Sumer Journal for Pure Science (ISSN: 2790-7031)
SJPS 2024 (December), Vol. 3, No. 2, p.p. 58-68

# Study the Effect of Phosphorous Impurities on Electronic and Optical Properties of Circumcoronene via DFT investigations

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**Abstract:**

The electronic and optical characteristics of circumcoronene are significantly impacted by phosphorus doping. Improved stability, smaller energy gaps, and changed Fermi levels are some of the main results, which make these doped systems attractive options for use in energy devices, photonics, and nanoelectronics. Phosphorus doping significantly alters the chemical indices of circumcoronene, increasing its stability, reactivity, and suitability for uses requiring robust electron interaction. The design of nanoscale materials, including catalysts, sensors, and energy-storage devices, will be significantly impacted by these discoveries. The structures can be appropriate for applications that need absorption in the far-infrared or electronic devices with decreased optical loss by modifying the high-energy transitions with a considerable oscillator strength. The optical characteristics of circumcoronene are markedly altered by phosphorus doping, as seen by longer absorption wavelengths, lower transition energies, and weaker oscillators. Because of these changes, phosphorus-doped circumcoronene retains its adjustable electronic behavior for certain optoelectronic applications while being extremely versatile for usage in infrared photodetection, optical sensors, and energy storage.

**Keywords:** Circumcoronene; Optical Properties ; Electronic properties ; DFT; Energy gap; Chemical doping.

# دراسة تأثير الشوائب الفسفورية على الخواص الالكترونية والبصرية للسيركومكورونين من خلال تحقيقات DFT

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**الملخص**: تتأثر الخصائص الالكترونية والبصرية للسيركومكورونين بشكل كبير بالتشويب بالفوسفور. ومن بين النتائج الرئيسية التي توصلنا إليها أن التحسن في الاستقرار، وتقليص فجوات الطاقة، وتغير مستويات فيرمي، تجعل هذه الأنظمة المعززة بالفوسفور خيارات جذابة للاستخدام في أجهزة الطاقة، والفوتونيات، والإلكترونيات النانوية. ويغير التشويب بالفوسفور بشكل كبير المؤشرات الكيميائية للسيركومكورونين، مما يزيد من استقراره وتفاعليته وملاءمته للاستخدامات التي تتطلب تفاعلًا إلكترونيًا قويًا. وسوف يتأثر تصميم المواد النانوية، بما في ذلك المحفزات، وأجهزة الاستشعار، وأجهزة تخزين الطاقة، بشكل كبير بهذه الاكتشافات. ويمكن أن تكون الهياكل مناسبة للتطبيقات التي تحتاج إلى امتصاص في الأشعة تحت الحمراء البعيدة أو الأجهزة الإلكترونية مع انخفاض الخسارة البصرية عن طريق تعديل التحولات عالية الطاقة بقوة مذبذب كبيرة. وتتغير الخصائص البصرية للسيركومكورونين بشكل ملحوظ عن طريق التشويب بالفوسفور، كما يتضح من أطوال موجية أطول للامتصاص، وطاقات انتقال أقل، ومذبذبات أضعف. وبسبب هذه التغييرات، يحتفظ السيركومكورونين المضاف إليه الفوسفور بسلوكه الكهربائي القابل للتعديل لبعض التطبيقات البصرية الإلكترونية.

**الكلمات المفتاحية:** سيركومكورونين؛ الخواص البصرية؛ الخواص الإلكترونية؛ DFT؛ فجوة الطاقة؛ التشويب الكيميائي.

# 1. Introduction

Graphene, a single layer of $sp^2$-hybridized carbon atoms arranged in a two-dimensional honeycomb lattice, has emerged as one of the most promising materials in nanotechnology due to its remarkable electronic and optical properties [1-4]. Its vast surface area and unique structure make graphene an ideal material for various photonic and optoelectronic applications [5, 6]. The ability to manipulate its properties using advanced computational methods like density functional theory (DFT) has significantly expanded its potential in research and development [7, 8].

The DFT, known for its accuracy and computational efficiency, has become a cornerstone in graphene research [9-11]. Its effectiveness is driven by the development of more precise density functions, improved functionality, and the superior balance between accuracy and computational cost compared to other ab initio methods [10]. Studies reveal that the edge effects and boundary termination of graphene heavily influence its electronic properties [1, 12-15]. These effects can be precisely examined through DFT calculations, especially when incorporating heteroatom doping, such as phosphorus.

The unique optoelectronic characteristics of graphene have fueled extensive research, particularly in its applications in solar cells, photodetectors, light-emitting devices, touchscreens, and ultrafast lasers [1, 16-20]. The material's anisotropic optical properties, sensitive to light polarization and electronic structure, enhance its role in nanophononics and optoelectronics. However, pristine graphene's transparency in the visible spectrum limits its absorption capabilities for specific wavelengths, which is where impurity doping becomes advantageous. By introducing heteroatoms like phosphorus into graphene-based systems, the electronic structure and absorption spectrum can be precisely tailored [7, 10, 16, 21, 22].

Circumcoronene (CC), a large polycyclic aromatic hydrocarbon, is of special thickness due to its privileged electronic, optical and structural properties [23-27]. It belongs to the family of graphene-like molecules and therefore can be considered as a model system for tests of polymers with longer π-systems and, hence, has significance in material science and nanoelectronics. It has good applicability in organic light emitting diodes (OLEDs) [28, 29], thermoelectric and batteries/supercapacitors owing to its efficient charge transport networks and strong photoluminescence [26, 30]. Apart from this, the robust circumcoronene's aromatic structure is quite suitable for catalytic and environmental applications while its derivatives are currently investigated for biomedical imaging and drug delivery [24, 31]. Given this wide array of functionalities, circumcoronene can be regarded as a fundamental building block molecule for the development of materials and enhancement of energy and health science research [32].

In this study, we aim to elucidate the impact of phosphorus doping on the electronic and optical properties of CC. The investigation includes a systematic analysis of one to five phosphorus-doped rings in CC. The goal is to explore how such modifications influence the absorption spectrum and optical behavior of CC, paving the way for potential advancements in nanoelectronics and optoelectronics.

## 2. Computational Details

The electronic and optical properties of circumcoronene were analyzed using both time-independent and time-dependent density functional theory DFT [24, 33-35] and TDDFT [17, 36-38]. The B3LYP functional paired with the 6-31G(d) basis set was employed for all geometric optimizations and property calculations. This combination, implemented in the Gaussian 09W software package, has been widely recognized for its efficiency in handling systems with complex electronic structures. Here, CC models with varying degrees of phosphorus doping (from one to five rings) were constructed. Both the pristine and phosphorus-doped structures underwent full geometric optimization, ensuring that the calculations captured the intrinsic electronic and optical behaviors without external constraints. The B3LYP functional was chosen for its robust performance in describing the exchange-correlation effects critical to molecular systems like CC.

The 6-31G(d) basis set provided an optimal balance between computational cost and accuracy, particularly for systems with significant electronic interactions. This level of theory enabled precise modeling of the absorption spectrum, bandgap variations, and optical anisotropy introduced by phosphorus doping. By comparing the doped and un doped CC systems, this study offers a comprehensive understanding of how phosphorus impurities modulate the electronic and optical characteristics of CC.

Electronic characteristics of CC include energy gap ($E_{\mathrm{gap}}$), Fermi level ($E_{\mathrm{FL}}$), LUMO orbitals energies ($E_{\mathrm{LUMO}}$), HOMO orbitals energies ($E_{\mathrm{HOMO}}$), and DOS resolution. The density functional theory (DFT), which includes the chemical reactivity parameters, is a very helpful instrument for the investigation of reactivity patterns, excited states, and toxicity investigations. These parameters included chemical hardness ($\eta$), chemical softness ($S$), chemical potential ($\mu$), and the electrophilicity index ($\omega$). These parameters can give by [3, 6, 26, 27]:

$$\mu = -\frac{(IP + EA\,)}{2} \tag{1}$$

$$\eta = \frac{(IP - EA\,)}{2} \tag{2}$$

$$S = \frac{(IP - EA\,)}{2} \tag{3}$$

$$\omega = \frac{\mu^2}{2\eta} \tag{4}$$

The ionization potential ($IP$) and the electron affinity ($EA$) may both be calculated with the use of Koopman's theorem, which gives the following formula [28-31]:

$$IP = -E_{\mathrm{HOMO}} \tag{5}$$

$$EA = -E_{\mathrm{LUMO}} \tag{6}$$

In addition, we use the following formula to calculate the electronic band gap as well as the energy of the Fermi level [32]:

$$E_{\mathrm{g}} = E_{\mathrm{LUMO}} - E_{\mathrm{HOMO}} \tag{7}$$

$$E_{\mathrm{FL}} = \frac{(E_{\mathrm{HOMO}} + E_{\mathrm{LUMO}})}{2} \tag{8}$$

Cohesive energies for each structure were computed in order to examine the structural stability of the P-codoped CC. The doped structures with the highest stability are those with the highest negative value [18].

## 3. Results and discussions

### 3.1. Geometric and Electronic Properties

Based on the results shown in Fig. 1(a), it can be seen that pure CC contain a 7-benzene ring, which has a typical C-C bond length of about 1.42 Å [31]. This value is in agreement with the values that have been reported in the previous articles [8, 23, 24, 31]. The density of states (DOS) of pure CC be analyzed for both before and after the replacement of carbon atoms with phosphorous. This is necessary in order to get a comprehensive knowledge of the changes that occur in the electronic characteristics of pure CC.

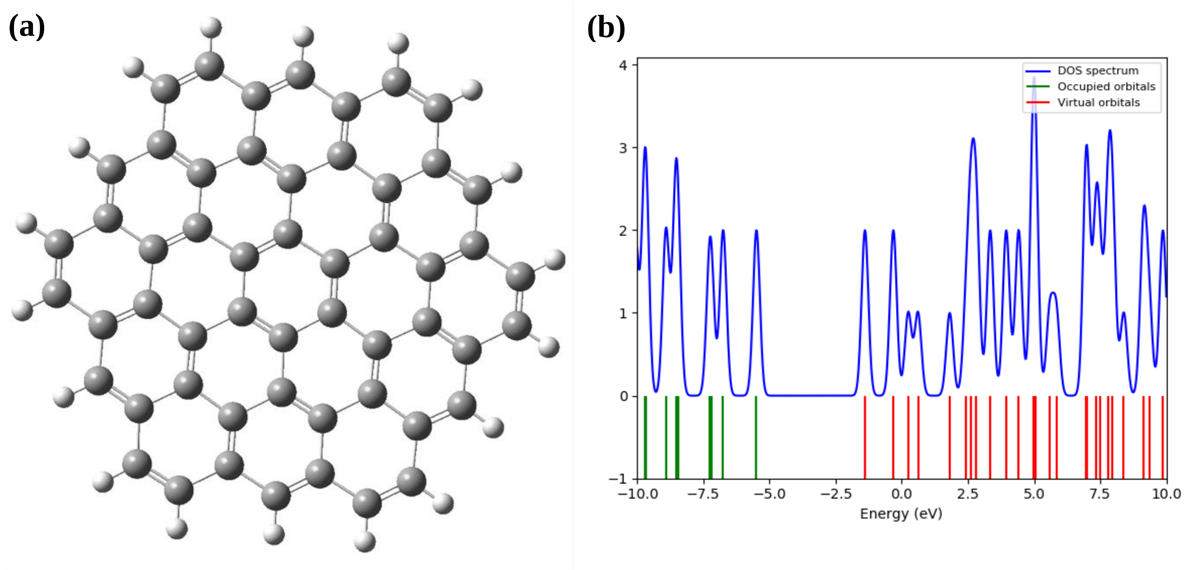

**Figure 1-** (**a**) The geometrical structure of pure circumcoronene, and their (**b**) density of state.

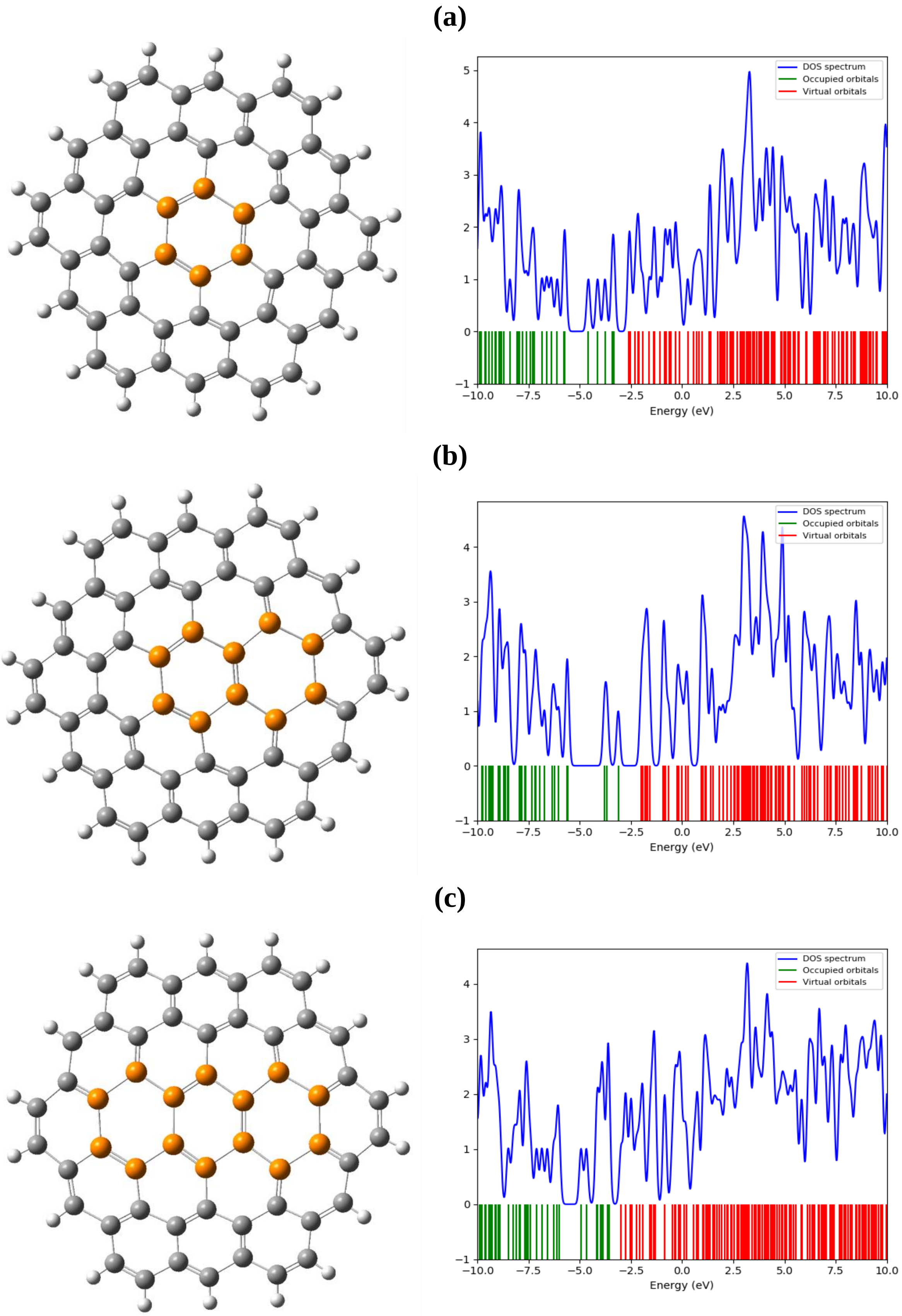

**Figure 2-** Shows the CC configurations with P generating the following structures: (a) CC-P1, (b) CC-P2, (c) CC-P3 with their density of state.

**Table 1** The values of the total energy ($E_T$), dipole moment (DM), Fermi level energy ($E_{FL}$), work function (ϕ), HOMO ($E_{HOMO}$) and LUMO ($E_{LUMO}$) energies, and energy gap ($E_g$) for the structures under study, all energies in eV unit.

| **Structure** | $E_t$ | **DM** | $E_{FL}$ | **ϕ** | $E_{HOMO}$ | $E_{LUMO}$ | $E_g$ |
|---|---|---|---|---|---|---|---|
| **CC** | -56291.3 | 0.029 | -3.588 | 3.588 | -5.134 | -2.043 | 3.091 |
| **CC-1P** | -105767.8 | 0.392 | -2.563 | 2.563 | -3.121 | -2.006 | 1.115 |
| **CC-2P** | -138756.4 | 5.166 | -2.965 | 2.965 | -3.334 | -2.595 | 0.739 |
| **CC-3P** | -171746.9 | 2.198 | -3.159 | 3.159 | -3.446 | -2.872 | 0.574 |

**Table 2** All chemical indices were calculated, including the ionization potential ($IP$), electron affinity ($EA$), hardness ($H$), softness ($S$), and electronegativity ($\mu$) and electrophilicity ($\omega$), all indices in eV unit.

| **Structure** | $IP$ | $EA$ | $H$ | $S$ | $\mu$ | $\omega$ |
|---|---|---|---|---|---|---|
| CC | 5.134 | 2.043 | 1.545 | 0.324 | 3.588 | 4.166 |
| CC-1P | 3.121 | 2.006 | 0.557 | 0.897 | 2.563 | 5.895 |
| CC-2P | 3.334 | 2.595 | 0.370 | 1.353 | 2.965 | 11.893 |
| CC-3P | 3.446 | 2.872 | 0.287 | 1.742 | 3.159 | 17.378 |

**Table 3** The maximum absorption wavelength (λmax ), transition energy ($E_{opt}$), and oscillator strength (*f*) of these structures calculated by using time-dependent density-functional theory (TD-DFT) B3LYP/6-31G(d) for all structures.

| **Sample** | $\lambda max$ **(nm)** | $E_{opt}$ **(eV)** | $f$ |
|---|---|---|---|
| CC | 395.240 | 3.137 | 0.6106 |
| CC-1P | 1850.670 | 0.669 | 0.0000 |
| CC-2P | 8304.910 | 0.149 | 0.0003 |
| CC-3P | 7095.940 | 0.174 | 0.0002 |

The data in **Tables 1-3** provides a comprehensive comparison of various energy parameters and properties for circumcoronene (CC) and its phosphorus-doped structures (CC-1P to CC-3P). We can summarize and discuss the results as follows:

- **Total Energy**: The total energy becomes more negative with increasing phosphorus doping, indicating enhanced stability of the doped structures [39].
- **Dipole Moment (DM):** The dipole moment increases notably from 0.029 (CC) to 5.166 (CC-2P), then fluctuates with further doping. This reflects the asymmetric electronic charge

distribution induced by phosphorus impurities, which affects the molecule's polarization properties.

- **Fermi Level Energy**: There is a progressive decrease in the Fermi level energy from -3.588 (CC) to -2.563 (CC-1P). This indicates that phosphorus doping lowers the Fermi level, suggesting changes in the electronic density of states and potential shifts in electrical conductivity.
- **Energy Gap**: The energy gap decreases significantly with phosphorus doping, from 3.091 eV (CC) to 0.574 eV (CC-3P). This narrowing of the energy gap suggests that doping introduces mid-gap states or reduces the separation between the conduction and valence bands, enhancing electronic conductivity. Such behavior aligns with phosphorus's role as a dopant that modifies the electronic structure and creates localized electronic states.
- **Enhanced Conductivity**: The decrease in Fermi level energy and energy gap suggests that phosphorus-doped circumcoronene could exhibit higher electronic conductivity.
- **Chemical Reactivity**: Changes in electron affinity and softness suggest potential applications in sensing, where doping influences the interaction of the molecule with external species.
- **Optoelectronic Applications**: The reduction in the energy gap with phosphorus doping makes the system more suitable for optoelectronic devices that require materials with tunable electronic properties.
- **Ionization Potential:** Decreases with phosphorus doping, from 5.134 eV (CC) to 3.446 eV (CC-3P). Lower values indicate that doped structures require less energy to remove an electron, suggesting increased reactivity.
- **Electron Affinity**: Increases their values with doping reflects a greater ability to accept electrons, which enhances the electron-withdrawing properties of the system.
- **Hardness**: Decreases significantly with phosphorus doping, hardness suggests that the doped structures are more resistant to deformation in their electron clouds, indicating greater chemical stability.
- **Softness:** Shows an inverse trend. Lower softness values indicate reduced polarizability and less flexibility in electron distribution, consistent with increasing doping concentration.
- **Electronegativity:** Higher electronegativity indicates a stronger tendency to attract electrons, reflecting the influence of phosphorus atoms in altering the electron distribution.
- **Electrophilicity:** Increases sharply with doping, the dramatic rise in $\omega$ highlights the doped structures' enhanced ability to stabilize additional charges, making them more reactive in electrophilic interactions.
- **Maximum Absorption Wavelength:** The absorption wavelength increases significantly with doping, reaching up to 8304.910 nm for CC-2P, compared to 395.24 nm for pristine CC. This redshift suggests that doping introduces states that lower the energy required for electronic transitions, likely due to the creation of mid-gap states or significant changes in the molecular electronic structure [40].
- **Transition Energy:** The transition energy decreases dramatically with doping, from 3.137 eV (CC) to 0.149 (CC-2P). Lower transition energy indicates that less energy is required for electronic excitations in the doped structures.
- **Oscillator Strength:** Pristine CC has a moderate oscillator strength of 0.6106, but doping reduces significantly. For most doped structures, $f$=0.000 for (CC-1P). Low oscillator

strengths for doped structures suggest reduced probability of direct optical transitions in these systems. Doping introduces impurities or additional carriers into a material, altering its electronic structure and transition probabilities. This reduction can occur due to:

**(a) Increased Carrier Concentration**: Free carriers introduced by doping can screen the electric field associated with the optical transition, decreasing the probability of such transitions.

**(b)Changes in Band Structure**: Doping may lead to band filling (Pauli blocking) or modify the density of states, thereby reducing available states for transitions.

**(c) Non-Radiative Recombination**: Doping can increase defects or traps, which favor non-radiative over radiative recombination, indirectly affecting the oscillator strength.

It can note that the phosphorus doping increases both electron affinity and electrophilicity, making the doped systems more chemically active. Although reactivity increases, the rising hardness values suggest that doped circumcoronene systems are also chemically stable, with well-defined electronic structures. The systematic changes in indices such as ionization potential, hardness, and electrophilicity show that doping allows precise tuning of the chemical and electronic behavior of circumcoronene. Also, it is noted that the phosphorus doping systematically lowers the excitation energy levels, demonstrating its role in tuning the material’s electronic structure. The drastic reduction in oscillator strength with increased doping suggests that phosphorus impurities disrupt the symmetry of the electronic transitions, leading to less optically active states.

## 4. Conclusion

Phosphorus doping has a profound impact on the electronic and optical properties of circumcoronene. Key outcomes include enhanced stability, reduced energy gaps, and altered Fermi levels, making these doped systems promising candidates for applications in nanoelectronics, photonics, and energy devices. Phosphorus doping introduces significant changes to circumcoronene's chemical indices, making the material more reactive, stable, and suitable for applications requiring strong electron interaction capabilities. These findings have profound implications for designing materials in nanotechnology, such as catalysts, sensors, and energy-storage devices. By modifying the High-energy transitions with significant oscillator strength, the structures can be suitable for applications requiring absorption in the far-infrared or electronic devices with reduced optical loss. Phosphorus doping significantly shifts the optical properties of circumcoronene, as evidenced by extended absorption wavelengths, reduced transition energies, and diminished oscillator strengths. These modifications make phosphorus-doped circumcoronene highly adaptable for applications in infrared photodetection, optical sensors, and energy storage, while maintaining tunable electronic behavior for specific optoelectronic uses.

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