



Application of Graphene/Nickel Oxide Composite as a Humidity Sensor

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Abstract

Molecular modeling analyses at Density functional theory DFT level was used to study the possible application of modified graphene (G) as gas sensor. A model molecules of graphene sheet was constructed then modified with nickel oxide NiO attached to graphene through covalent bonds forming G/NiO composite. DFT at B3LYP/6-31G(d,p) was utilized to investigate the physical properties of G; G/NiO; G/NiO/2H₂O. Results show that interacting G/NiO composite with water molecules lowers the calculated energy of the formed structure reflecting the possibility of exposing G/NiO structure to humidity, since it forms more energetically stable composition that can be detected by a proper circuit. However, water addition results in significant reduction in the TDM which would enhance its stability. This would increase the efficiency of G/NiO material as a humidity sensor. Mapping molecular electrostatic potential indicated that, the impact of interacting with G/NiO composite through Ni end increases electron cloud on the terminals ensuring the great ability of this region to sense different water molecules. It is concluded that, the change in the physical properties of G/NiO under the influence of water molecules took place. Collecting these data together, it is clear that the studied G/NiO composite could act as humidity sensor.

Keywords: Graphene; Molecular Modeling; DFT; Geometrical parameters; MESP

1. Introduction

Graphene-based structures have witnessed incredible attention regarding the next-generation as super electronic materials due to its unique features particularly its strong current density, ballistic transport property, optical transmittance, good thermal conductivity, inert nature, and super hydrophobicity at nano size [1, 2]. They were firstly synthesized using graphite source via micro-mechanical cleavage method [3] which allowed easy way for graphene production with high-quality and as well led to vast experimental activities [4] with the reverse magnetic features. Nanotechnology ensure always that it is capable of controlling the assembling

procedures of various chemical compounds at nano size [5]. Consequently, nanomaterials are sometimes found to be emerged within the concentration of advanced research papers [6, 7]. Developments in different materials in the nanoscale are not limited to techniques of preparation and characterizations, but also include the theories specialized at interactions in this tiny scale [8, 9]. Nickel oxide (NiO) has received also great attention due to its size-dependent crystal construction, its various vibration modes and as well magnetic characteristics, and its applications in different fields such as storage devices, catalysis, antiferromagnetic (AFM) layer, energy conversion, battery electrodes, multidisciplinary sensors, transparent conducting films and electrochromic films [10, 11]. Extensive research papers have been

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Receive Date: 20 July 2020, Accept Date: 09 August 2020

DOI: 10.21608/EJCHEM.2020.36453.2753

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described in the start of this century on particle size-magnetic characteristics relationships [12-14] and finite-size against surface impacts on magnetism [15], the marvelous effect of replacement [16], and magnetism-matter crossover at room temperature [17-20]. Early on 2013 graphene oxide acts as ultrafast sensor for humidity [21]. Later on, the existence of metal oxide enhances the ability of graphene to act as sensor [22]. Moreover, the effect of metal oxide such as NiO upon graphene dedicate it for many applications especially biomedical applications as reported earlier [23, 24]. Still the mechanism of enhancement need to be elucidated which requires computational efforts on molecular scale. Molecular modelling aspects are usually used to study different properties of various chemical structures such as geometrical, structural, dynamical, and thermodynamical properties of great number of structures [25-27]. Such computational methods are now used to model the molecular behavior in order to investigate chemical, physical, and biological features in various science fields and applications [28-30]. Molecular electrostatic potential (MESP) maps are currently considered as one of the unique properties which can be investigated by molecular modeling concepts. They are valuable in describing the active sites of different chemical samples [31]. This concept is theoretically suitable as it determine the nature of the chemical addition through which a chemical structure may undergo; either electrophilic or nucleophilic chemical addition. Possible interaction between graphene and nicker oxide is indicated in our previous work [32]. DFT was used to describe the electronic properties of Gr/NiO compsite.

This work is devoted to investigate the ability of graphene/NiO composites to act as a humidity sensor using Density Functional Theory (DFT) model.

2. Calculation Details

All computations are conducted via GAUSSIAN 09 soft code which at Spectroscopy Department, National Research Centre, NRC [33]. They are carried out by Density Functional Theory (DFT) at Becke-style 3-Parameter Density Functional Theory (using the Lee-Yang-Parr correlation functional) (B3LYP) [34-36] and 6-31G(d,p) as a basis set.

Then, constructing molecular electrostatic potential (MESP) maps are

3. Results and Discussion

3.1. Modified Graphene as Sensor

In the present work graphene is supposed to be modified with NiO in order to act as a sensor for humidity. The modification of graphene with such metal oxide is supposed to change the physical properties of the G/NiO surface which in turn dedicate this composite as sensor for humidity.

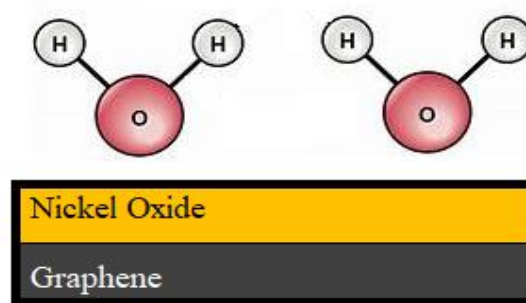


Fig 1. Schematic diagram for graphene/nickel oxide (G/NiO).

3.2. Building Model Molecules

The model molecule could be described as a graphene sheet of 42 C atom was constructed and NiO attached to graphene via covalent bonds with C₁₆ and C₁₇ atoms. In addition in this paper, two water molecules in the vapor state are added through hydrogen bonds, as illustrated in figure 2. To follow up the changes in the surface total dipole moment and mapping electrostatic potential are two important parameters needed to fulfill the change in the surface and could be good descriptors for the ability of such surface to further interact with water molecules. It is stated earlier that total dipole moment, HOM/LUMO band gap energy as molecular electrostatic potential are good descriptors for reactivity of a given structure [37-41].

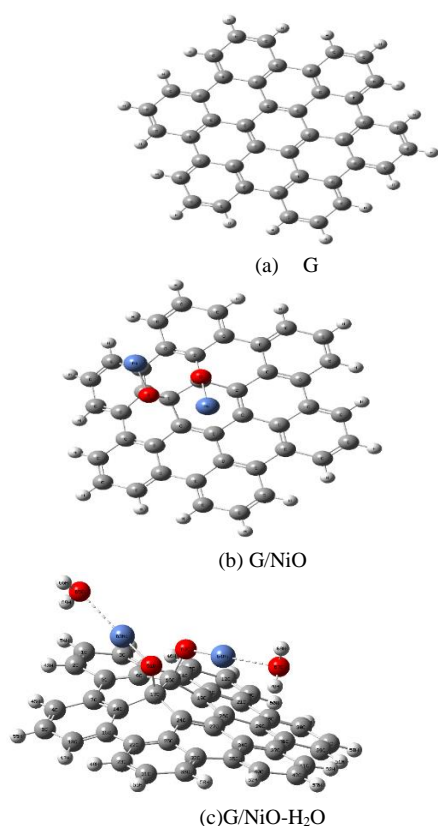


Fig 2. Model molecules of (a) Graphene sheet (G), (b) graphene-NiO composite (G/NiO), (c) graphene-NiO composite interacting with water vapor (G/NiO-H₂O)

3.3. DFT Energy Calculations

Computations of energy are carried out by DFT at B3LYP method and 6-31G(d,p) as a basis set in order to compare some physical and geometrical parameters of graphene/NiO composite before and after interaction with water vapor. Table 1 presents data which calculated at the DFT level as indicated earlier in the previous molecular modeling work [32] regarding graphene, NiO and graphene/NiO composites to compare it with the newly computed ones of graphene/NiO composite after interaction with water vapor (G/NiO-H₂O). The selected physical parameters are total energy (E), total dipole moment (TDM) and HOMO/LUMO band gap energy (ΔE).

Table 1: Calculated physical parameters such as energy (E) as eV, total dipole moment (TDM) as Debye and band gap energy as eV for graphene sheet (G), NiO, graphene functionalized with NiO (G/NiO), and graphene-NiO composite interacting with water vapor (G/NiO-H₂O) using B3LYP/6-31G(d,p) method.

Structure	E (keV)	TDM (Debye)	ΔE (eV)
G	-43.8459	0.0082	0.0928

NiO	-43.0809	3.9303	0.0799
G/NiO	-130.0085	8.9544	0.0040
G/NiO-H ₂ O	-134.1679	3.4685	0.0040

Energy is always considered as the conjugate physical parameter for structures' stability which is one of the valuable parameters for studying structures on the molecular scale theoretically. The lower the energy of some chemical structure, the more is its stability [37]. It was previously mentioned the energies of graphene, NiO and graphene/NiO composite to be -43.8459, -43.0809 and -130.0085 keV referring to the stability of the formed composite with respect to pristine graphene. Interacting G/NiO composite with two water molecules in the gaseous state lowers the calculated energy of the formed structure which equals -134.1679 keV. This reflects the possibility of exposing G/NiO structure to humidity, since it forms more energetically stable composition that can be detected by a proper circuit. Moreover, dipole moment (TDM) is a powerful parameter in assessing structures' reactivity [30]. Those structures of great TDM results are considered highly reactive compared to others. Similarly and as previously stated, addition of NiO for graphene 2D sheet enhances its electronic features and causes a significant increment in its TDM from 0.0082 to 8.9544 Debye. However, the addition of water to the proposed G/NiO composite results in noteworthy reduction in the previously mentioned TDM result to equal 3.4685 Debye. This decline in reactivity would enhance the stability for the G/NiO structure after adsorbing water molecules. This would increase the efficiency of G/NiO material as a humidity sensor. Finally HOMO/LUMO band gap energies, interacting water with G/NiO does not affect the electrical conductivity of the proposed structure allowing it to be a part from an electrical sensor circuit easily. HOMO/LUMO band gap energies of both G/NiO and G/NiO-H₂O are the same and equal 0.0040 eV.

Then, various geometrical parameters are investigated for G, G/NiO and G/NiO-H₂O structures utilizing the same output files calculated at B3LYP/6-31G(d,p) theoretical level. Table 2 lists some of the interested parameters. LC₁₆-C₁₇ is the length of the bond linking C₁₆ atom with C₁₇ one. It equals 1.3546 Å in the graphene sheet, while addition of NiO to G either before or after interaction with water vapor causes its increase to 1.5949 and 1.5968 Å, respectively. The bond lengths of C-O in both

terminals have nearly the same range from 1.4297 to 1.4330 Å and interaction with water has no significant effect on them. Similarly, the bond lengths of Ni- O in the two terminals range from 1.8099 to 1.8213 Å and also the interaction with water has no significant effect on them. The investigated angles follow the same manner, the angles between C, O and Ni increase slightly due to water interaction from

109.4823° to 109.9263° in C₁₆O₆₂Ni₆₄ and to 110.0750° in C₁₇O₆₁Ni₆₃. In Contrary, the values of the O₆₁C₁₇C₁₆ bond angle suffers from little decrease due to adsorption of water where it lowers from 103.52° to 103.3751°. However, it has little increase in the other terminal at O₆₂C₁₇C₁₆ from 103.8605° to 104.0104°.

Table 2. Calculated geometrical parameters involving bond lengths (L) and bond angles (A) for graphene (G), graphene/NiO composite (G/NiO) and graphene-NiO composite interacting with water vapor (G/NiO-H₂O) calculated using DFT at B3LYP/6-31G(d,p).

Structure	LC ₁₆ -O ₆₂ (Å)	LC ₁₇ -O ₆₁ (Å)	LC ₁₆ -C ₁₇ (Å)	LNi ₆₃ -O ₆₁ (Å)	LNi ₆₄ -O ₆₂ (Å)	AC ₁₆ O ₆₂ Ni ₆₄ °	AC ₁₇ O ₆₁ Ni ₆₃ °	AO ₆₁ C ₁₇ C ₁₆ °	AO ₆₂ C ₁₆ C ₁₇ °
G	-----	-----	1.3546	-----	-----	-----	-----	-----	-----
G/NiO	1.4301	1.4297	1.5949	1.8099	1.8101	109.4823	109.4823	103.5200	103.8605
G/NiO-H ₂ O	1.4330	1.4319	1.5968	1.8213	1.8172	109.9263	110.0750	103.3751	104.0104

3.4. Molecular Electrostatic Potential (MESP)

Maps

Maps of MESP are constructed for investigating the chemical reactivity of the proposed structures at DFT level using B3LYP/6-31G(d,p) method. MESP maps are often important in providing simple and quite informative way for studying the charge distribution over chemical structures and therefore their most probable active sites. Figure 3 shows the mapped molecular electrostatic potentials (MESP) for graphene (G), NiO, graphene functionalized with NiO (G/NiO) before and after interacting with water vapor molecules. As illustrated in our previous works [38, 39], MESP are always constructed of different colors ranging from red color to light and dark blue referring to extreme negative regions for red and positive sites for blue. They follow the order of red, orange, yellow, green, light blue and dark blue corresponding the most negative to most positive regions, respectively. The MESP distributions can be correlated to the electronegativity of the involved atoms. Highly electronegative atoms appear in red color when linking to another atom of lower electronegativity. Bonding of two atoms or more of similar electronegativity makes color distributions much narrower. Therefore, MESP maps can be a feasible method in determining whether the investigated active site is most probable undergo electrophilic or nucleophilic interactions.

MESP map of the 2D graphene sheet (G), NiO and graphene functionalized with NiO (G/NiO) were previously constructed and explained in our previous article [28]. MESP of graphene consists mainly of three colors; red, blue and dark blue. Red is focused in the centers of benzene rings composing graphene sheet reflecting the impact of electron delocalization phenomenon. This leads to the suggestion that nucleophilic interactions are the most proper for graphene core. On the other hand, its terminals appear in light and dark blue due to the presence of H atoms, suggesting that electrophilic pathway to be most proper there. Regarding graphene functionalized with NiO structure as previously stated, it is featured by yellow regions in general except some regions colored by light red due to O presence on the upper surface suggesting that addition of NiO turn graphene to less electronegative structure. However, addition of two water molecules increases the electronegativity around O atoms which appear in deep red color. By comparing the two adjacent figures, the impact of interacting with G/NiO composite through Ni end increases electron cloud on the terminals ensuring the great ability of this region to sense different structure such as water vapor molecules enhancing its usage as a humidity sensor.

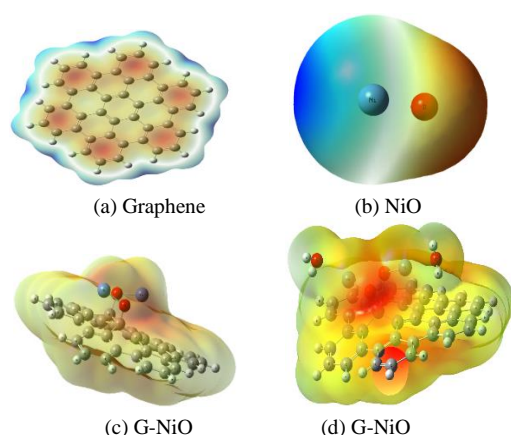


Fig. 3. Calculated molecular electrostatic potential (MESP) maps of (a) Graphene sheet (G), (b) NiO, (c) graphene functionalized with NiO (G/NiO), and (d) graphene-NiO composite interacting with water vapor (G/NiO-H₂O) on DFT using B3LYP/6-31G(d,p) method.

4. Conclusions

Density functional theory is conducted to indicate the ability of G/NiO composite to act as humidity sensors. The change in the studied physical properties indicates that changes in the calculated physical and electronic parameters are observed under the influence of two water molecules. Interacting G/NiO composite with water molecules lowers the calculated energy of the formed structure reflecting the possibility of exposing G/NiO structure to humidity, since it forms more energetically stable composition that can be detected by a proper circuit. However, water addition results in significant reduction in the TDM which would enhance its stability. This would increase the efficiency of G/NiO material as a humidity sensor. MESP maps illustrate that water addition increases the electronegativity around O atoms as well as increases electron cloud on the structure's terminals ensuring the great ability of this region to sense different structure such as water vapor molecules enhancing its usage as a humidity sensor. In conclusion, this work is confirming the suitability of DFT for elucidating the surface as well as physical properties for emerging materials such as graphene to functionalize its structure in one hand and direct the application in the other hand. This finding is in good agreement with those obtained previously [42-44].

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