Sumer Journal for Pure Science (ISSN: 2790-7031)
2nd International Scientific Conference on Pure and Medical Sciences/University of Sumer 2024

Theoretical Investigation of Zinc Oxide Impurities Effect on The Electronic Properties of Circumcoronene

Alaa M. Khudhair[1]*, Hussein Ghafel Shakier [2], Ahmed. J. Almusawe[3]

[1]Department of Physics, College of Science, University of Sumer, Iraq
[2]Directorate of Education, Thi-Qar, Ministry of Education, Iraq
[3]Department of Physics, College of Science, University of Basrah, Iraq
*Corresponding author: alaa5alrikabi@gmail.com

Abstract

In this work, density functional theory (DFT) has been used to calculate the electronic properties of Circumcoronene (CC) and CC-doped by zinc oxide (ZnO). The doping produced five new structures regarding to ZnO position and number in CC structure. Result shows the electronic properties such as density of state (DOS), total energy(E_T), Fermi level energy (E_{FL}), E_{HOMO} , E_{LUMO}, and energy gap (E_g). The interesting result in this study was the (E_g) affected by the ZnO position in the CC structures, in another word it can controlled by the position and number of doping atom (ZnO). It's equal to 3.091 eV for pure CC structure and equal to 1.791 eV for one CC-ZnO, while its equal to 2.642 eV for CC-ZnO in another position, this difference gradient in (E_g) values represent an interesting result in addition to Circumcoronene properties which made it a promising material for many electronic applications such as nanoelectronics device, biosensors, and nanomedicine.

Keywords: ZnO, doping, Circumcoronene, DFT calculation, electronic properties.

دراسة نظرية لتأثير شوائب أوكسيد الزنك على الخواص الإلكترونية للسيركوم كورونين

علاء محسن خضير[1], حسين غافل شخير[2], احمد جواد الموسوي[3]

[1]قسم الفيزياء/ كلية العلوم / جامعة سومر / ذي قار/ العراق
[2]مديرية تربية ذي قار/ ذي قار / وزارة التربية / العراق
[3]قسم الفيزياء/ كلية العلوم / جامعة البصرة / البصرة/ العراق

الخلاصة

تم استخدام نظرية كثافة الدالة الوظيفية في حساب الخصائص الالكترونية لواحد من تراكيب الكاربون السطحية المعروفة باسم (circumcoronene) ومن ثم تم تطعيم هذا التركيب بأوكسيد الخارصين ZnO . تمت عملية التطعيم من خلال استبدال ذرتي كاربون في حلقة البنزين بواسطة ZnO ، ومن خلال تغيير موضع التطعيم في حلقة البنزين وأيضا من خلال مضاعفة عدد أوكسيد الخارصين ب 2ZnO ومن ثم ZnO انتجت هذه العملية خمسة تراكيب جديدة. تم حساب الخواص الالكترونية مثل كثافة الحالة، فجوة الطاقة ، الطاقة الكلية و طاقة مستوى فيرمي فضلا عن المعاملات الكيميائية مثل معامل الصلابة لجميع هذه التراكيب . بينت النتائج المتحصل عليها في هذه الدراسة ان هناك علاقة وثيقه بين فجوة الطاقة وموضع وعدد جزئية ZnO في حلقة البنزين. اذا كانت فجوة الطاقة لتركيب CC قبل عملية التطعيم مساوية الى 3.091 eV وبعد اجراء عملية التطعيم قلت لتصل الى 1.791 eV لتركيب ZnO-CC (الثالث) وتعتبر هذه نتيجة مثيرة للاهتمام اذ ان التحكم في فجوة الطاقة لهذه المركبات يجعلها ملائمة للعديد من التطبيقات والأجهزة والتي تعتمد بصورة مباشرة او غير مباشرة على قيمة فجوة الطاقة للتركيب مثل تطبيقات المتحسسات الحيوية النانوية وتطبيقات الأجهزة النانوية.

الكلمات المفتاحية: أكسيد الزنك، المنشطات، السيركومكورونين، حساب DFT، الخواص الإلكترونية.

1. Introduction

Graphene is one of the most studied nanoscale materials regarding to their electronic properties [1]. Graphene sheets have a high technological promise due to its ability to be overlap semi-metal (both electrons and holes carry a charge), it has sparked a lot of interest in a range of applications where high conductivity has been a barrier [2, 3]. It has a unique electrical band structure that is accentuated by the massless Dirac spectrum, resulting in remarkable physical properties. The zero-band gap problem, on the other hand, can be handled by breaking graphene into nanoribbons [4] or quantum dots (QDs), which minimizes the material's lateral dimensions [5]. Graphene quantum dots, or GQDs, are nanoparticles formed of graphene that are less than 100 nanometers in size [6]. Because of their low toxicity, persistent photoluminescence, chemical stability, and a large quantum confinement effect, GQDs are recognized as a unique material for usage in biological, optoelectronic, energy, and environmental applications [7, 8].

In order to operationalize materials composed of graphene, it is essential to manipulate the electronic characteristics of the material. Hetero atoms doping is a regularly employed method for manipulating electronic properties. The synthesis of nitrogen/boron-doped graphene via chemical vapor decomposition techniques has been documented [9] [10, 11]. The stability of modification in graphene structures has been the subject of extensive theoretical investigation [12]. The stability of nitrogen/boron-doped graphene, characterized by a uniform doping configuration, has been established under specific conditions. This is discernible through the structure of the electrons and symmetry of the doping configuration [13]. The charge transfer that occurs between the additives and the edge states explains the stabilization mechanism of heteroatom doping [16][17].

In this study, we investigated the electronic properties of Circumcoronene (CC). The electronic properties of pure and doped CC structure were studied, the doping done by replacing two carbon atoms by ZnO to produced CC-ZnO, and when change the ZnO position in the benzene ring which produced a new structure of CC with ZnO doped.

2. Theory and computational details

Gaussian 09 package program [18-20] used in this work with DFT method to investigate the electronic properties for all six structures. All the six CC structures optimized via unrestricted B3LYP / 6-31G level of the DFT [21-24]. It is widely known that the 6-31G core group performs effectively in engineering enhancements related with closed-shell organic compounds. So, for this reason it was selected as an option for utilization [25]. Before and after performing the energy calculations, all the atoms on CC structures with and without ZnO were given the opportunity to relax. the electronic and of CC including DOS resolution, total energies, highest energies of occupied molecular orbitals ((E_{HOMO}), Fermi level (E_{FL}), lowest energies of unoccupied molecular orbitals (E_{LUMO}), and bandgap (Eg) are studied for pure CC and new five structures.

The adaptability of CC as a material has been related to their ability to create and modify their properties via the management of their form and components. The chemical reactivity parameters, which in the context of the DFT include chemical hardness, chemical potential, and the electrophilicity index, are highly useful for analyzing toxicity, evaluating reactivity trend, and exploring excited states [26-28]. The following expressions can be used to define chemical potential and chemical hardness, respectively.

$$\boldsymbol{\eta = \frac{(IP - EA\,)}{2}} \tag{1}$$

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

$$\boldsymbol{\omega = \frac{\mu^2}{2\eta}} \tag{3}$$

It is possible to use Koopman's theorem to get an estimate of the ionization potential (IP) and the electron affinity (EA) [29, 30]:

$$\boldsymbol{IP = -E_{\mathrm{HOMO}}} \tag{4}$$

$$\boldsymbol{EA = -E_{\mathrm{LUMO}}} \tag{5}$$

where E_{HOMO} and E_{LUMO} are the energy levels of the HOMO and LUMO orbitals, respectively. In addition, we determine the electronic band gap and the Fermi level energy using the following formula [30-32]:

$$\boldsymbol{Eg = E_{\mathrm{LUMO}} - E_{\mathrm{HOMO}}} \tag{6}$$

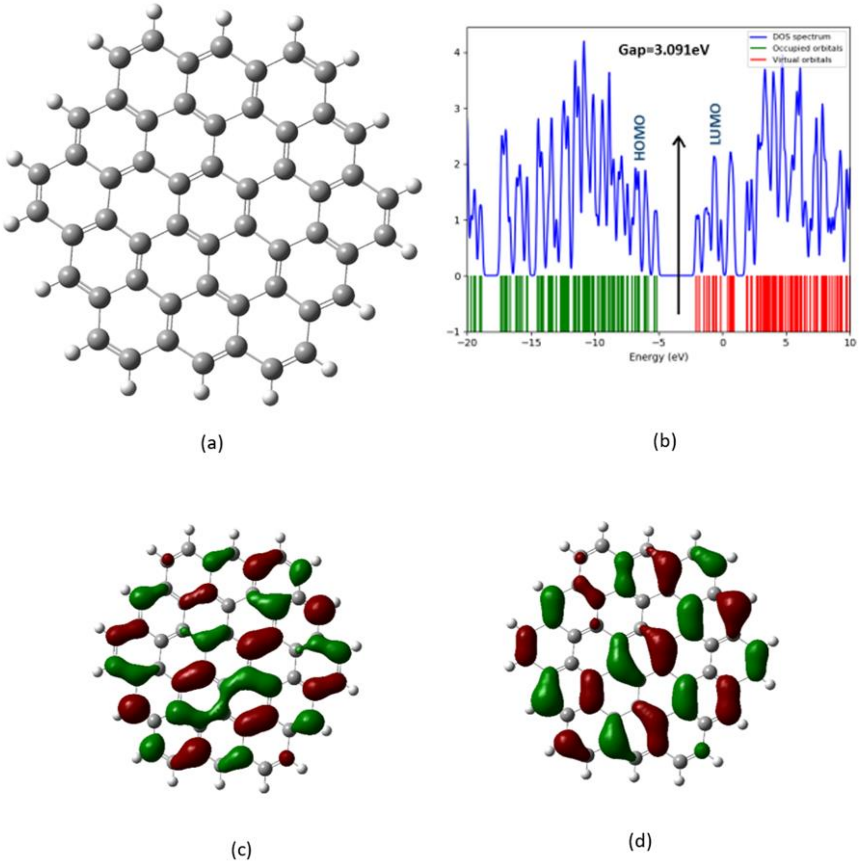
$$\boldsymbol{{}_{\mathrm{FL}} = (E_{\mathrm{HOMO}} + E_{\mathrm{LUMO}})\;/2} \tag{7}$$

To investigate the structural stability of the ZnO-codoped CC, the formation energies EF for all structures were also calculated [33-35]:

3. Results and discussion

3.1 The electronic properties

We investigated how ZnO impurities affect the geometrical and electrical characteristics of CC. The geometries of carbon-carbon (CC) structures with varying amounts of ZnO impurities in different positions are optimized using the B3LYP functional with a 6-31G (d) basis set. At first, a pure circumcoronene determined its lattice constant to be 2.43 Å, somewhat lower than the experimental measurement of 2.46 Å. We discovered that the bond length of C-C in CC is 1.43 Å, which matches the reference [36]. Additionally, the electronic density of states (DOS) and optimization geometry of PGNFs were examined, as illustrated in Figure 1.



(a) (b)

(c) (d)

Figure - 1 (a) Optimizations geometric and (b) DOS, (c) HOMO, and (d) LUMO of CC

After examining the pure characteristics of the CC, we analyzed the varying electrical properties of the CC with different levels of ZnO impurities. We begin our computation by examining the impact of a single ZnO impurity on the electronic characteristics. In terms of electronic characteristics, we observed that the electronic band gap is diminished, and the electronic DOS is altered in comparison to the immaculate case of the CC. As depicted in Figures 2–6 (b), relocating the location of the ZnO impurity in the CC yields a highly intriguing result. In accordance with the data depicted in Figures 2-6 (c and d), it can be observed that the LUMO has a lower value and fewer peaks than the HOMO. Total energy constitutes an additional noteworthy attribute. By exchanging the location of the S impurity in the pristine CC for the exchanged CC, we were able to decrease the total energy. As table 1 demonstrates, ZnO impurities at various sites decrease the total energy value of CC, resulting in increased stability and decreased reactivity.

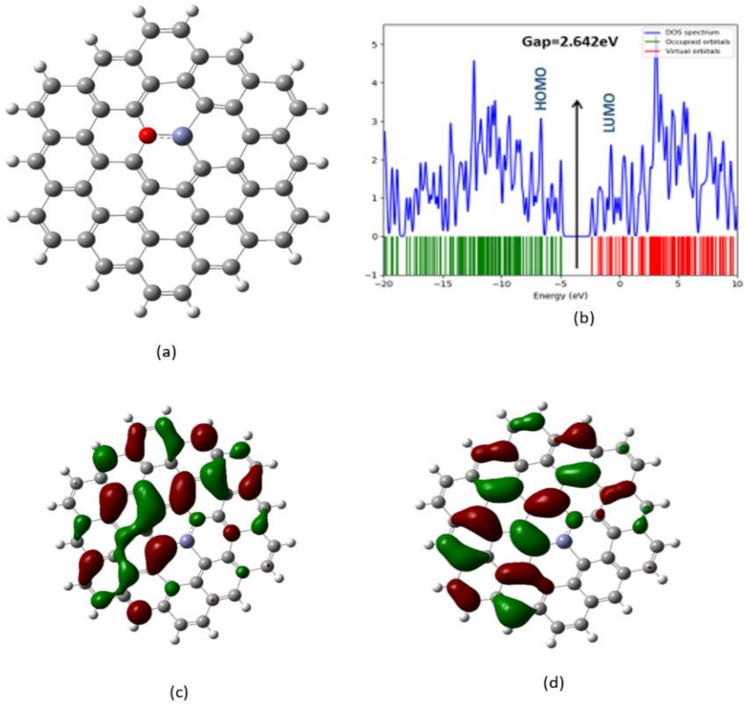


Figure - 2 (a) Optimizations geometric ZnO-doped CC, (b) DOS, (c) HOMO, and (d) LUMO

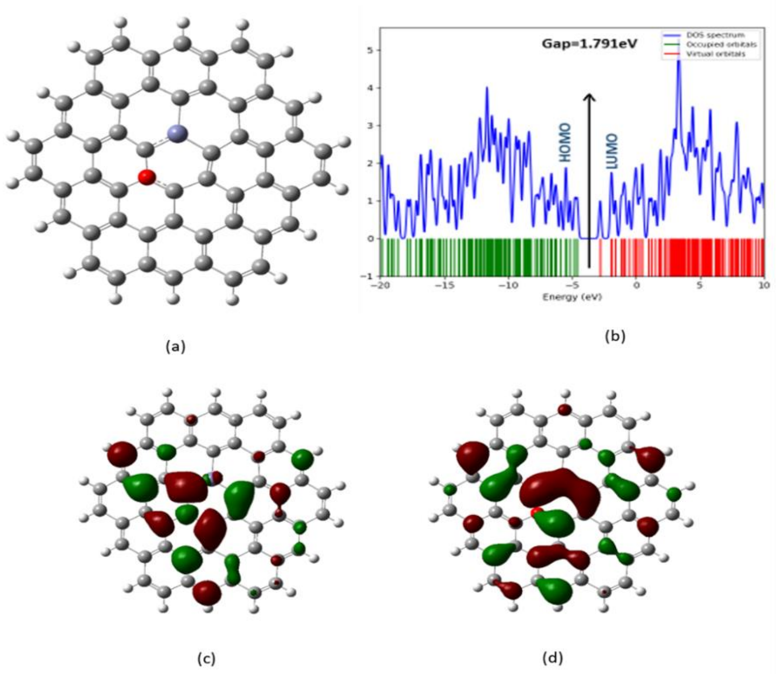
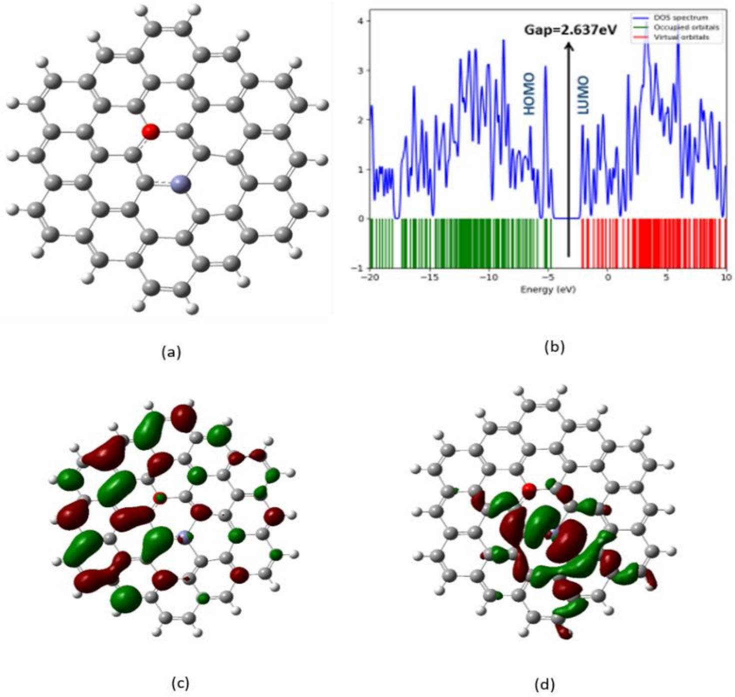


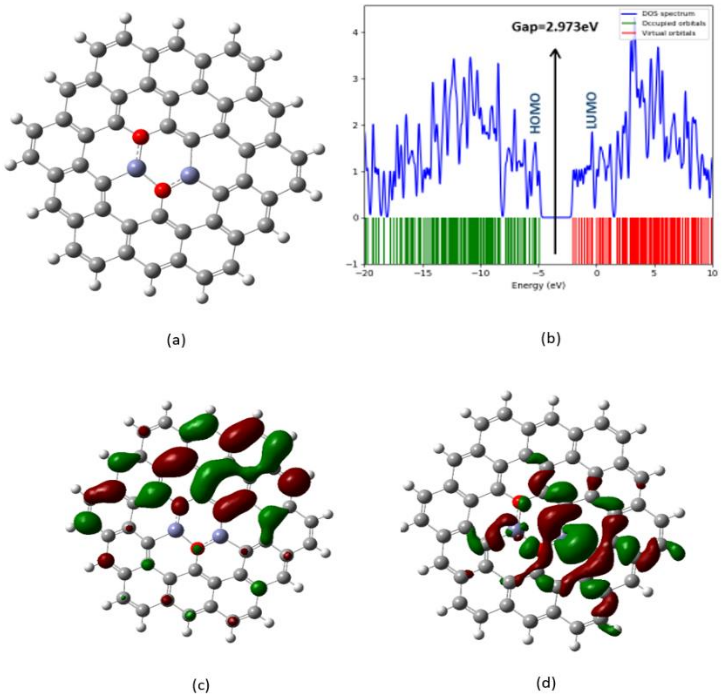
Figure - 3 (a) Optimizations geometric ZnO-doped CC, (b) DOS, (c) HOMO, and (d) LUMO



(a) (b)

(c) (d)

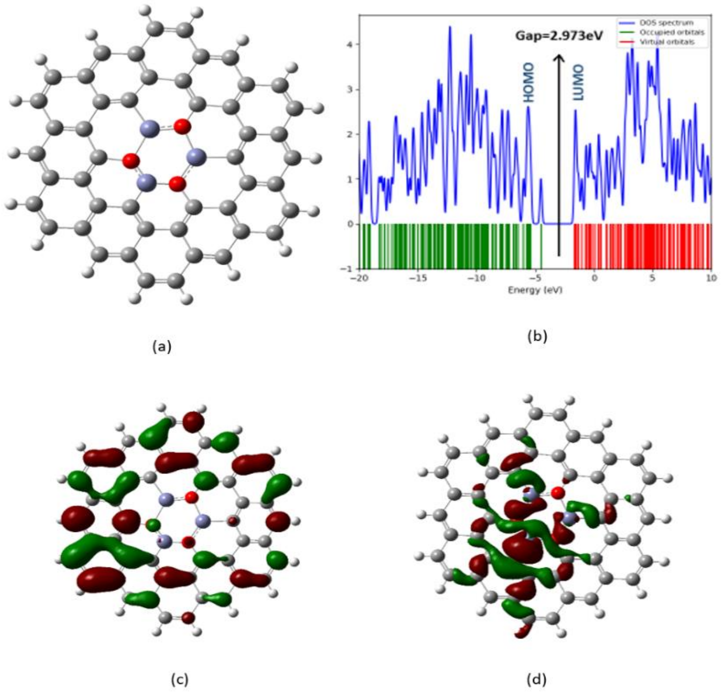
Figure - 4 (a) Optimizations geometric ZnO-doped CC, (b) DOS, (c) HOMO, and (d) LUMO



(a) (b)

(c) (d)

Figure - 5 (a) Optimizations geometric 2ZnO-doped CC, (b) DOS, (c) HOMO, and (d) LUMO



(a)

(b)

(c)

(d)

Figure - 6 (a) Optimizations geometric 3ZnO-doped CC, (b) DOS, (c) HOMO, and (d) LUMO.

The orbitals of molecules (MO) of ZnO-doped CC showed interaction with their border orbitals, including HOMO and LUMO. We discovered that the HOMO LUMO is destabilized, as seen in Figure (2-6) (c and d). Additionally, the relationship between the CC and ZnO impurity can be elucidated through the application of frontier molecular orbitals. In the event that the molecule acquires an unstable state, a higher value of the HOMO will result in increased reactivity; conversely, a lower value will render the molecule less reactive. The electrons are transmitted from the ZnO impurity to the CC as a consequence of the decrease in HOMO energy caused by the impurity. In order to validate our findings, we exchanged four carbon atoms for ZnO impurities in order to augment their concentrations. The findings corroborated our identification of ZnO impurity, as illustrated in Table 1. Thus, extremely exciting discoveries have been made. In addition to the concentrations of ZnO impurities, the location of specific ZnO impurities within the CC also influences the electronic properties of CC doped with ZnO at different concentrations.

Table 1- The values of the total energy (E_t), Dipole moment (DM), Fermi level energy (E_{fl}), Work Function (**ϕ**), $\boldsymbol{E_{HOMO}}$, $\boldsymbol{E_{LUMO}}$, and energy gap (E_g) in eV unit

Structure	E_t	DM	E_{fl}	ϕ	E_{HOMO}	E_{LUMO}	E_g
CC (Fig 1 (a))	-56291.363	0.029	-3.588	3.588	-5.134	-2.043	3.091
CC-ZnO (Fig 2 (a))	-104670.152	3.879	-3.621	3.621	-4.942	-2.301	2.642
CC-ZnO (Fig 3 (a))	-104665.244	6.229	-3.697	3.697	-4.593	-2.802	1.791
CC-ZnO (Fig 4 (a))	-104665.940	6.343	-3.426	3.426	-4.744	-2.108	2.637
CC-2ZnO (Fig 5 (a))	-153054.616	4.638	-3.454	3.454	-4.940	-1.967	2.973
CC-3ZnO (Fig 6 (a))	-201428.037	0.376	-3.062	3.062	-4.502	-1.622	2.880

3.2. Global reactivity descriptions

Our investigation revealed that the chemical activity of these structures is diminished in comparison to pure CC, as evidenced by their reduced chemical potential values (absolute values) as shown in Table 2. The Koopmans' theorem indicates that the HOMO and LUMO magnitudes are a good approximation of the negative experimental ionization potential (−IP) and negative electron affinity (−EA), respectively [4, 32]. Through the calculation of the Ionisation Potential (IP) and Electron Affinity (EA), it was shown that CC-3ZnO (Fig 6 (a)) has a greater tendency to donate an electron and form a cation in comparison to other structures, as it possesses a lower IP value. Additionally, CC-ZnO (Fig 3 (a)) has a greater capacity for accepting an electron due to its higher electron affinity value, as shown in Table 2. Furthermore, it has been observed that the pristine CC exhibits a greater ability for electron transfer in comparison to the other structures being investigated, owing to its higher H value. We observed that the separation between the valence and conduction bands in CC-ZnO (Fig 3 (a)) is considerably narrower than in other materials, as a result of the CC-ZnO's (Fig 3 (a)) higher S value. Additionally, we demonstrated that a minor interaction exists between pristine CC and different concentrations of ZnO impurities, as evidenced by the fact that the ω values of these structures (CC-2ZnO (Fig 5 (a) and CC-3ZnO (Fig 6 (a)) are lower than those of pristine CC, as shown in Table 2. And this behavior is similar to results in the reference [29].

Table 2- All chemical indices were calculated, including the ionization potential (IP), electron affinity (EA), hardness (H), softness (S), and electronegativity (μ) and electrophilicity (ω), in (eV) unit

Structure	IP	EA	S	H	μ	ω
CC (Fig 1 (a))	5.134	2.043	0.324	1.545	3.588	4.166
CC-ZnO (Fig 2 (a))	4.942	2.301	0.379	1.321	3.621	4.964
CC-ZnO (Fig 3 (a))	4.593	2.802	0.558	0.895	3.697	7.634
CC-ZnO (Fig 4 (a))	4.744	2.108	0.379	1.318	3.426	4.451
CC-2ZnO (Fig 5 (a))	4.940	1.967	0.336	1.486	3.454	4.013
CC-3ZnO (Fig 6 (a))	4.502	1.622	0.347	1.440	3.062	3.256

4. Conclusion

In this paper we study the ground state electronica properties of pure Circumcoronene (CC) and CC doped by zinc oxide using density functional theory calculations. The results show the position of ZnO has been affect to the electronic properties of curcumin. It was demonstrated that the antiaromatic structure of meta ZnO contributes to the low band gap. In contrast, the band gap of ortho and para ZnO is modest, with the band gap of the para ZnO structure being lower than that of the ortho ZnO structure. In addition, the presence of zinc oxide has been observed to affect the global chemical markers of CC. The HOMO-LUMO gap is dramatically changed as a result of the HOMO, Fermi and LUMO levels of the systems being pushed to higher energies. This change is critical in many applications because a simple shift in the band gap can change the electrical conductivity. Finally, we can control the electronic properties CC by doping by zinc oxide at different position and number of doping atoms.

Reference

[1] M. H. Al-Abboodi, F. N. Ajeel, and A. M. Khudhair, "Influence of oxygen impurities on the electronic properties of graphene nanoflakes," *Physica E: Low-dimensional Systems and Nanostructures,* vol. 88, pp. 1-5, 2017.

[2] M. H. Mohammed, F. N. Ajeel, and A. M. Khudhair, "Adsorption of gas molecules on graphene nanoflakes and its implication as a gas nanosensor by DFT investigations," *Chinese journal of physics,* vol. 55, no. 4, pp. 1576-1582, 2017.

[3] A. Silva, M. Pires, V. Freire, E. Albuquerque, D. Azevedo, and E. Caetano, "Graphene nanoflakes: thermal stability, infrared signatures, and potential applications in the field of spintronics and optical nanodevices," *The Journal of Physical Chemistry C,* vol. 114, no. 41, pp. 17472-17485, 2010.

[4] F. Ajeel, A. Khudhair, M. Mohammed, and K. M. Mahdi, "DFT investigation of graphene nanoribbon as a potential nanobiosensor for tyrosine amino acid," *Russian Journal of Physical Chemistry A,* vol. 93, pp. 778-785, 2019.

[5] F. P. García de Arquer, D. V. Talapin, V. I. Klimov, Y. Arakawa, M. Bayer, and E. H. Sargent, "Semiconductor quantum dots: Technological progress and future challenges," *Science,* vol. 373, no. 6555, p. eaaz8541, 2021.

[6] C. Cheng, S. A. Iyengar, and R. Karnik, "Molecular size-dependent subcontinuum solvent permeation and ultrafast nanofiltration across nanoporous graphene membranes," *Nature Nanotechnology,* vol. 16, no. 9, pp. 989-995, 2021.

[7] Y. R. Kumar, K. Deshmukh, K. K. Sadasivuni, and S. K. Pasha, "Graphene quantum dot based materials for sensing, bio-imaging and energy storage applications: a review," *RSC advances,* vol. 10, no. 40, pp. 23861-23898, 2020.

[8] T. D. Thangadurai, N. Manjubaashini, D. Nataraj, V. Gomes, and Y. I. Lee, "A review on graphene quantum dots, an emerging luminescent carbon nanolights: Healthcare and Environmental applications," *Materials Science and Engineering: B,* vol. 278, p. 115633, 2022.

[9] S. Chung, R. A. Revia, and M. Zhang, "Graphene quantum dots and their applications in bioimaging, biosensing, and therapy," *Advanced Materials,* vol. 33, no. 22, p. 1904362, 2021.

[10] S. Miao, K. Liang, J. Zhu, B. Yang, D. Zhao, and B. Kong, "Hetero-atom-doped carbon dots: Doping strategies, properties and applications," *Nano Today,* vol. 33, p. 100879, 2020.

[11] Y.-B. Tang *et al.*, "Tunable band gaps and p-type transport properties of boron-doped graphenes by controllable ion doping using reactive microwave plasma," *Acs Nano,* vol. 6, no. 3, pp. 1970-1978, 2012.

[12] J. Rawal, U. Kamran, M. Park, B. Pant, and S.-J. Park, "Nitrogen and Sulfur Co-Doped Graphene Quantum Dots Anchored TiO2 Nanocomposites for Enhanced Photocatalytic Activity," *Catalysts,* vol. 12, no. 5, p. 548, 2022.

[13] S. A. Kulkarni, N. Yantara, K. S. Tan, N. Mathews, and S. G. Mhaisalkar, "Perovskite nanostructures: leveraging quantum effects to challenge optoelectronic limits," *Materials Today,* vol. 33, pp. 122-140, 2020.

[14] D. Hoat *et al.*, "Opening the germanene monolayer band gap using halogen atoms: An efficient approach studied by first-principles calculations," *Applied Surface Science,* vol. 551, p. 149318, 2021.

[15] A. Chaves *et al.*, "Bandgap engineering of two-dimensional semiconductor materials," *npj 2D Materials and Applications,* vol. 4, no. 1, p. 29, 2020.

[16] F. N. Ajeel, K. H. Mohsin, H. G. Shakier, S. K. Khamees, and M. N. Mutier, "Theoretical insights into tunable electronic properties of graphene quantum dots through ZnO doping," *Chemical Physics Impact,* vol. 7, p. 100305, 2023.

[17] A. K. Bhardwaj, A. Kant, A. Rehalia, V. Singh, and R. Sharma, "A review on nanomaterials for drug delivery systems and application of carbon based nanomaterials," *ES Materials & Manufacturing,* vol. 21, p. 824, 2023.

[18] F. N. Ajeel, A. M. Khudhair, and A. A. Mohammed, "Density functional theory investigation of the physical properties of dicyano pyridazine molecules," *Int. J. Sci. Res,* vol. 4, no. 1, pp. 2334-2339, 2015.

[19] F. N. Ajeel, M. H. Mohammed, and A. M. Khudhair, "Effects of lithium impurities on electronic and optical properties of graphene nanoflakes: A DFT–TDDFT study," *Chinese Journal of Physics,* vol. 58, pp. 109-116, 2019.

[20] F. N. Ajeel, M. H. Mohammed, and A. M. Khudhair, "SWCNT as a model nanosensor for associated petroleum gas molecules: via DFT/B3LYP investigations," *Russian Journal of Physical Chemistry B,* vol. 13, pp. 196-204, 2019.

[21] F. N. Ajeel, M. H. Mohammed, and A. M. Khudhair, "Tuning the electronic properties of the fullerene C 20 cage via silicon impurities," *Russian Journal of Physical Chemistry B,* vol. 11, pp. 850-858, 2017.

[22] F. N. Ajeel, M. H. Mohammed, and A. M. Khudhair, "Energy bandgap engineering of graphene nanoribbon by doping phosphorous impurities to create nano-heterostructures: A DFT study," *Physica E: Low-dimensional Systems and Nanostructures,* vol. 105, pp. 105-115, 2019.

[23] M. H. Mohammed, F. N. Ajeel, and A. M. Khudhair, "Analysis the electronic properties of the zigzag and armchair single wall boron nitride nanotubes with single Li impurity in the various sites," *Journal of Electron Spectroscopy and Related Phenomena,* vol. 228, pp. 20-24, 2018.

[24] A. Alrikabi, "Theoretical study of the design dye-sensitivity for usage in the solar cell device," *Results in physics,* vol. 7, pp. 4359-4363, 2017.

[25] A. M. Khudhair, F. N. Ajeel, and M. H. Mohammed, "Engineering and design of simple models from dye-sensitive of solar cells and photovoltaic cells applications: Theoretical study," *Chemical Physics Letters,* vol. 713, pp. 166-171, 2018.

[26] A. M. Khudhair and A. Ben Ahmed, "Pure and Stone-Wales Defect Armchair Boron Nitride Graphene Nanoribbons as Anticancer Drug Delivery Vehicles: A Theoretical Investigation," *Journal of Cluster Science,* pp. 1-10, 2023.

[27] M. H. Mohammed, F. N. Ajeel, S. H. Mohammed, A. M. Khudhair, and F. H. Hanoon, "Engineering and controlling the electronic properties of zigzag and armchair boron nitride nanotubes with various concentrations of oxygen impurities," *Chinese Journal of Physics,* 2023.

[28] A. M. Khudhair and A. B. Ahmed, "Utilizing Circumcoronene and BN Circumcoronene for the delivery and adsorption of the anticancer drug floxuridine," *Computational and Theoretical Chemistry,* vol. 1222, p. 114075, 2023.

[29] F. N. Ajeel, Y. W. Ouda, and A. M. Khudhair, "Graphene Nanoflakes as a New Nanobiosensor for Histidine Amino Acid in Fish with Gas, Ethanol, DMSO and Water Environment," *Journal of Basrah Researches (Sciences),* vol. 45, no. 2A, 2019.

[30] A. M. Khudhair and A. Ben Ahmed, "Anticancer drugs delivery and adsorption computations in pure and Stone–Wales defect armchair graphene nanoribbons," *Optical and Quantum Electronics,* vol. 55, no. 9, p. 812, 2023.

[31] A. M. Khudhair, M. H. Mohammed, F. N. Ajeel, and S. H. Mohammed, "Enhancement the electronic and optical properties of the graphene nanoflakes in the present S impurities," *Chemical Physics Impact,* vol. 6, p. 100154, 2023.

[32] F. Nimr Ajeel, A. Mohsin Khuodhair, and S. Mahdi AbdulAlmohsin, "Improvement of the optoelectronic properties of organic molecules for nanoelectronics and solar cells applications: via DFT-B3LYP investigations," *Current Physical Chemistry,* vol. 7, no. 1, pp. 39-46, 2017.

[33] F. N. Ajeel, K. H. Bardan, S. H. Kareem, and A. M. Khudhair, "Pd doped carbon nanotubes as a drug carrier for Gemcitabine anticancer drug: DFT studies," *Chemical Physics Impact,* vol. 7, p. 100298, 2023.

[34] F. N. Ajeel, M. H. Mohammed, and A. M. Khudhair, "Electronic, thermochemistry and vibrational properties for single-walled carbon nanotubes," *Nanoscience & Nanotechnology-Asia,* vol. 8, no. 2, pp. 233-239, 2018.

[35] A. M. Khudhair, F. N. Ajeel, and M. H. Mohammed, "Theoretical Study of the Electronic and Optical Properties to Design Dye-Sensitivity for Using in Solar Cell Device," *Russian Journal of Physical Chemistry B,* vol. 12, pp. 645-650, 2018.

[36] A. G. Garcia, S. E. Baltazar, A. H. R. Castro, J. F. P. Robles, and A. Rubio, "Influence of S and P doping in a graphene sheet," *Journal of Computational and Theoretical Nanoscience,* vol. 5, no. 11, pp. 2221-2229, 2008.