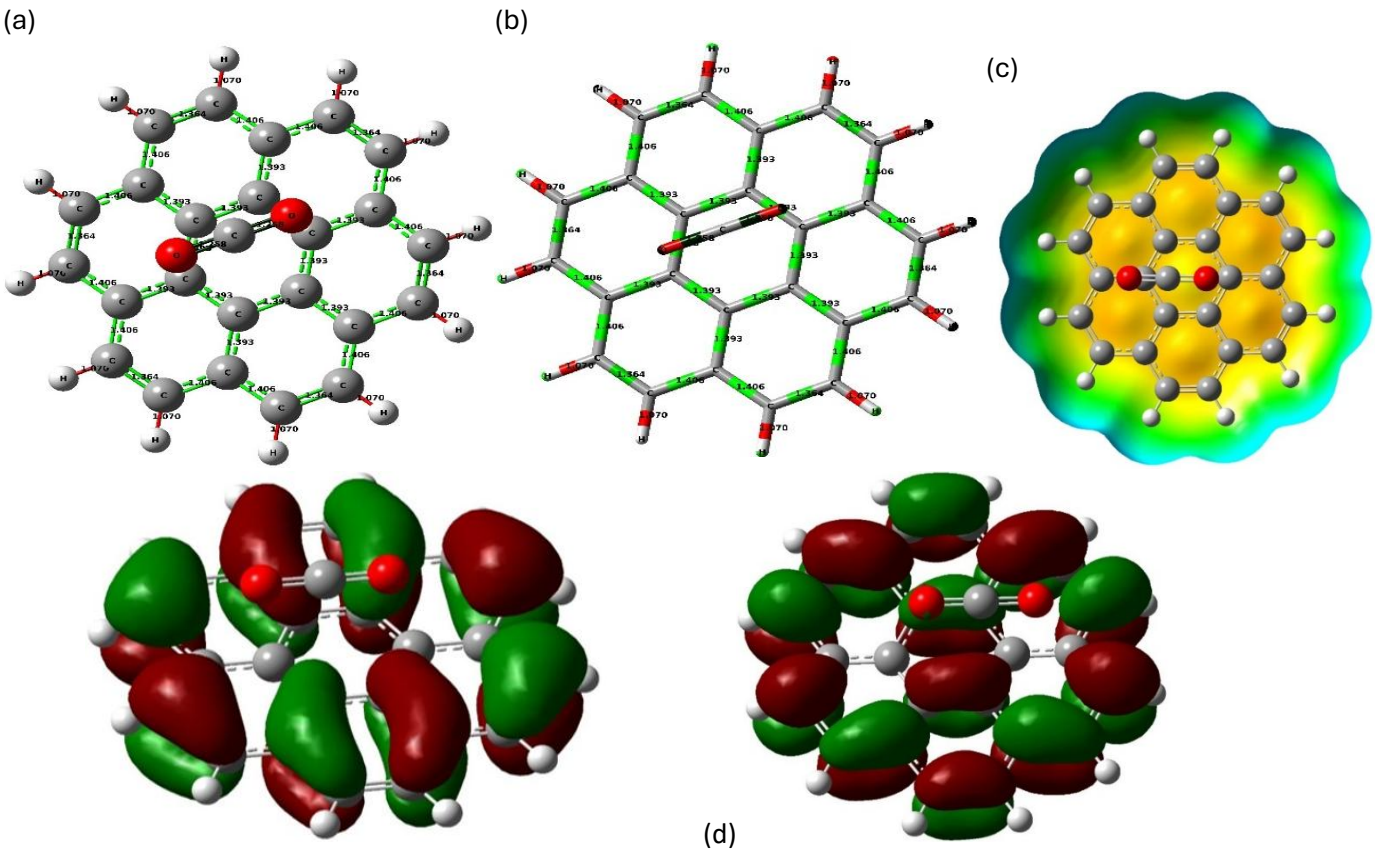


Figure 3: The most stable structure for adsorption of CO_2 molecule on the surface of pristine coronene quantum dot and its (a, b) and molecular electrostatic potential (MEP) with CO_2 (c) HOMO-LUMO plots (d).

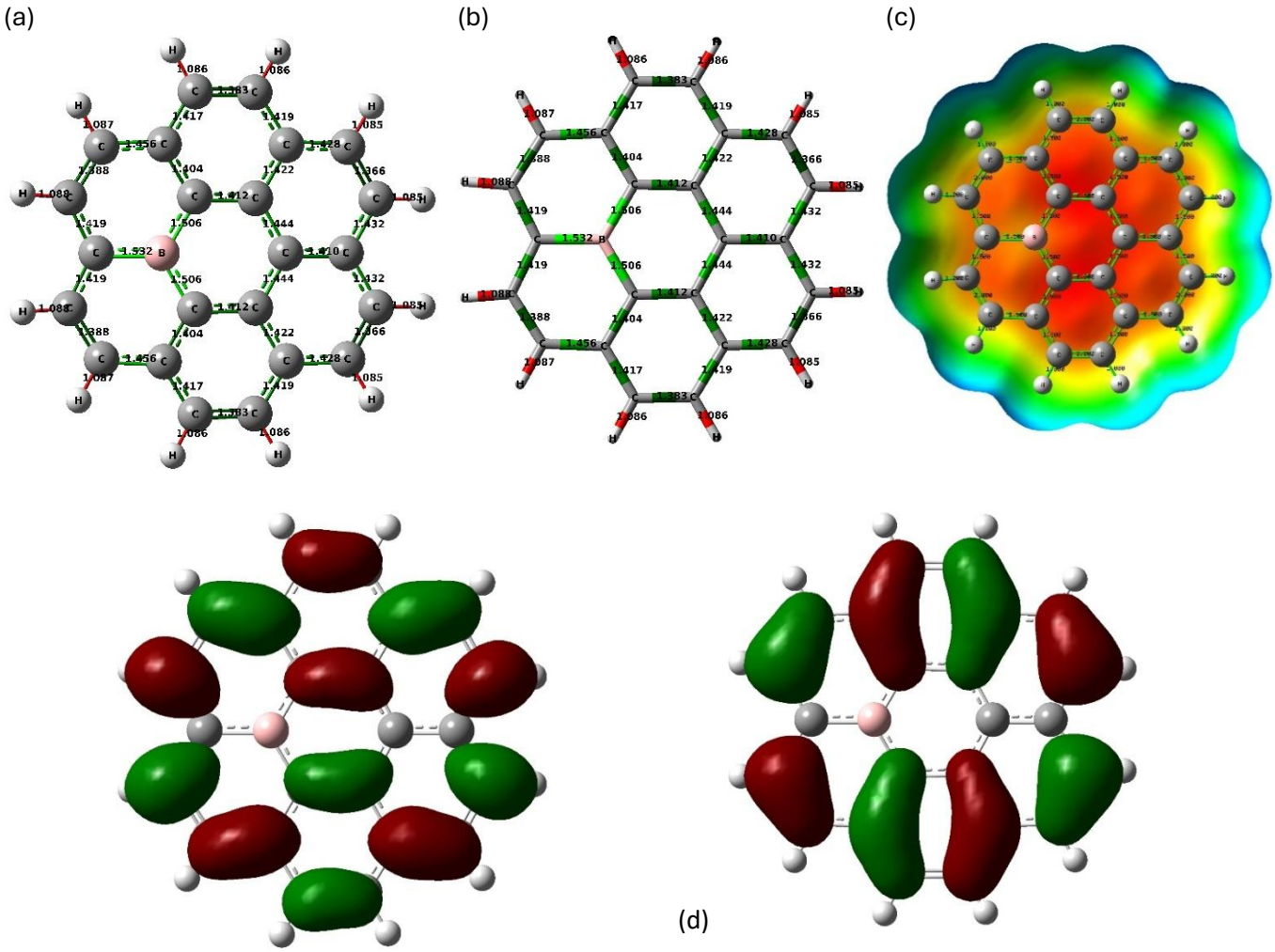
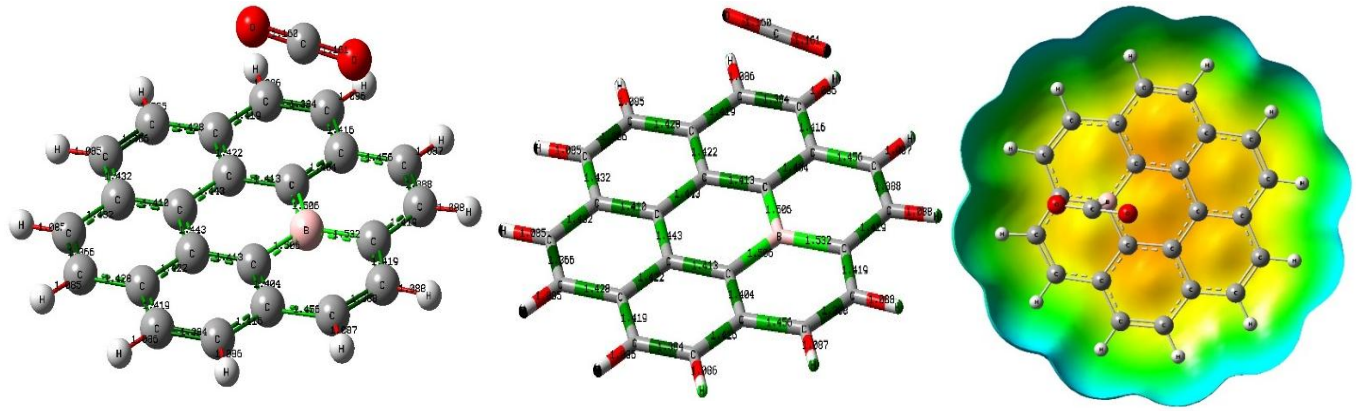
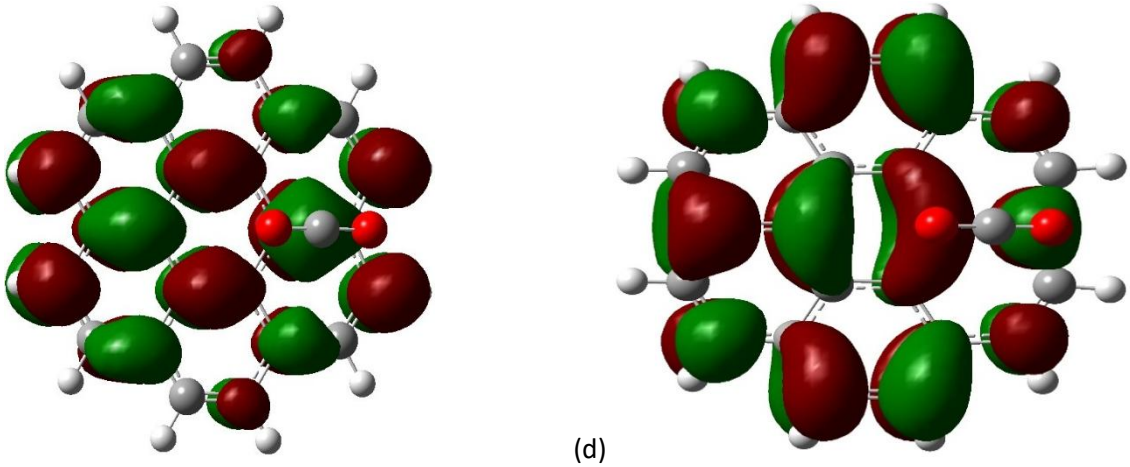


Figure 4: The structured geometries (a), the bond lengths (in angstrom unit) (b), molecular electrostatic potential (MEP), (c) and the HOMO-LUMO plots (d) of boron-doped coronene quantum dots (B-CQDs).





(d)

Figure 5: The most stable structure for adsorption of CO_2 molecule on the surface of of boron-doped coronene quantum dots (B-CQDs) its (a, b) and molecular electrostatic potential (MEP) with CO_2 (c) HOMO-LUMO plots (d).

Table 1: Calculated energetic data, HOMO energies (E_{HOMO}), Fermi level energy (E_{FL}), LUMO energies (E_{LUMO}), and energy gap energy (E_g), and the dipole moment (Dm), calculated for pristine coronene quantum dot CQDs and B-doped CQDs at room temperature

Complex	$E_{HOMO}(eV)$	$E_{FL}(eV)$	$E_{LUMO}(eV)$	$E_g(eV)$	$E_{coh}(eV)$	D_m
CQD-Pristine	-5.705	-3.694	-1.684	4.021-	-5.889	0.00000
CO_2/CQD	-5.661	-3.651	-1.642	4.018	-5.880	0.047349
B-CQD	-5.627	-3.681	-1.735	3.892	-5.847	0.147043
CO_2/CQD	-5.650	-3.706	-1.762	3.888	-10.925	0.251051

Table 2: The global chemical indexes: chemical potential (μ), chemical hardness (η), chemical softness (S) and electrophilicity (ω) and electronegativity (X) calculated for coronene quantum dot (CQDs) with and without B element, all these parameters are measured in unite eV

Complex	μ	η	S	ω	X
CQD-Pristine	3.694	2.010	0.2487	3.394	-3.694
CO_2/CQD	3.651	2.009	0.2488	3.317	-3.651
B-CQD	3.681	1.946	0.2569	3.481	-3.681
CO_2/CQD	3.706	1.944	0.2572	3.532	-3.706

Table 3: The total electronic energy (E_{tot}), energy gap energy (E_{gap}), change in E_{gap} (ΔE_{gap}), adsorption energies (E_{ads}), and absorption threshold (λ_{abs}) calculated in the gas phase for CO_2/CQDs and CO_2/B-CQDs at room temperature

Complex	$E_{tot}(eV)$	$E_g(eV)$	$\Delta E_g(\%)$	$E_{ads}(eV)$	$\lambda_{abs}(nm)$
CQD-Pristine	-25091.44	4.021	-	-	308.3
CO_2/CQD	-30222.56	4.018	-0.10%	-0.902	308.6
B-CQD	-24729.48	3.892	-	-	318.6
CO_2/B-CQD	-29862.69	3.888	-0.11%	-1.632	318.9

Table 1 summarizes the calculated electronic characteristics for the pristine coronene, the B-doped coronene, and the corresponding gas adsorption complexes (Ajeel & Ben Ahmed, 2023; Khamees et al., 2024). The results obtained are informative about the effect of Boron doping and subsequent interactions with target gases on the electronic structure and stability of coronene system. For example, the HOMO energy level changes from -5.705 eV for the pristine coronene to -5.627 eV for the B-doped configuration. This shift implies a large reduction of the ionization potential and thus a strong increase of the capacity of the system to donate electrons and participate in charge transfer processes (Feng et al., 2018; Khamees et al., 2024). Also, the LUMO energy level shifts from -1.684 eV to -1.735 eV and these effects together lead to the reduction in energy band gap as

mentioned above. The LUMO energy of B-doped coronene is -1.684 eV in the pristine system and -1.735 eV indicating an increase in electronic affinity (Ajeel & Ben Ahmed, 2023; Khamees et al., 2024). This affects the charge transport properties of the material as the Fermi level shifts towards the conduction band. The most significant change is observed in the energy gap (E_g), which is considerably reduced from 4.021 eV (pure coronene) to 3.892 eV (B-doped coronene) with a reduction of -0.11 %. This large decrease indicates the successful enhancement of the conductivity of coronene framework by Boron doping which is more suitable for the gas sensing applications (Glasser & Sheppard, 2016; Vig et al., 2023). Also, the cohesive energy (E_{coh}) is employed to evaluate the thermodynamic stability and the degree of atomic incorporation in the modified nanostructure. The more negative value of Ecoh indicates more stable configuration. The results show a slight decrease in stability from -5.889 eV (pristine coronene) to -5.880 eV for the B doped structures. This means that although the total binding energy is slightly reduced due to the incorporation of Boron, the structures are still energetically stable and experimentally feasible. The negative values of Ecoh confirm the exothermic nature of the B-doped coronene formation and guarantee the structural stability of the nanostructure throughout the entire sensing application (Ajeel & Ben Ahmed, 2023; Khamees et al., 2024). The dipole moment needs to be considered in order to understand fully the charge distribution and polarisation properties of the modified system of coronene with the Boron dopant. Table 1 shows that the charge distribution of pristine coronene is very symmetric, with a very small dipole moment of 0.251051 Debye. However, the Boron dopant changes this symmetry considerably and results in significant differences in the values of dipole moment for the studied configurations. The dipole moment of B-doped coronene and its adsorption complexes with CO_2 are 0.047349, 0.147043 and 0.251051 Debye, respectively. The enhancement of dipole moment indicates the asymmetry of charge distribution due to the electron-deficient nature of the Boron atom, which results in localized charge density fluctuations. This configuration has the highest dipole moment (0.251051 Debye) due to the strong spatial polarization throughout the molecule. This polarization is further increased in the case of gas adsorption due to the electronic interaction and charge redistribution between the gas molecules and the Boron active site. Structural distortion and increased atomic separation in the B-doped framework improve the charge separation and lead to a larger dipole moment (Almansour et al., 2026). These enhanced polarization effects are highly advantageous for sensing applications where sensitivity to external molecular interactions is extremely important. Strong polarization is helpful to the detection of target gas CO_2 by increasing the electrostatic attraction between the surface and the gas molecules, which is important for high-performance chemical sensors. Fig. 4 shows the optimized geometries and characteristic bond lengths of the coronene system, including the B-doped configurations and their interaction with gas molecules. These configurations show different structural differences that directly affect the electronic properties as predicted by the DFT calculations. The figure illustrates the various adsorption sites and the spatial orientation and bonding interactions between the Boron active site and the target gas molecules (CO_2 and Formaldehyde) inside the nanostructure (Feng et al. 2018; Khamees et al. 2024). The detailed analysis of the structural geometries provides important information on the electronic and environmental changes essential for the development of advanced functionalities in coronene-based systems. The atomic size mismatch and the difference in electronegativity are responsible for unprecedented distortions in the bond lengths of neighboring carbon atoms upon the introduction of the Boron dopant. Studies of the electronic states confirm that this spatial arrangement results in the formation of new states around the Fermi level that play a decisive role in the modulation of the energy band gap (E_g) (Ajeel & Ben Ahmed, 2023; Khamees et al., 2024). Moreover, these bond length variations are a direct measure of an increased dipole moment, which greatly increases the sensitivity of the system to external molecular interactions. In some topologies, elongation of the B–C bonds leads to a particularly pronounced distortion of the structure, and a modified charge distribution pattern within the framework. This modified electronic environment is very useful for the fabrication of high-performance heterostructures in gas sensing applications where efficient charge separation and surface reactivity are of utmost importance (Feng et al. 2018; Khamees et al. 2024). In conclusion, the analyzed configurations show the possibility to fine tune the electronic properties of the coronene system through the interactions between the Boron dopant and the target gas molecules. Given the strong impact of changes in the adsorption sites and bond lengths on the charge transfer and the total electronic properties, these systems are interesting prospects for high-end gas sensing and environmental monitoring applications (Ajeel & Ben Ahmed, 2023; Khamees et al., 2024). Table 2. Chemical potential (μ), chemical hardness (η), softness (S) and electrophilicity index (ω). These parameters give the basic insights about the chemical reactivity and electronic stability of the pristine and B-doped coronene systems. The LUMO decreases from -1.762 eV in B-CQDs to -1.642 eV in pristine coronene CO_2 configuration, indicating the trend of promoted electronic activity (Feng et al., 2018; Khamees et al., 2024; Almansour et al., 2026). The chemical potential remains fairly constant with moderate variations across the doped structures, indicating that the

addition of Boron does not greatly affect the average energy of the frontier molecular orbitals (HOMO and LUMO) of the system. A great reduction of the chemical hardness (μ) is predicted from 3.694 eV in the pristine coronene to 3.706 eV in the B-doped configuration, which indicates an enhanced electronic sensitivity and thus a higher reactivity to external molecular perturbations. In parallel, a significant increase of chemical softness (S), the inverse of hardness, is observed, which points to higher susceptibility to electronic interactions and surface reactivity. Moreover, the electrophilicity index (ω), which is a measure of the energy stabilisation of a system due to receiving an electron transfer, is significantly enhanced for the B-doped structures with a maximum value of 3.532 eV for the 3.394 eV structure. These results indicate that B-doped coronene exhibits excellent charge transfer properties, and thus is a highly promising candidate for advanced gas sensing and environmental remediation applications. The observed decreases in energy gap and hardness along with increase in softness and electrophilicity show that Boron doping greatly optimizes the electronic properties of the framework. The tunable conductivity due to the change in electronic energy levels indicates the potential of these engineered nanomaterials to be incorporated into modern environmental monitoring devices and highly sensitive chemical sensors (Feng et al., 2018; Khamees et al., 2024; Almansour et al., 2026). The structural asymmetry induced by the Boron dopant not only modifies the electrostatic environment of the nanostructure but also enhances interatomic orbital interactions, particularly at the active defect sites introduced by the dopant. Such structural deformation facilitates the delocalization of charge carriers by creating mid-gap states, which effectively reduces the energy band gap (Eg) and improves the total electrical conductivity. At the same time the predicted large dipole moments for the highly distorted configurations are a result of an increased charge separation across the framework. The observed phenomenon is a clear manifestation of the direct correlation of the modified molecular geometry with the optimized electronic behavior, which ultimately determines the enhanced sensitivity of the material toward the target gas molecules (Khamees et al., 2024; Almansour et al., 2026).

CONCLUSION

We have studied the interaction of pristine and B-doped CQDs (coronene quantum dots) with CO_2 molecules using Density Functional Theory (DFT) at B3LYP level of theory. The results show that the CO_2 molecule is physically adsorbed on the surface of the pristine Coronene, while it is strongly chemisorbed on the surface of the Boron-doped Coronene with a large adsorption energy. The pristine Coronene recovery time towards the CO_2 molecule is found to be low enough to enable the practical detection of this molecule. Later, the sensitivity performance of the B-Coronene clusters was greatly enhanced by replacing a carbon atom in the Coronene structure by a Boron atom. Moreover, a significant change in the energy gap was found after the interaction of CO_2 molecules with the B-Coronene surface, which means a considerable increase in its electrical conductivity. Therefore, the complex shows a high electronic sensitivity to the CO_2 molecules, which indicates its potential as an effective nanosensor for the detection of this gas. Finally, our results on sensitivity and recovery time clearly reveal that the studied B-doped Coronene material is a promising and efficient sensor for the detection of CO_2.

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