

Phthalates Adsorption on Nanostructures for Environmental Remediation: an *ab initio* Study

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Phthalates are organic molecules found in various everyday materials, such as plastics, but they do not bond chemically to the product. Consequently, they are released and contaminate the environment. In humans, ingesting phthalates can stimulate a functionality similar to estrogen hormones, acting as endocrine disruptors, thus requiring selective adsorption. This paper demonstrates the use of cyclodextrins (CDs), which are useful due to their capacity for selective adsorption by the inclusion of organic molecules in their internal cavities to remove pollutants from water. Graphene (Gr) is also evaluated due to its interesting electronic properties and a large surface, making this nanomaterial ideal for molecule adsorption. Through *ab initio* simulations, three phthalate molecules, benzyl butyl phthalate (BBP), dicyclohexyl-phthalate (DCHP), and dipropyl phthalate (DPP) interacting with β -CD and Gr, were evaluated. The results indicate that a weak interaction occurs, through physical adsorption. β -CD interacting with phthalates tends to form a host-guest complex. In the case of Gr, weak adsorption is favored by π - π interactions and H-bonds. Therefore, this study shows that these nanosystems are promising for removing phthalate molecules from wastewater.

Keywords: environmental applications, DFT, nanomaterial, physics adsorption, simulation

Introduction

Phthalates are organic esters with wide industrial applications as plasticizers, used to improve plasticity and softness in various consumer products, for example, water and beverage bottles, food containers, cosmetics, and others.¹ However, they do not chemically bond to the product and are released into the environment and contaminate water, food, soil, and air. In humans, phthalates stimulate a functionality similar to estrogen hormones, thus acting as endocrine disruptors and killing sperm, for example.²⁻⁶ They have adverse effects on the liver and kidneys and are suspected to be carcinogens in humans. Due to the large industrial use and the environmental risk, mainly due to their adverse effects on human and animal health, the adequate removal of these molecules is essential, especially from aquatic environments.⁷⁻¹⁰

Cyclodextrins (CDs) are cyclic oligosaccharides with several applications,¹¹ including a new generation

for removing pollutants from the wastewater as they are deemed efficient, selective, and reusable.¹¹⁻¹⁶ Specifically, β -CDs are considered a perfect tool in environmental remediation due to their low cost, with a cavity diameter that offers the most suitable size for removing organic and inorganic pollutants. The hydrophilic exterior and hydrophobic interior of β -CD can host a variety of molecules through host-guest adsorption, establishing hydrophobic interaction in aqueous media with most organic targets, such as phthalate.^{9-13,16} Experimental studies show the capacity for selective phthalate adsorption by forming inclusion complexes with β -CD. At the same time, the inclusion of phthalate in the internal cavity of β -CD proved to be the main mechanism for successfully removing phthalate from water.^{9-13,16-20}

Due to the hydrophobic nature of phthalate and hydrophobic core of the cavity, the phthalate molecule could be inserted into the cavity of the β -CD in aqueous media. In aqueous or high-polar solvents, the slightly hydrophobic β -CD cavity is occupied by water molecules energetically unfavorable (polar-non-polar interaction). It can, therefore, be readily substituted by phthalate, which is more hydrophobic than water.⁹

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Prof. Oswaldo's fervor for science, nationwide talent support, and Nanoscience promotion beyond academia render him unforgettable.



A few hexagonal layers compose graphene (Gr), the same layers that form graphite.²¹ The electronic properties and the large surface area are some of the most interesting features for the adsorption of molecules of chemical or biological interest.^{22,23} In addition, the aromatic structure and the numerous delocalized π electrons make Gr promising for environmental decontamination applications, especially in organic systems.²²⁻²⁵ In recent years, graphene materials have attracted great interest in their potential use in purifying organic pollutants in the aqueous system.²⁵⁻²⁷ Studies involving the adsorption of phthalates on graphene material sheets have already been demonstrated experimentally and by classical molecular dynamics.²⁷⁻²⁹

A few studies have explored quantum computer simulations involving pristine graphene interacting with phthalates such as benzyl butyl phthalate (BBP), dicyclohexyl-phthalate (DCHP), and dipropyl phthalate (DPP). In this paper, β -CD and Gr through first-principles calculations based on the density functional theory (DFT) as nanomaterials with potential for absorbing or including phthalate molecules were evaluated. These simulations consider three phthalate molecules (BBP, DCHP, and DPP) interacting with β -CD or Gr to assess the electronic, energetic, and structural properties of the resulting systems. Additionally, understanding the differences between the interactions of phthalates with graphene and/or CD is crucial due to variations in chemical conditions and surface shapes.

Methodology

To evaluate energetic, structural, and electronic properties of the phthalate molecules (BBP, DCHP, and DPP) with Gr or β -CD, calculations of the first-principles were performed using the SIESTA computational code,³⁰ based on DFT. In these calculations, double-zeta polarized (DZP) basis functions were employed. The potential for exchange-correlation was described by local density approximation (LDA).³¹ This choice was justified primarily by similar works in the literature^{23,32-36} where LDA demonstrated better agreement for binding energies and binding distance values in weakly interacting systems compared to experimental results. In the same way, LDA shows good agreement for weakly interacting systems, particularly in the presence of π -stacking interactions in sp^2 -type materials.³⁶⁻⁴¹

The charge density was represented using a 200 Ry cut-off radius for the real-space integration grid. Structural optimizations were performed via a conjugate gradient method, ensuring residual forces were below $0.05 \text{ eV } \text{\AA}^{-1}$ in all atomic coordinates. For simulations involving Gr

and phthalate molecules (BBP, DCHP, or DPP), periodic boundary conditions were applied with the unit cell dimensions set at $24.68 \times 14.85 \times 40.00 \text{ \AA}^3$. The Gr [β -CD] isolated system consists of 144 [147] atoms in the supercell. Similar computational methodologies have been employed in previous studies by our research group.^{22,23,36,42}

To calculate the binding energy (E_b), the BSSE method (base set superposition error) is considered (equation 1):⁴³

$$E_b = - [E(A + B) - E(A + B_{\text{ghost}}) - E(A_{\text{ghost}} + B)] \quad (1)$$

where the ghost subscript refers to the atomic base placed in the positions of Gr/ β -CD or phthalates but without atomic potentials representing real atoms in those positions. In the BSSE method, the correction is performed from the initial geometry of the system AB (interacting systems) and calculating the total energy of the system A[B] (isolated system), considering the entire set of basis functions, where the set of basis functions B[A] is located in the position corresponding to the system B[A] (isolated system), without the explicit presence of atoms. It is worth noting that positive energy values indicate an attractive system.

Results and Discussion

Initially, the isolated structures of β -CD, Gr, BBP, DCHP, and DPP were evaluated. β -CD has a HOMO (higher occupied molecular orbital) and LUMO (lowest unoccupied molecular orbital) difference of 5.72 eV, close to that described in the literature with similar methodology.^{42,44} The HOMO-LUMO difference observed in BBP, DCHP, and DPP is, respectively, 3.44, 3.51, and 3.44 eV (Table 1). Singh *et al.*⁴⁵ obtained 3.88 eV for the HOMO/LUMO difference for DCHP molecule with DFT/B3LYP (6-311G) basis set.⁴⁶

The interaction of β -CD with phthalate molecules (BBP, DCHP, or DPP) has been proposed in various atomic arrangements. The phthalate molecules interacting through the largest and smallest cavity and the external part of the β -CD were analyzed. Figure 1 illustrates the most stable chemical structures for each interacting system. Table 1 shows the values of the binding energy (eV), shortest distance (\AA), HOMO/LUMO difference (eV) ($\Delta_{\text{HOMO/LUMO}}$), and charge transfer (e^-) between the nanostructures (β -CD or Gr) and the molecules.

BBP interacts with β -CD (Figure 1a) through the inner part of the largest cavity, considering the molecular dimensions of the β -CD cavity (diameter 6.0-6.5 \AA), with a binding energy of 0.94 (21.69) eV (kcal mol^{-1}). The HOMO-LUMO difference is 2.85 eV, which decreases compared with isolated BBP and β -CD, 3.44 and 5.72 eV,

Table 1. Most stable configurations studied for the interaction of phthalate molecules (BBP, DCHP, and DPP) with β -CD or Gr. Binding energy, shortest distance, $\Delta_{\text{HOMO/LUMO}}$, and charge transfer

Phthalate molecule		E_b / eV	E_b / (kcal mol ⁻¹)	Shortest distance / Å	$\Delta_{\text{HOMO/LUMO}}$ / eV	Charge transfer / e ⁻
BBP	β -CD	0.94	21.68	1.80	2.85	+0.22
	Gr	0.42	9.68	3.35	–	+0.09
DCHP	β -CD	1.12	25.83	1.76	2.56	+0.16
	Gr	0.55	12.68	2.96	–	+0.09
DPP	β -CD	1.04	23.98	2.02	3.22	-0.08
	Gr	0.18	4.15	2.99	–	+0.08

BBP: benzyl butyl phthalate; DCHP: dicyclohexyl-phthalate; DPP: dipropyl phthalate; CD: cyclodextrin; Gr: graphene; +: sign indicates that the phthalate acts as an electron acceptor.

respectively. β -CD acts as an electron donor of +0.22 e⁻ in the presence of the BBP molecule. Saini *et al.*⁴² also showed that β -CD interacts with bisphenol. The electronic charge plot in HOMO is located on β -CD and in LUMO on BBP, more precisely on the aromatic ring inside the β -CD cavity. These results show that electronic levels in previous theoretical/experimental⁴⁷ studies state that BBP can partially enter the beta-CD cavity. This complexation is favorable for the degradation of BBP. β -CD has

hydrophobic internal cavities, and Zhou *et al.*¹⁹ used this strategy to capture BBP molecules.

When the β -CD interacts with the DCHP (Figure 1b), the binding energy is around 1.12 (25.83) eV (kcal mol⁻¹), in this case, the molecule interacts perpendicularly over the largest cavity of the β -CD. The interaction distance (minimum distance between interacting atoms of DCHP and β -CD) is 1.76 Å, and β -CD acts as an electron donor to the DCHP molecule, resulting in a charge transfer of +0.18 e⁻. The HOMO-LUMO difference is 2.56 eV, a smaller value than that of the isolated DCHP molecule (3.51 eV). The charge plot in the HOMO region is concentrated on β -CD, while in the LUMO, it is exclusively on the DCHP molecule. In this case, the inclusion of DCHP in the β -CD cavity is unfavorable; nevertheless, this system was the most stable among the studies. Despite the binding energy value, the system exhibits physical adsorption characteristics, as evidenced by the absence of significant changes in electronic properties, interaction distance value, and low charge transfer.

The most stable system of DPP phthalate interacting with β -CD (Figure 1c) occurs through encapsulation of the larger CD cavity; the binding energy is 1.04 (23.98) eV (kcal mol⁻¹). In this case, the β -CD in the presence of DPP is an electron acceptor (0.08 e⁻), contrasting with the BBP and DCHP interaction. This behavior can be understood as a result of the electronegativity variation within the region where phthalate molecules enter the cavity of β -CD. A HOMO-LUMO difference of 3.22 eV is observed, a value close to that of the isolated DPP molecule (3.44 eV). The charge plot in HOMO reveals that the charge is mainly concentrated on β -CD and LUMO in the DPP aromatic ring in the β -CD cavity.

In Figure 2, the most stable configurations of Gr interacting with BBP, DCHP, and DPP, the energy bands

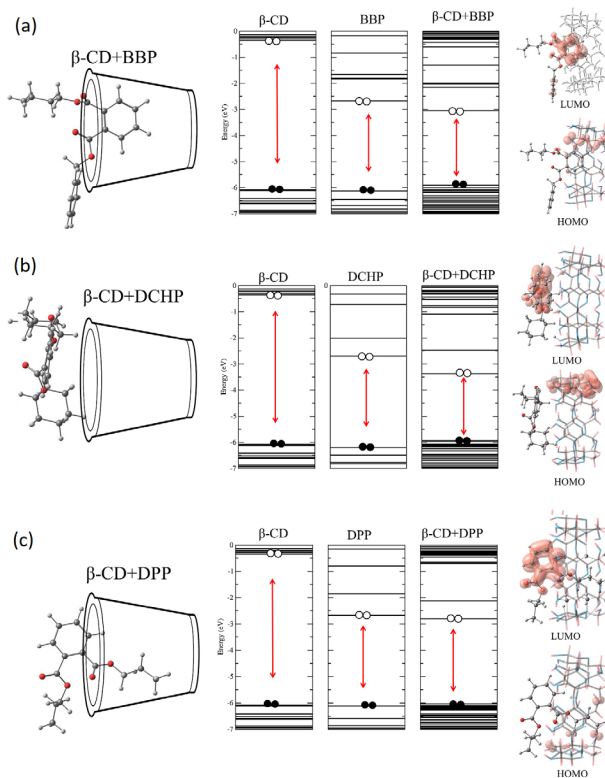


Figure 1. β -CD interacting with (a) BBP, (b) DCHP, and (c) DPP: most stable configuration, energy levels, and charge plot on HOMO and LUMO (isosurface value $1 \times 10^{-3} e \text{ \AA}^{-3}$).

of the isolated systems and the most stable configurations, and the charge plot in the valence (VB) and conduction band (CB) are presented.

In the interaction of BBP with Gr (Figure 2a), the most stable system presents a binding energy of 0.42 (9.68) eV (kcal mol⁻¹), with an electronic charge transfer from Gr to the phthalate molecule of +0.09 e⁻, that is, BBP is a charge acceptor. The smallest distance between structures is 3.35 Å. There are no significant changes in electronic properties compared to isolated Gr. The charge plots on the VB and CB are concentrated mainly on Gr.

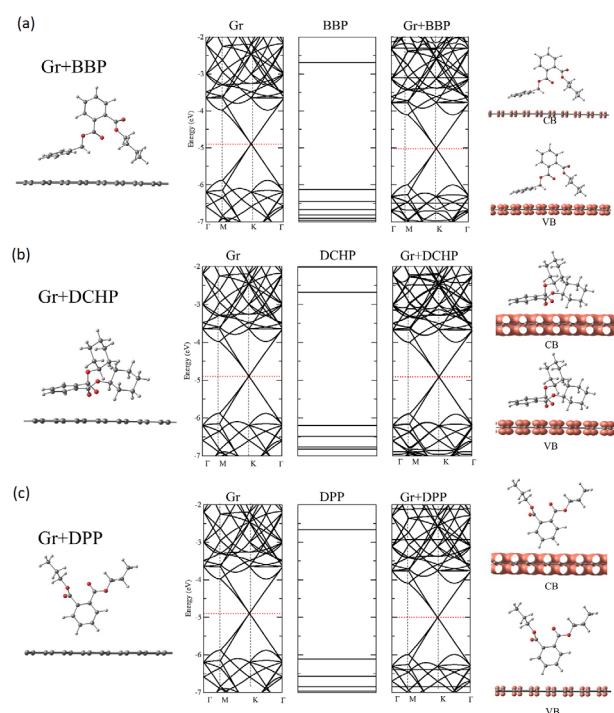


Figure 2. Gr interacting with (a) BBP, (b) DCHP, and (c) DPP: most stable configuration, energy levels, and charge plot on HOMO and LUMO (isosurface value $1 \times 10^{-3} e \text{ \AA}^{-3}$).

DCHP interacting with Gr (Figure 2b) exhibits a binding energy of 0.55 (12.68) eV (kcal mol⁻¹), with a distance of 2.96 Å. A slight charge transfer of +0.09 e⁻ from Gr to DCHP is observed in this case. Additionally, there are no significant changes in electronic properties compared to isolated Gr, indicating a weak interaction, namely physical adsorption.

In the interaction of BBP and DCHP with Gr, it is notable that in the two most stable cases, one of the phthalate aromatic rings interacts in a planar structure with Gr. Previous studies^{23,36} show that planar molecules, or planar portions of molecules, interact through π - π type.

In the case of the interaction of DPP with Gr (Figure 2c), the phthalate molecule interacts perpendicularly. In this case, the binding energy is 0.18 (4.15) eV (kcal mol⁻¹),

with a smaller distance between the structures of 2.99 Å. As in the previous cases, Gr donates an electronic charge to phthalate (0.08 e⁻). The electronic properties remain unchanged to isolated Gr, and the charge plot in VB and CB are concentrated over Gr.

The interaction of BPP, DCHP, and DPP molecules with Gr present binding energy in the order of 0.42 (9.68), 0.55 (12.68), and 0.18 (4.15) eV (kcal mol⁻¹), respectively. In these systems, the bonding distance is around 3 Å. Studies demonstrate that other pollutants, such as analgesics, are adsorbed through non-covalent interactions (van der Waals and π - π interactions) with graphene.⁴⁸ demonstrate that the structures are optimized at a relatively long distance (3–4 Å) compared to typical C–H and C–C bond lengths, and the negligible change in electronic properties indicates that the adsorption mechanism is of a physical nature. The interaction occurs within a physical adsorption regime, indicating weak interaction between the constituents.

Experimental studies on the adsorption of phthalates onto carbon nanotubes have revealed that not only does the small diameter of the nanotubes contributes to higher adsorption efficiency, but also that it is an endothermic process, whereby an increase in ambient temperature leads to increased adsorption efficiency.^{49,50} Moreover, in all these instances, the adsorption of a broad spectrum of phthalates with varying polarities was observed to be relatively non-selective.⁵¹

The results presented in this paper collaborate with previous experimental studies.⁵¹ It is observed that β -CDs and graphene can be utilized for the adsorption of phthalates in a physical regime. β -CD provides better stabilization for the interaction with phthalates molecules compared to Gr. This adsorption preference occurs through the cyclodextrin cavity, which increases the number of possible chemical interactions between the systems.

Conclusions

In this paper, first-principle DFT-based calculations to assess the interaction of phthalate molecules (BPP, DCHP, and DPP) with both Gr and β -CD nanomaterials were conducted. The energetic, structural, and electronic properties estimation results indicate that the interactions occur through a physical adsorption regime. This suggests that the interaction is weak, with no significant changes observed in the electronic and structural properties of the systems. In the case of β -CD[Gr] interacting with phthalate molecules, the binding energy obtained are 0.94 / 21.68 [0.42 / 9.68] eV / kcal mol⁻¹, 1.12 / 25.83 [0.55 / 12.68] eV / kcal mol⁻¹, and 1.04 / 23.98 [0.18 / 4.15] eV / kcal mol⁻¹, for BBP, DCHP,

and DPP, respectively. However, all binding energies were less than 1.12 (25.83) eV (kcal mol⁻¹), indicating a physical adsorption regime. The absence of chemical bonds between the systems is one of the essential conditions for utilizing Gr and β -CD as a potential nanofilter platform for phthalate molecules BBP, DCHP, and DPP. Thus, we demonstrate that both β -CD and Gr are promising nanomaterials for removing phthalate molecules, offering the prospect of reusable systems.

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Author Contributions

Mariana Z. Tonel was responsible for investigation, methodology, validation; Jaine Schemmer for investigation, methodology; Laura O. Vendrame for investigation, visualization, writing original draft; Ivana Zanella for formal analysis, investigation, supervision, validation; Solange B. Fagan for conceptualization, funding acquisition, project administration, supervision, writing review and editing.

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