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Tuning the Electronic Properties of Graphene through MgO Impurities: DFT Investigations

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Abstract

Nanoelectronics devices, which are crucial for numerous applications, are created by modifying the electronic properties of manufactured graphene. Graphene nanoflake (GNF) with tunable electronic characteristics is studied through chemical doping. We used the density function theory (DFT) method to examine the GNF with and without different dopants of MgO dimers because we thought that we might create electronic features in a GNF by changing its geometrical arrangement of MgO dimers. The three forms of MgO dimers are made from ortho, meta, and para position dimers of Mg and O atoms. The bandgap values of the GNF structure have been found to be significantly impacted by the presence of MgO dimers. Our results indicate that the presence of MgO dimers as well as their geometric arrangement in the GNF, will greatly affect its electronic properties.

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

تنغيم الخواص الإلكترونية للكرافين من خلال شوائب MgO : فحوصات DFT

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الملخص

يتم إنشاء أجهزة الإلكترونيات النانوية، والتي تعتبر ضرورية للعديد من التطبيقات، عن طريق تعديل الخصائص الإلكترونية للجرافين المصنع. رقاقة الكرافين النانوية (GNF) ذات الخصائص الإلكترونية القابلة للتنغيم تم دراستها مع المنشطات الكيميائية. استخدمنا طريقة نظرية دالة الكثافة الوظيفية (DFT) لفحص GNF مع وبدون مواد منشطة مختلفة لثنائيات MgO لأننا نعتقد بإمكانية انشاء ميزات إلكترونية في GNF عن طريق تغيير الترتيب الهندسي لهذه الثنائيات. الأشكال الثلاثة من ثنائيات MgO تشكل ثنائيات أورثو ortho، ميتا meta، وبارا para الموضعية لذرات Mg وO. وجد بان قيم فجوة النطاق لبنية GNF تتأثر بشكل كبير بوجود ثنائيات MgO. وتشير نتائجنا إلى أن إضافة ثنائيات MgO وكذلك ترتيبها الهندسي داخل GNF يؤثر بشكل ملحوظ على خواصها الإلكترونية.

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

1. Introduction

Graphene has been the subject of much experimental and theoretical investigation in the last twenty years due to its excellent mobility, high thermal conductivity, outstanding elasticity, and high optical transparency [1-4]. However, pristine graphene has no bandgap, which limits its electro-optical applications. Surface functionalization, mechanical fields, and nano-patterning have all been used to construct semiconducting graphene structures (graphene nanoflake). In most cases, a bandgap may be opened by altering the electronic properties of graphene by modifying its structure [3, 5-9].

Graphene flakes (GNFs) are structures of finite size that exhibit a HOMO-LUMO gap due to quantum confinement. Many experimental approaches have been used to create GNFs, and they can have a variety of topologies [5-9]. Its potential uses are limited by the fact that graphene without an energy gap, which makes it unsuitable for use as a semiconductor [10, 11]. Graphene nanoflakes are graphene nanoclusters in which charge carriers are contained in all three directions. They are a prospective rival that may increase the applications of graphene as a semiconductor material [12-14]. Recently, there has been a lot of interest in zero-dimensional graphene nanoflake due to its unique electronic and optoelectronic properties and its applications in photovoltaics, biosensors, nanoelectronics, nanomedicine, and supercapacitors [15, 16]. But as recent studies have demonstrated, doping GNFs with additional atoms and functionalizing them can lead to very good modifying of their optoelectronic characteristics [1, 17-22]. The functionalizing GNFs provirus's enhanced physical features and biological activity open up new application opportunities for it [4, 23-25].

This paper uses first principles DFT simulations to study the effects of MgO dimers on the structural and electronic properties of graphene. Three types of MgO dimers are identified: ortho, meta, and para. The aim is to find the structure that is the most stable among them. In order to design the electronic characteristics that are wanted, substitutional impurities may be introduced into the system.

2. Computational Methods

As a model, we used a graphene nanoflake ($C_{24}H_{12}$), which is a 7-benzene ring. Using the DFT in Gaussian package 09, B3LYP and 6-31G(d,p) were the levels at which the structure of the $C_{24}H_{12}$ was optimised. Electronic characteristics of GNFs include energy gap (E_{gap}), Fermi level (E_{FL}), LUMO orbitals energies (E_{LUMO}), HOMO orbitals energies (E_{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 (η), chemical softness (S), chemical potential (μ), and the electrophilicity index (ω).

These parameters can give by [3, 6, 26, 27]:

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

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

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

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

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]:

$$IP = -E_{\mathrm{HOMO}} \quad (5)$$

$$EA = -E_{\mathrm{LUMO}} \quad (6)$$

In addition, we use the following formula to calculate the electronic band gap as well as the energy of the Fermi level [32-35]:

$$E_{\mathrm{g}} = E_{\mathrm{LUMO}} - E_{\mathrm{HOMO}} \quad (7)$$

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

Cohesive energies for each structure were computed in order to examine the structural stability of the MgO-codoped GNFs, which are defined as [21, 36-38]:

$$E_{\mathrm{coh}} = (E_{\mathrm{tot}} - n_{\mathrm{i}}\, E_{\mathrm{i}})/n\ , \quad (\mathrm{i} = \mathrm{C, H, Mg, and\ O}) \quad (9)$$

where E_{coh} is the cohesive energy per atom. E_{i} and E_{tot} correspond to the energy of an individual element in the same supercell and the total energy of the system, respectively. n represents the total number of atoms in the supercell.

, the energies of carbon atom and MgO atoms, respectively. Also, m and n indexes refer to the number of carbon and MgO atoms in the system, respectively. The doped structures with the highest stability are those with the highest negative value [1, 39].

3. Results and discussions

Based on the results shown in Figure 1(a), it can be seen that pure graphene nanoflakes contain a 7-benzene ring, which has a typical C-C bond length of about 1.42 Å [3, 5, 6, 8]. This value is in agreement with the values that have been reported in the previous articles. The density of states (DOS) of pure GNFs must be analysed both before and after the replacement of carbon atoms with MgO dimers. This is necessary in order to get a comprehensive knowledge of the changes that occur in the electronic characteristics of pure GNFs.

The data that are shown in figure 1(b) exhibit the density of states investigation of pure GNF. The energy gap, which is equal to 4.101 eV, is also included in this study. The energy gap is the difference in energy between the HOMO and the LUMO. According to the reference, the energy gap value that was found demonstrates features that are characteristic of a semiconductor material that has a large energy gap. In order to confirm the true absolute minimum, the harmonic vibrational frequencies were computed at the same theoretical level. The presence of such frequencies on surface of the potential energy indicates that the structure is now in a stationary state.

The purpose of this work is to investigate how the electronic properties of GNF are affected by the introduction of MgO dimer at various places. Our assumptions on the following four forms of magnesium oxide dimers are shown in the diagram included in figure 2: (a) Mg and O atoms are fixed at ortho position (MgO-1); (b) Mg or O atoms are positioned close to other atoms in meta position (MgO-2); (c) Mg and O are at the para-position (MgO-3); and (d) MgO pair is at ortho position but there is a big space between two MgO pairs (MgO-4) [10, 11, 20].

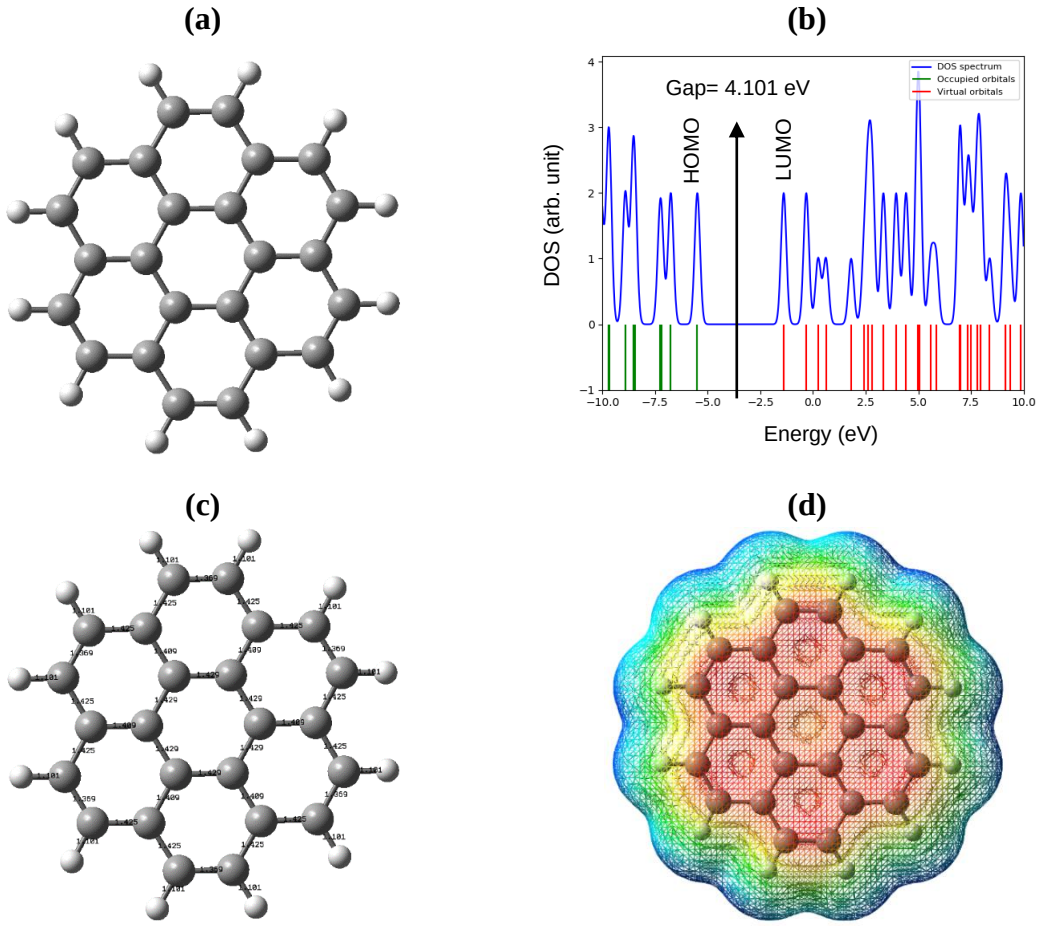

Figure -1 (**a**) Pure graphene nanoflakes, (**b**) The density of state, (**c**) Both the bond lengths and the structured geometries, and (**d**) Gas-phase molecular electrostatic potential.

It has been shown that the gaps between the valence and conduction bands and the electronic DOS alter with the introduction of MgO impurities. It was also discovered that the

DOS diagrams and the electronic energy gap (E_g) are affected when the positions of the MgO impurities are changed while the concentrations remain constant. Changes in the positions of Mg and O atoms in GNF structures, for example, cause the energy gap to shift from -39.365% to -88.335%, and this is relevant in numerous cases. GNF has the potential to be transformed into a semiconductor with a small energy gap by the process of doping its structures with MgO dimers, which reduces the energy gap.

The combination of magnesium and oxygen atoms into GNFs via the process of substitutional doping leads to the identification of a large number of bonds in addition to the alteration of bond lengths to a substantial degree. When sorted in the order of longest to shortest bond length, the average bond length may be arranged as follows: > C-C > Mg-C > Mg-O > C-O. In MgO-codoped GNFs, the sublattice symmetry would be broken as a result of the distortion that resulted from the varied bond lengths. Due to this, the electronic properties of GNFs exhibit a significant transformation when they are exposed to high concentration ratios of magnesium oxide dimers.

Furthermore, Table 1 presented the data that were computed for the energetic state and included the following: the HOMO energies (E_{HOMO}, eV), Fermi level energy (E_{FL}, eV), LUMO energies (E_{LUMO}, eV), band gap (E_g, eV), change of E_g (ΔE_g) and cohesive (E_{coh}, eV) for graphene nanoflake with and without MgO dimers. The energies of HOMO and LUMO for the pure GNF are -5.490 and -1.389 eV, respectively, according to the results of the study that was carried out on the molecular orbital frontier. Figure 4 illustrates how these values gradually increase as a result of the addition of magnesium oxide dimers. As is evident from the data shown in Table 1, not only is the E_g altered, but the energy of Fermi level (E_{FL}) is also being altered. In addition, this impact results in an increase in the work function, that is an essential component in applications involving field emission [10, 11].

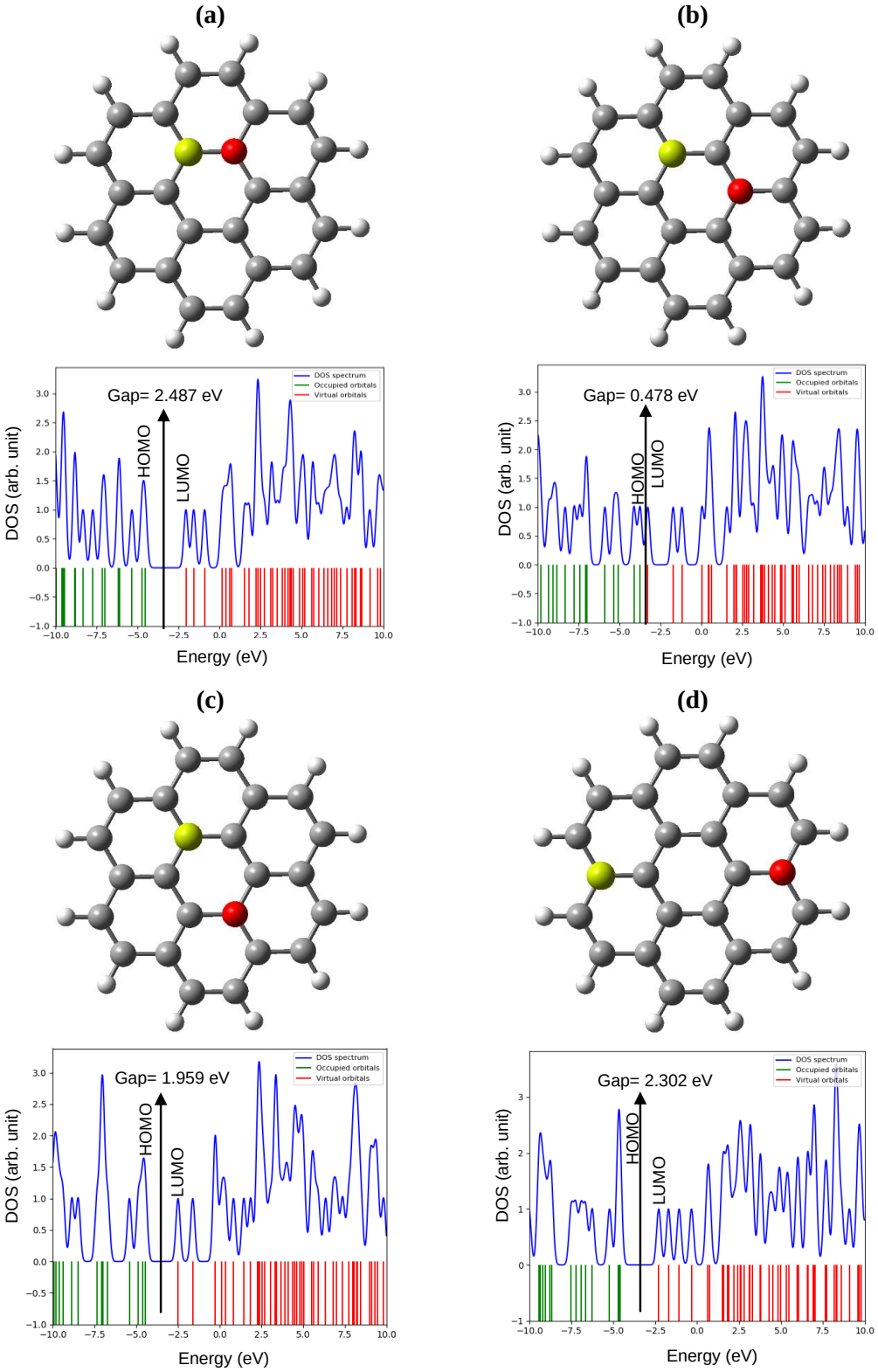

Figure -2 Shows the graphene nanoflakes configurations with MgO dimers generating the following structures: (**a**) MgO-1, (**b**) MgO-2, (**c**) MgO-3, and (**d**) MgO-4, along with their density of state.

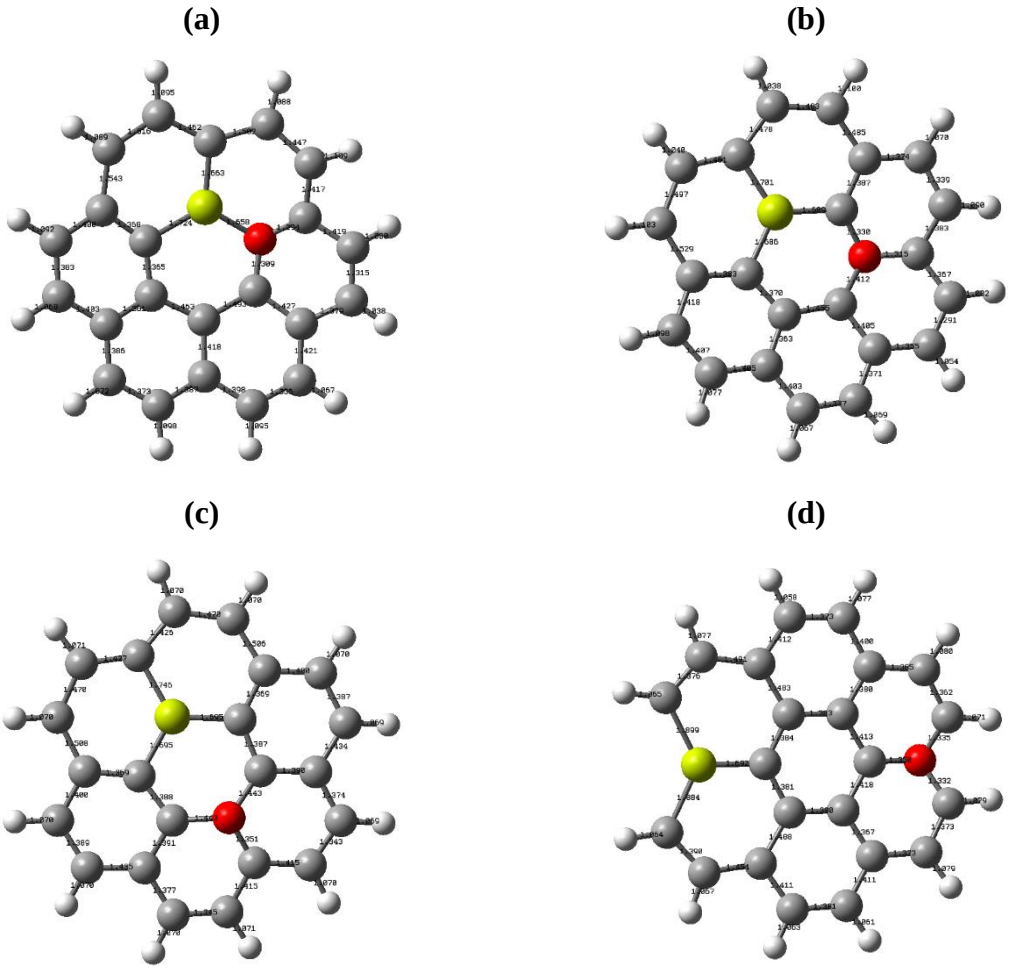

Figure -3 Bond lengths (in Å unit) and structured geometries of a graphene nanoflake with MgO dimers creating the structures: MgO-1, MgO-2, MgO-3, and MgO-4.

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 MgO 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	-5.490	-3.440	-1.389	4.101	-	-11.39
(MgO-1)-codoped GNF	-4.538	-3.295	-2.052	2.487	-39.365	-208.53
(MgO-2)-codoped GNF	-3.750	-3.511	-3.272	0.478	-88.335	-208.74
(MgO-3)-codoped GNF	-4.455	-3.476	-2.496	1.959	-52.225	-208.64
(MgO-4)-codoped GNF	-4.591	-3.440	-2.289	2.302	-43.857	-208.58

* The change of E_{g} is calculated by $\Delta E_{\mathrm{g}} = \left(\frac{E_2 - E_1}{E_1}\right) \times 100$. [18, 19]

To examine the reactivity descriptors which are displayed in Table 2, Koopman's theorem is used to perform an analysis. Characteristics such as ionization potential, electron affinity, electronegativity, chemical hardness, chemical softness, and electrophilicity are included in this category. When it comes to analyzing the reactivity trends and the excited states, as well as assessing toxicity, each of these properties is very helpful [6, 26, 29].

According to the Koopman theorem, HOMO energy is very close to the experimentally determined negative ionization potential. This is in contrast to the LUMO energy, which is a representation of the negative electron affinity. When it comes to determining the stability and reactivity of a molecule, one of the most helpful indications is the mechanical and chemical hardness of the system. In a manner that is analogous to the observation of the meta site for (MgO-2)-codoped GNF, it is expected that molecules that have the minimal chemical hardness values will be useful in inhibiting corrosion.

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 MgO dimers. All indexes are in eV unit.

System	I_P	E_A	μ	η	S	ω
GNF Pure	5.490	1.389	3.440	2.050	1.025	2.885
(MgO-1)-codoped GNF	4.538	2.052	3.295	1.243	0.622	4.366
(MgO-2)-codoped GNF	3.750	3.272	3.511	0.239	0.120	25.771
(MgO-3)-codoped GNF	4.455	2.496	3.476	0.980	0.490	6.165
(MgO-4)-codoped GNF	4.591	2.289	3.440	1.151	0.576	5.139

Lastly, the equation $\sigma \propto \exp(-E_g/2k_\beta T)$ must be taken into consideration in order to account for how MgO dimers impact the electronic properties of GNFs [40]. This suggests that a slight change in E_g may alter the electrical conductivity of the GNF. Where $T, k_\beta,$ and σ stand for temperature, Boltzmann's constant, and electric conductivity, respectively, at 298.14 K. According to the equation, greater levels of electric conductivity are produced by lower values of E_g at a given temperature. Consequently, the presence of MgO dimers in pure GNF influences a notable vary in the electrical conductivity. Therefore, by adding MgO dimers, we may change the electronic characteristics of the GNFs.

4. Conclusion

Here, we analyze the electronic ground state of both pure and MgO-codoped graphene nanoflake by means of DFT calculations. There is evidence that the present and location of MgO dimers affects the electronic structure of GNF which has big energy gap 4.101eV. Because of their antiaromatic structure, it has been shown that meta MgO dimers have a low energy gap 0.478 eV. By comparison, the energy gap of the ortho (2.487 eV) and para (1.959 eV) MgO dimers is modest, but the energy gap of the para ZnO dimer structure is narrower than that of the ortho ZnO. It investigated into the density of state to find the energies of the energy gaps between the various states and to calculate the MgO dimer contributions. According to results, the presence of MgO dimers also modifies the global chemical indices of GNF. The systems are driven to higher energies in terms of HOMO, Fermi level, and LUMO, which causes a significant change in the HOMO-LUMO gap. Small shifts in the HOMO-LUMO gap may change the electrical conductivity, which makes this adjustment valuable for many different applications.

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