Sumer Journal for Pure Science (ISSN: 2790-7031)

nd International Scientific Conference on Pure and Medical Sciences/University of Sumer 20242

Investigating the Effects of TiO Impurities on the Electronic Properties of Graphene Nanoflakes Using DFT Method

Mustafa K. Salman[1], Noora B. Shwayyea[2], Fouad N. Ajeel[3,*], Alaa M. Khudhair[4]

[1,2,3,4] Department of Physics, College of Science, University of Sumer, Iraq

***Corresponding author:** fouadnimr2@gmail.com

Abstract

Modifying the electronic characteristics of produced graphene allows for the creation of nanoelectronics devices, which are essential for a wide variety of applications. Through the process of chemical doping, graphene nanoflake (GNF) with electronic properties that can be tuned may be successfully produced. We utilised the density function theory (DFT) approach to investigate the GNF with and without various dopants of TiO dimers. This was done because we believed that we might potentially produce electronic characteristics in a GNF by altering the geometrical arrangement of the TiO dimers. In order to create the three different types of TiO dimers, ortho, meta, and para position dimers of titanium and oxygen atoms are used. It has been found that the presence of TiO dimers has a considerable influence on the bandgap values achieved by the GNF structure. According to the findings that we obtained, the electronic characteristics of the GNF are affected by both the arrangement of the TiO dimers that are included inside the GNF and the total amount of GNF dimers that are present.

Keywords: Graphene nanoflake; Electronic properties; DFT; Energy gap; Chemical doping.

دراسة تأثير شوائب TiO على الخواص الالكترونية لرقائق الكرافين النانوية بأستخدام طريقة DFT

مصطفى كاظم سلمان[1]، نوره بلبول شويع[2] ، فؤاد نمرعجيل[3,*] ، علاء محسن خضير[4]

[1,2,3,4] جامعة سومر – كلية العلوم – قسم الفيزياء

الخلاصة

ان إمكانية تعديل الخصائص الإلكترونية للكرافين المستخدم لصناعة الأجهزة إلالكترونية نانوية تعتبر عملية ضرورية لمجموعة واسعة من التطبيقات. فمن خلال عملية التنشيط الكيميائية، يمكن إنتاج رقاقات الكرافين النانوية (GNF) ذات الخصائص الإلكترونية التي يمكن ضبطها. استخدمنا نظرية الدالة الوظيفية للكثافة (DFT) للتحقيق في الخواص الالكترونية لـ GNF مع وبدون شوائب ثنائيات TiO. تم ذلك لأننا نعتقد امكانية أن ننتج خصائص إلكترونية في GNF عن طريق تغيير الترتيب الهندسي لثنائيات TiO. ومن أجل إنشاء ثلاثة أنواع مختلفة من ثنائيات TiO، تم استخدام ثنائيات أورثو ortho، ميتا meta، وبارا para الموضعية لذرات التيتانيوم والأكسجين. لقد وجد أن وجود ثنائيات TiO له تأثير كبير على قيم فجوة النطاق التي يحققها هيكل GNF. وفقًا للنتائج التي حصلنا عليها، تتأثر الخصائص الإلكترونية لـ GNF بكل من بوجود وترتيب ثنائيات TiO المضمنة داخل GNF

.

الكلمات المفتاحية: رقاقة الكرافين النانوية؛ الخصائص الإلكترونية؛ فجوة الطاقة؛ المنشطات الكيميائية.

1. Introduction

Graphene has been thoroughly researched by several scientists in recent years due to its favorable characteristics and its uses. Graphene's great carrier movement, saturate velocity, and lengthy spin diffusing length have opened up opportunities for creating advanced electronics and spintronics using graphene [1-8]. However, insufficient energy in the form of a band gap renders graphene unsuitable for use in transistor applications. Creating a limitless energy gap in graphene can be accomplished by reducing the material to graphene nanoflakes [9]. The characteristics of graphene nanoflakes may be significantly affected by their forms, sizes, and peripheral circumstances [10-16]. Therefore, it is critical to investigate the manner in which these variables influence the characteristics of graphene nanoflakes in order to maximize the encouraging prospects of graphene in the fields of electronic and spintronics. GNFs' features make them ideal for future electronics and spintronics devices, which need nanoscale materials to maximize performance while remaining compact. GNFs are often employed in current nanotechnology because to their rational, repeatable, predictable, and stable nature [11, 15, 17].

Various studies have studied ways to control the band gap energy. As the size of a graphene cluster increases, the band gap energy decreases [18]. Doping and functionalizing GNFs may result in significant modifications to their optoelectronic properties [19, 20]. Chemical doping is a potential strategy to enhance the electronic characteristics of graphene nanoflakes (GNFs) and is recognized as one of the most effective approaches to manipulate and design the electronic properties for two-dimensional nanomaterials [21]. Different levels of impurity concentration resulted in the emergence of mid-gap states in the DOS and, at sufficient concentrations, a transition from semiconductor to semimetal behavior. Furthermore, the electron thermal conductivity of monolayer hydrogenated graphene is influenced by both a diluted charged impurity and a magnetic field that surrounds it. The behavior of the hydrogenated graphene was altered to semiconducting by the impurity and the magnetic field, and the electronic band gap was decreased as a result of the symmetry disruption [22].

In this work, we employed first-principles DFT simulations to investigate the impact of TiO doping on the structural and electronic characteristics of graphene nanoflakes. Three varieties of TiO have been identified: ortho, meta, and para. The goal is to identify the structure that is the most stable among them. To design the desired electronic properties, substitutional impurities may be introduced into the system.

2. Theory and Computational Methods

Studying the electronic characteristics of graphene ($C_{24}H_{12}$), which includes a 7-benzene ring in its structure, is what we are attempting to accomplish here. The $C_{24}H_{12}$ structure was optimized at B3LYP and 3-21G levels using the DFT in Gaussian package 09. The electronic properties of GNFs. All of the atoms on GNFs, both with and without TiO_2, were given time to unwind both before and after the energy computations. Electronic attributes include bandgap (Egap), Fermi level (EFL), lowest energies of unoccupied molecular orbitals (ELUMO), highest energies of occupied molecular orbitals (EHOMO), total energies, and DOS resolution. Another highly useful tool for examining reactivity patterns and excited states is the density functional theory (DFT), which also contains the chemical reactivity parameters [3, 8, 16, 23-26]. These parameters, which were determined for graphene nanoflakes with and without TiO2 dimers, included chemical hardness (η), chemical softness (S), chemical potential (μ), and electrophilicity (ω). The versatility of graphene nanofibers (GNFs) as a material has been ascribed to the capacity to engineer and modify their characteristics by adjusting their structure and constituent parts. The chemical reactivity metrics, such as chemical hardness η, chemical potential μ, and the electrophilicity index ω, are highly useful within the context of the DFT for evaluating excited states and reactivity trends [27]. The following definitions of chemical potential and chemical hardness can be used to express these parameters, which can be given by [12, 15, 28, 29]:

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

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

$$S = \frac{1}{2\eta} \tag{3}$$

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

Koopman's theorem, which provides the following formula, can be used to compute both the ionization potential (IP) and the electron affinity (EA). [8, 23, 25, 30]:

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

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

Furthermore, we compute the electronic band gap and the Fermi level energy using the following formula [31-34]:

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

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

In order to examine the structural stability of the TiO_2-codoped GNFs, the cohesive energy per atom (E_{coh}) is calculated by subtracting the energy of the individual atom from the total energy per atom of the nanoribbons system by:

$$E_{\mathrm{coh}} = \frac{(E_{atom} - E_{\mathrm{tot}})}{n} \tag{9}$$

where E_{tot} is the total energy of the nanoribbon and n is the number of atoms of the structure [35, 36].

3. Results and discussions

The analysis of figure 1(a) indicates the presence of a 7-benzene ring in pure graphene nanoflakes, characterized by a typical C-C bond length of approximately 1.42 Å. This observation aligns with values reported in previous articles, reinforcing the consistency of the findings. To comprehensively understand changes in the electronic characteristics of pure graphene nanoflakes (GNFs), it is crucial to conduct a density of states (DOS) analysis both before and after the substitution of carbon atoms with TiO dimers.

In Figure 1(b), the density of states investigation for pure GNFs is presented, revealing an energy gap of 4.20 eV. This energy gap, representing the difference between the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO), is indicative of semiconductor characteristics, aligning with references that associate a large energy gap with semiconductor materials. The computation of harmonic vibrational frequencies further confirms the stability of the structure, as the presence of such frequencies on the potential energy surface signifies a stationary state.

The primary objective of this study is to explore the impact of introducing TiO dimers at various locations on the electronic properties of GNFs. Four assumed forms of Titanium oxide dimers are illustrated in Figure 2: (a) Ti and O atoms fixed at the ortho position (TiO-1); (b) Ti or O atoms positioned close to other atoms in the meta position (TiO-2); (c) Ti and O at the para-position (TiO-3); and (d) TiO pair at the ortho position with a significant gap between two TiO pairs (TiO-4).

This investigation aims to elucidate how these different configurations of TiO dimers influence the electronic characteristics of GNFs. The assumptions set the stage for a comprehensive exploration, shedding light on potential variations in the electronic structure and paving the way for a deeper understanding of the interactions between graphene nanoflakes and TiO dimers.

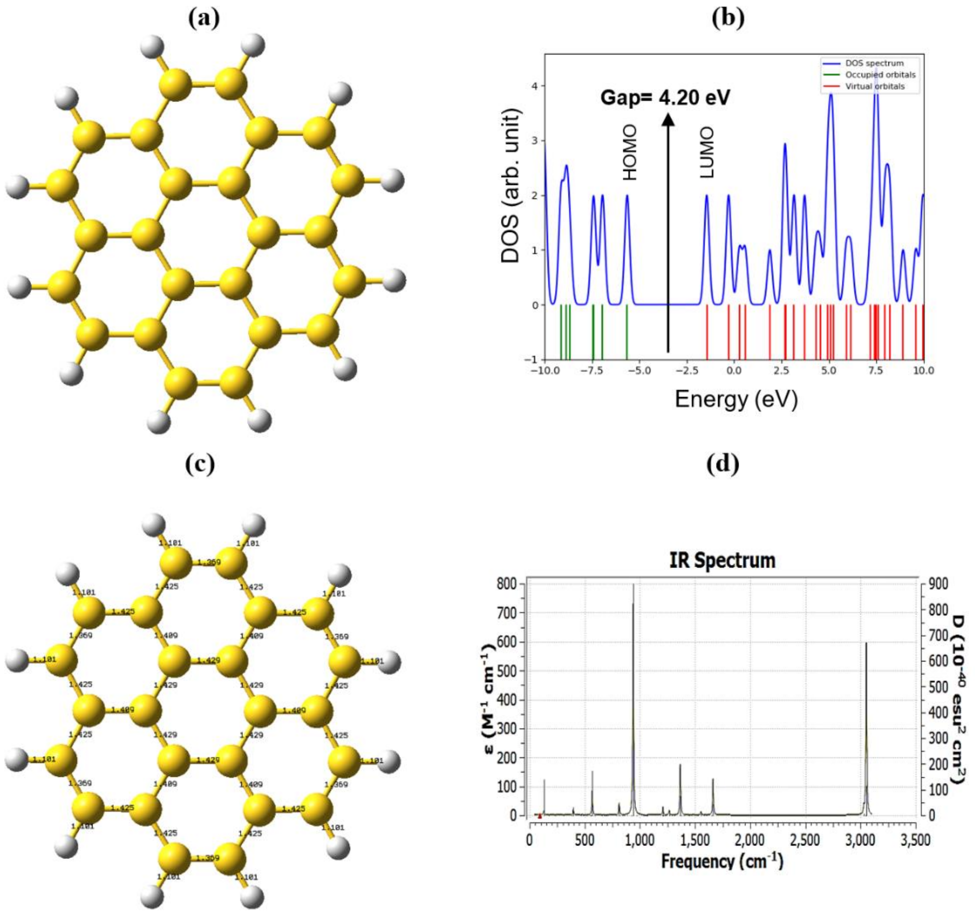
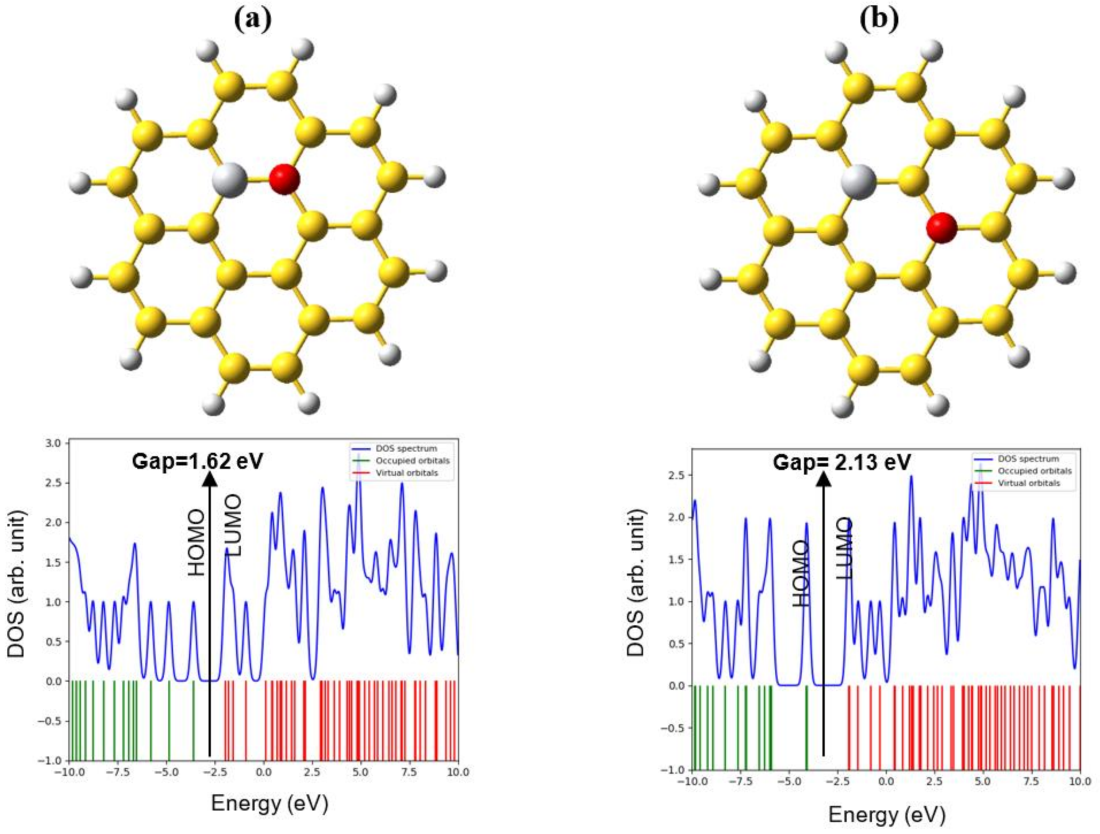


Figure -1 (**a**) Pure graphene nanoflakes, (**b**) The density of state, (**c**) Both the bond lengths and the structured geometries, and (**d**) Gas-phase molecular electrostatic potential

The study has revealed notable alterations in the gaps between the valence and conduction bands, as well as changes in the electronic density of states (DOS), upon the introduction of TiO impurities into graphene nanoflakes (GNFs). Furthermore, it was observed that the DOS diagrams and the electronic energy gap (Eg) undergo modifications when the positions of TiO impurities are varied, while the concentrations remain constant.

In particular, shifts in the positions of Ti and O atoms within GNF structures result in a significant change in the energy gap, transitioning from -74.777% to -84.658%. This shift holds relevance in various scenarios, indicating a sensitivity of the electronic structure to the spatial arrangement of TiO impurities within the graphene matrix.

The findings suggest a compelling potential for transforming GNF into a semiconductor with a reduced energy gap through the intentional doping of its structures with TiO dimers. By strategically incorporating TiO impurities, the energy gap can be diminished, paving the way for the engineering of GNFs with specific electronic properties. This insight opens avenues for tailoring the electronic characteristics of graphene-based materials through controlled doping processes, offering possibilities for applications in semiconductor devices and beyond.



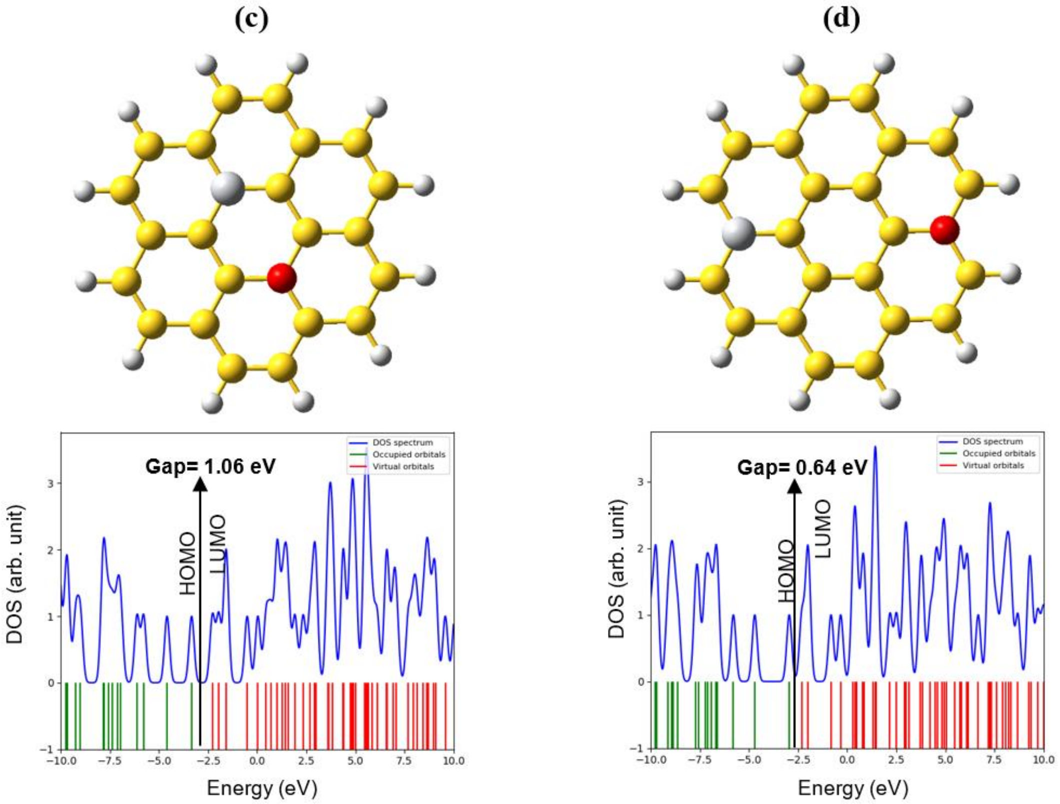


Figure -2 Shows the graphene nanoflakes configurations with TiO dimers generating the following structures: (**a**) TiO-1, (**b**) TiO-2, (**c**) TiO-3, and (**d**) TiO-4, along with their density of state

The incorporation of Titanium and oxygen atoms into graphene nanoflakes (GNFs) through the process of substitutional doping unveils a multitude of newly formed bonds, accompanied by substantial alterations in bond lengths. When arranged in descending order from longest to shortest bond length, the average bond lengths follow the sequence: C-C > Ti-C > Ti-O > C-O. This ordering of bond lengths underscores the significant impact of Titanium and oxygen incorporation on the structural characteristics of GNFs. The introduction of TiO dimers through doping disrupts the sublattice symmetry, leading to a distortion in bond lengths. As a result, the electronic properties of GNFs undergo a noteworthy transformation, particularly when subjected to high concentration ratios of titanium oxide dimers.

The observed distortion-induced asymmetry in the sublattice structure contributes to the overall modification of GNFs' electronic properties. This insight into the relationship between structural changes and electronic characteristics offers valuable information for understanding and potentially engineering the electronic behavior of graphene-based materials through controlled doping processes. In addition, for the lowest energy structures, vibrational calculations were performed inside the harmonic approximation to confirm the identification of local minima and as a measure of structural stability; the results showed positive values, as shown in Fig. 4.

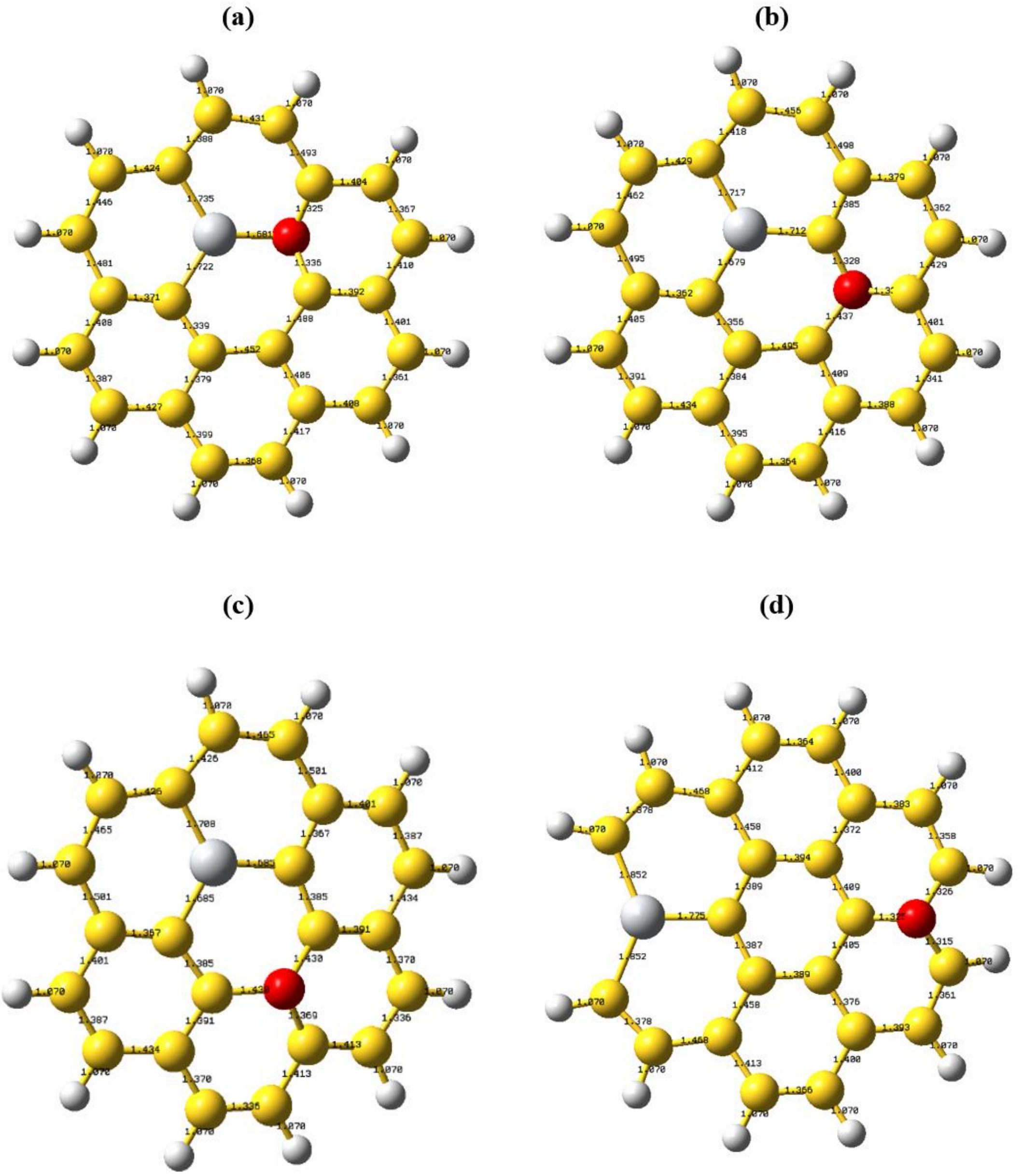


Figure -3 Bond lengths (in Å unit) and structured geometries of a graphene nanoflake with TiO dimers creating the structures: TiO-1, TiO-2, TiO-3, and TiO-4

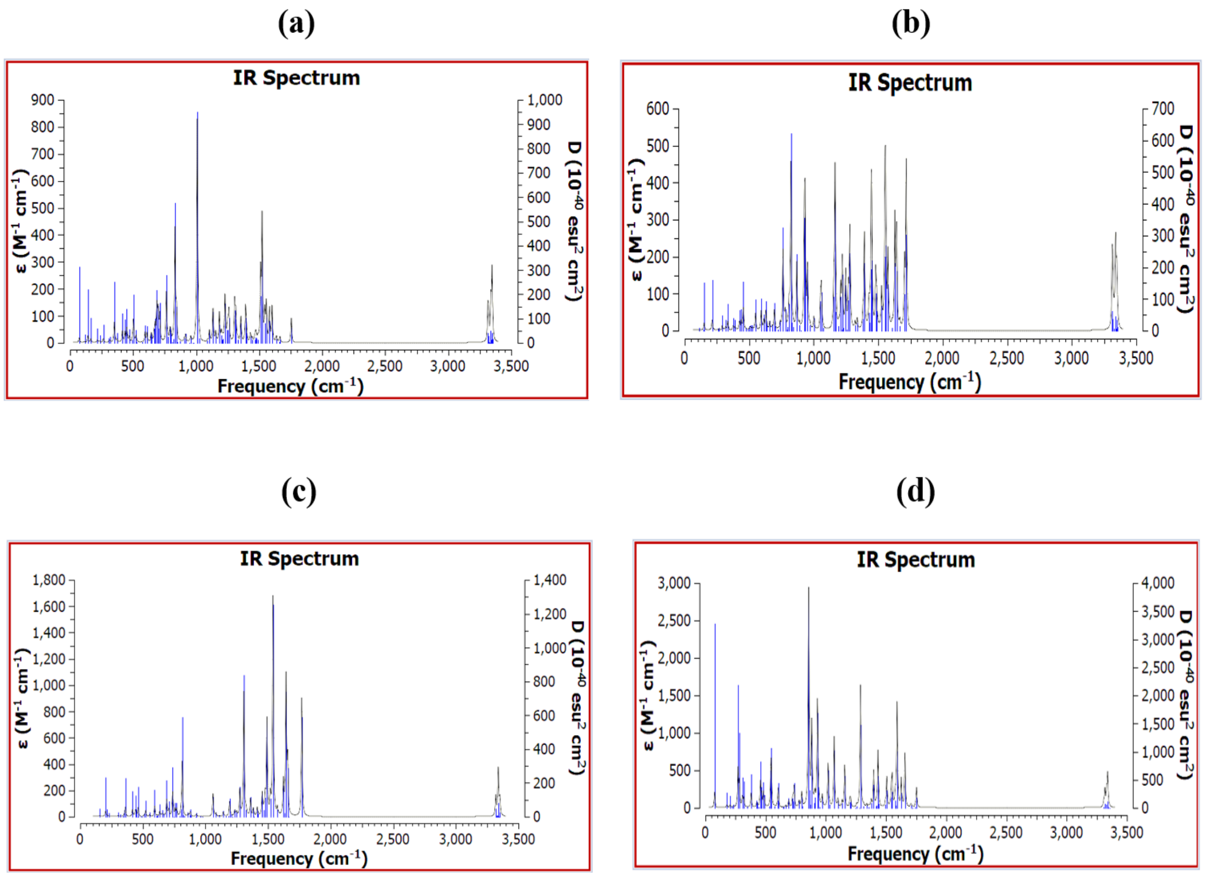


Figure -4 The vibrational spectrum for a graphene nanoflake with TiO dimers creating the structures: TiO-1, TiO-2, TiO-3, and TiO-4

Table 1 provides a comprehensive set of computed data on the energetic state, encompassing key parameters for both graphene nanoflakes (GNFs) with and without TiO dimers. The parameters include the highest occupied molecular orbital energies (EHOMO, eV), Fermi level energy (EFL, eV), lowest unoccupied molecular orbital energies (ELUMO, eV), band gap (Eg, eV), change in band gap (ΔEg), and cohesive energy (Ecoh, eV).

In the absence of TiO dimers, the HOMO and LUMO energies for pure GNF are reported as -5.644 and -1.445 eV, respectively, based on the molecular orbital frontier analysis. Figure 4 visually depicts the gradual increase in these values upon the introduction of Titanium oxide dimers. The data in Table 1 not only highlight the alteration in the band gap (Eg) but also emphasize changes in the Fermi level energy (EFL). Importantly, this influence results in an increase in the work function, a critical factor in applications involving field emission.

Table 1- The HOMO energies (E_{HOMO}), Fermi level energy (E_{FL}), LUMO energies (E_{LUMO}), energy gap (E_g), change of E_g (ΔE_g) and cohesive energy (E_{coh}) for graphene nanoflakes with and without TiO dimers. For all above energies, the eV unit is used

System	E_{HOMO}	E_{FL}	E_{LUMO}	E_{g}	ΔE_{g} (%)	E_{coh}
GNF Pure	-5.644	-3.544	-1.445	4.20	-	-7.53
(TiO-1)-codoped GNF	-3.595	-2.783	-1.972	1.62	-61.340	-2.74
(TiO-2)-codoped GNF	-4.052	-2.985	-1.918	2.13	-49.191	-2.60
(TiO-3)-codoped GNF	-3.337	-2.808	-2.278	1.06	-74.777	-2.58
(TiO-4)-codoped GNF	-2.950	-2.628	-2.305	0.64	-84.658	-2.64

The observed shifts in these energetic parameters underscore the impact of TiO dimers on the electronic structure of GNFs. The changes in band gap and Fermi level energy have implications for the material's conductivity and electronic behavior, with potential ramifications for applications such as field emission devices. These findings contribute valuable insights into the tailored modification of graphene nanoflakes through the controlled introduction of Titanium oxide dimers, enabling the fine-tuning of their electronic properties for specific applications.

In the examination of reactivity descriptors presented in Table 2, Koopman's theorem is employed to analyze characteristics such as ionization potential, electron affinity, electronegativity, chemical hardness, chemical softness, and electrophilicity. These descriptors play a crucial role in understanding reactivity trends, excited states, and toxicity assessment.

Koopman's theorem posits that the highest occupied molecular orbital (HOMO) energy is closely related to the experimentally determined negative ionization potential, providing insights into the ease of removing an electron. In contrast, the lowest unoccupied molecular orbital (LUMO) energy represents the negative electron affinity, indicating the willingness of a molecule to accept an electron. These parameters are instrumental in assessing the stability and reactivity of a molecule.

Mechanical and chemical hardness are particularly valuable in gauging the stability and reactivity of a system. Analogous to the observation of the ortho site for (TiO-4)-codoped graphene nanoflake (GNF), molecules with minimal chemical hardness values are anticipated to be effective in inhibiting corrosion. This insight offers a promising avenue for tailoring the reactivity of materials based on their electronic structure, providing a foundation for applications in corrosion inhibition and related fields.

Table 2- Show the global chemical indexes which include: the ionization potential (I_P), electron affinity (E_A), chemical potential (μ), chemical hardness (η), chemical softness (S), and electrophilicity (ω) calculated for graphene nanoflakes with and without TiO dimers. All indexes are in eV unit

System	I_P	E_A	μ	η	S	ω
GNF Pure	5.644	1.445	3.544	2.100	1.050	2.991
(TiO-1)-codoped GNF	3.595	1.972	2.783	0.812	0.406	4.771
(TiO-2)-codoped GNF	4.052	1.918	2.985	1.067	0.533	4.176
(TiO-3)-codoped GNF	3.337	2.278	2.808	0.530	0.265	7.441
(TiO-4)-codoped GNF	2.950	2.305	2.628	0.322	0.161	10.715

The equation $\sigma \propto \exp\left(-\mathrm{E_g}/2\mathrm{k_\beta T}\right)$ plays a crucial role in understanding how TiO dimers impact the electronic properties of graphene nanoflakes (GNFs). This equation suggests that even a slight change in the band gap (Eg) can significantly influence the electronic conductivity of GNFs. Here, T represents the temperature, kβ is Boltzmann's constant, and σ denotes electric conductivity, all measured at 298.14 K. According to above equation, lower values of Eg at a given temperature lead to higher electric conductivity. In practical terms, the presence of TiO dimers in pure GNF introduces a notable variation in the band gap, thereby influencing the electronic conductivity of the material. Consequently, the addition of TiO dimers presents a means to deliberately alter the electronic characteristics of GNFs, providing a pathway for tailoring their conductivity for specific applications. This insight underscores the potential for controlled doping strategies to engineer graphene-based materials with desired electronic properties.

4. Conclusion

We used density functional theory calculations to analyze the electronic ground state of pure and TiO_2 -doped graphene nanoflakes. It has been shown that the electronic structure of GNFs is influenced by the placement of TiO_2 dimers. It has been determined that the meta TiO_2 dimers' increased bandgap (2.13 eV) is a result of their antiaromatic structure. On the other hand, the bandgaps of the ortho and para TiO_2 dimers are moderate (1.62 and 1.06 eV), with the ortho TiO_2 dimer structure having a smaller bandgap than the para TiO_2 structure. Furthermore, it has been observed that TiO_2 dimers have an impact on the GQD global chemical indices. The systems are pushed to higher energies in terms of their LUMO, Fermi level, and HOMO, which considerably modifies the HOMO-LUMO gap. Since electronic conductivity may be changed by even a small bandgap shift, this modification is essential in many applications. Ultimately, the addition of TiO_2 dimers at various locations allows us to modify the electronic properties of GNFs, a valuable modification for a wide range of applications.

5. References

[1] K. S. Novoselov *et al.*, "Electric field effect in atomically thin carbon films," *science*, vol. 306, no. 5696, pp. 666-669, 2004.

[2] Z. Sun, Z. Yan, J. Yao, E. Beitler, Y. Zhu, and J. M. Tour, "Growth of graphene from solid carbon sources," *Nature*, vol. 468, no. 7323, pp. 549-552, 2010.

[3] 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.

[4] F. N. Ajeel and A. b. Ahmed, "Effect of ZnO dimers on the thermoelectric performance of armchair graphene nanoribbons," *Journal of Molecular Modeling*, vol. 29, no. 5, p. 145, 2023.

[5] F. N. Ajeel and A. B. Ahmed, "Influence of the boron doping and Stone–Wales defects on the thermoelectric performance of graphene nanoribbons," *The European Physical Journal B*, vol. 96, no. 10, p. 127, 2023.

[6] F. N. Ajeel and A. B. Ahmed, "Tuning the thermoelectric properties of graphene nanoribbons by vacancy defect with Ge-doping," *Chemical Physics Impact*, vol. 7, p. 100367, 2023.

[7] F. N. Ajeel and A. B. Ahmed, "Enhanced thermoelectric performances in graphene nanoribbons via BN dimers doping: Theoretical study," *Chemical Physics Impact*, vol. 8, p. 100413, 2024.

[8] 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.

[9] K. Nakada, M. Fujita, G. Dresselhaus, and M. S. Dresselhaus, "Edge state in graphene ribbons: Nanometer size effect and edge shape dependence," *Physical Review B*, vol. 54, no. 24, p. 17954, 1996.

[10] J. Lu, P. S. E. Yeo, C. K. Gan, P. Wu, and K. P. Loh, "Transforming C60 molecules into graphene quantum dots," *Nature nanotechnology*, vol. 6, no. 4, pp. 247-252, 2011.

[11] 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.

[12] F. N. Ajeel, Y. W. Ouda, and S. A. Abdullah, "Graphene nanoflakes as a nanobiosensor for amino acid profiles of fish products: Density functional theory investigations," *Drug Invention Today*, vol. 12, no. 12, 2019.

[13] 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.

[14] 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.

[15] 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.

[16] 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.

[17] W. L. Wang, S. Meng, and E. Kaxiras, "Graphene nanoflakes with large spin," *Nano letters,* vol. 8, no. 1, pp. 241-245, 2008.

[18] N. Kheirabadi and A. Shafiekhani, "The ground state of graphene and graphene disordered by vacancies," *Physica E: Low-dimensional Systems and Nanostructures,* vol. 47, pp. 309-315, 2013.

[19] 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.

[20] D. Mombrú, M. Romero, R. Faccio, and Á. W. Mombrú, "Electronic and optical properties of sulfur and nitrogen doped graphene quantum dots: A theoretical study," *Physica E: Low-dimensional Systems and Nanostructures,* vol. 113, pp. 130-136, 2019.

[21] A. Rycerz, "Strain-induced transitions to quantum chaos and effective time-reversal symmetry breaking in triangular graphene nanoflakes," *Physical Review B,* vol. 87, no. 19, p. 195431, 2013.

[22] T. A. Omeer and M. H. Mohammed, "Tuning the band gap in graphene nanoflakes via various impurities," *Nano-Structures & Nano-Objects,* vol. 35, p. 101009, 2023.

[23] 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.

[24] A. M. Khudhair, F. N. Ajeel, and H. M. Mohammed, "DFT Investigations for sensing capability of a single-walled Carbon nanotube for adsorptions H 2 , N 2 , O 2 and CO molecules," *International Journal of Nano Dimension,* vol. 8, no. 1, pp. 82-88, 2017.

[25] A. M. Khudhair, F. N. Ajeel, and M. H. Mohammed, "Theoretical (DFT and TDDFT) insights into the effect of polycyclic aromatic hydrocarbons on Monascus pigments and its implication as a photosensitizer for dye-sensitized solar cells," *Microelectronic Engineering,* vol. 212, pp. 21-26, 2019.

[26] 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.

[27] F. N. Ajeel, "Analytical Insight into the Effect of Electric Field on Molecular Properties of Homonuclear Diatomic Molecules," *Current Smart Materials,* vol. 2, no. 2, pp. 153-161, 2017.

[28] 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.

[29] A. M. Khudhair, K. H. Bardan, A. Almusawe, and F. N. Ajeel, "Enhancement the electronic and optical properties for the dye Disperse Orange 13 and using in the solar cell device," in *IOP Conference Series: Materials Science and Engineering,* 2020, vol. 928, no. 7: IOP Publishing, p. 072031.

[30] 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.

[31] 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.

[32] 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.

[33] M. T. Ahmed, A. A. Roman, D. Roy, S. Islam, and F. Ahmed, "Phosphorus-doped T-graphene nanocapsule toward O3 and SO2 gas sensing: a DFT and QTAIM analysis," *Scientific Reports*, vol. 14, no. 1, p. 3467, 2024.

[34] M. A. Ibrahim *et al.*, "A Comparative DFT Investigation of the Adsorption of Temozolomide Anticancer Drug over Beryllium Oxide and Boron Nitride Nanocarriers," *ACS omega*, 2024.

[35] A. Vig, E. Doan, and K. Yang, "First-Principles Investigation of Size Effects on Cohesive Energies of Transition-Metal Nanoclusters," *Nanomaterials*, vol. 13, no. 16, p. 2356, 2023.

[36] L. Glasser and D. A. Sheppard, "Cohesive energies and enthalpies: Complexities, confusions, and corrections," *Inorganic chemistry*, vol. 55, no. 14, pp. 7103-7110, 2016.