P- ISSN 1991-8941 E-ISSN 2706-6703 *Journal of University of Anbar for Pure Science (JUAPS)* Open Access
2023,(17), (1):129 – 136

Effect the concentration of NH3 gas adsorbed on the graphene sheet on the electrical and thermal properties: A theoretical study

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ARTICLE INFO

Received: 08 / 04 /2023
Accepted: 24 / 05/ 2023
Available online:11 /06/ 2023

DOI: 10.37652/juaps.2023.178874

Keywords:
2D materials,
Gas sensor,
DFT,
Graphene doped Pt .

ABSTRACT

To differentiate the potential of graphene sensors, research into how the grafted particles interact with the graphene sheet is essential. We employed calculations based on the "density functional theory DFT,"to analyze the characteristics of native and Pt-grafted graphene sheets with NH_3 gas adsorption on their surface. Our goal is to determine how will the material may serve as a gas sensor. Increased charge transfer was seen after NH_3 gas molecules were adsorbed on the surface of Pt-decorated graphene that was significantly larger, smaller intermolecular distance, and had higher orbital hybridization as compared to virgin graphene. also, that they showed excellent sensitivity to ammonia (NH_3) at room temperatures.

Introduction

The widespread prevalence of problems associated with air pollution exposure means that technology for the detection of gaseous air pollutants (such as ammonia gas, NH_3) is of paramount relevance. Human health is negatively impacted by the produced hazardous gases, particularly the skin and the respiratory system. So, creating a gas sensor for NH_3 is crucial in order to lessen the toll it has on human life. Building a gas- sensing material is the first requirement for creating a gas sensor[1]. Carbon nanotubes and other nanoscale materials have seen increased application as gas-sensing materials in recent years. In particular, graphene's sp^2-hybridized 2D hexagonal honeycomb structure has garnered a lot of interest for gas sensing applications[2]. However, platinum group metals are still needed for gas sensing[3]. In sensors based on graphene. There has been some research on whether or not graphene derivatives can boost gas sensors' sensitivity. Graphene oxide (GO), a graphene sheet having oxygen functional groups, is used in gas sensing applications[4-5].

Engineers and scientists are involved in graphene because of its physical and chemical properties, such as its high surface area, excellent thermal and electrical conductivity, and high mechanical strength. Graphene has also been suggested as a potential use in many fields, including electronics, energy, and biotechnology[6-7]. Carbon atoms in the graphene layer are exchanged for those of different valence electron positions in this procedure[8-9]. These atoms include Pt, which can improve the interaction and give way for molecules and chemical groups to "dock" on the surface of graphene. By incorporating the right kind of doping[10-11].

For example, graphene nanosheets that have phosphorus (P) got to add to them showed good sensitivity to ammonia (NH_3) at room temperature because the P atom becomes active for NH_3 adsorption [12-13].

Graphene has been investigated for application in gas sensors because of its huge specific surface area (2630 m^2g) and high sensitivity to electrical interruptions of gas molecule adsorption[14]. Graphene

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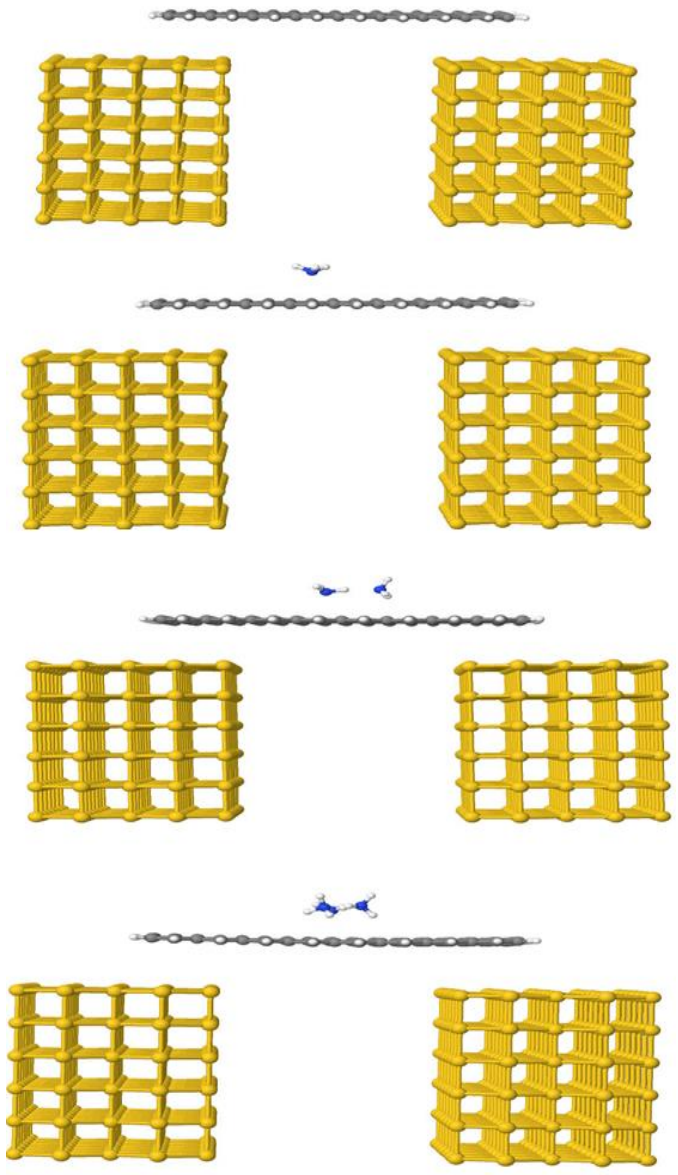
gas sensors are sensitive enough to detect molecules of gas that remain on or migrate away from the material's surface.They can tell when a gas molecule sticks to graphene because it changes the concentration of charge carriers in the graphene[15]. Different volumes of gases ended up causing resistance to change in different ways, gas is an electron acceptor (like NO_2, H_2O, or I) or an electron donor (the opposite) based on the direction of the change (like NH_3, CO, or ethanol)[16-17]. In this work, we use first- principles' "DFT" calculations to study what occurs when ammonia (NH_3) sticks to graphene layers that are doped to Pt.

Computing has helped model and simulate systems with millions of degrees of freedom. Among these fundamental questions is the nature of electron transfer between electrodes[18-20].



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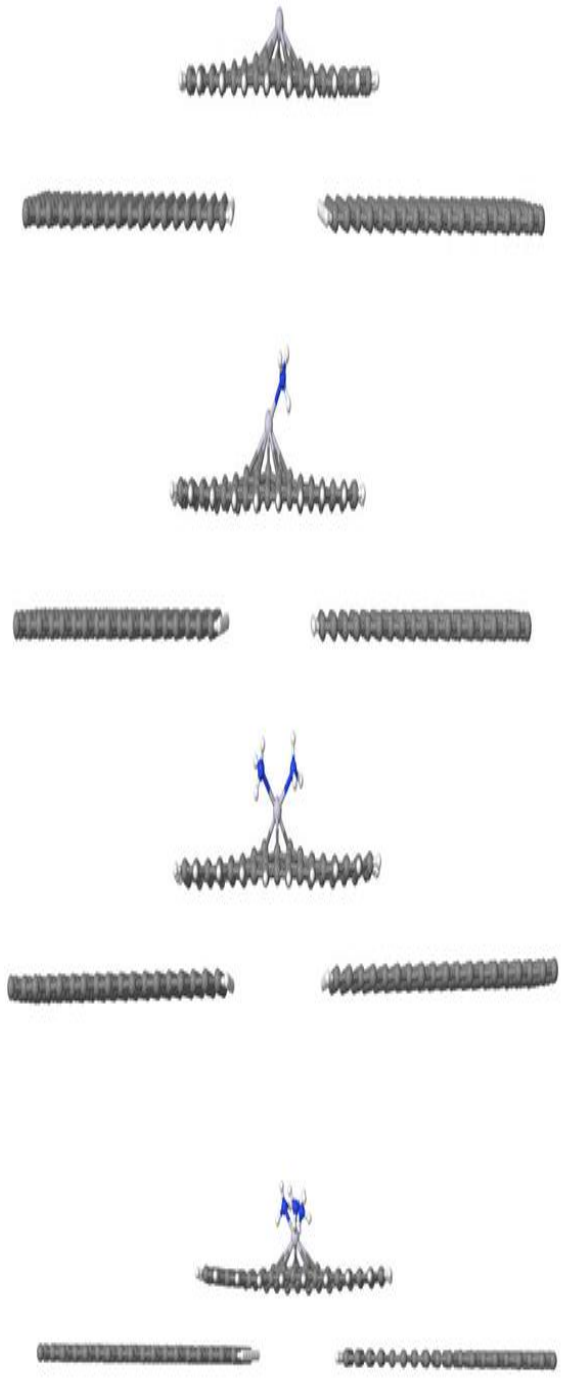


Figure 1. Structure of doped Graphene with Gold Electrodes and Graphene Electrodes

METHODS

The electronic structure was calculated by employing the "Density Functional Theory (DFT) code SIESTA"[19- 21]. Relaxing the geometries of the isolated single molecules until all forces on the atoms were less than 0.04 eV/ yielded the minimum geometries possible. Additionally, a 200 Rydberg energy cutoff was used to determine the real space grid, and a generalised functional gradient was used to determine the correlation of functional exchange for "the SIESTA (GGA)"[31-32]. The electrical conductivity of the gold and graphene electrodes was determined by attaching a sheet of graphene between them. The ideal distance for the gold atoms to bond to the surface graphene was calculated to be 4.5Å using Eq1. "The Gollum code" was used to study the zero-bias electronic "transport T(E)", and The whole structure of (gold-graphene-gold) was Hamiltonian explained using the SIESTA software (graphene-graphene-graphene)[22-23].

$$B.E = E_{ab} - (E_a + E_b) \qquad (1)$$

To determine the electrical conductance we used the Landauer formula [29].

$$G = \frac{1}{v} = G_{\circ} \int_{-\infty}^{\infty} dET(E) \left(-\frac{df(E)}{dE}\right) \qquad (2)$$

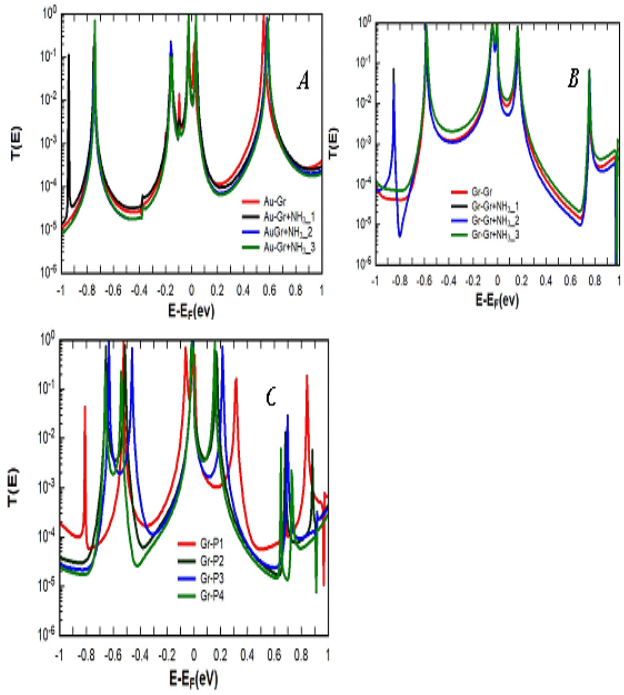
Where "the quantum of conductance" is $G = \frac{2e^2}{h}$ and f (E, T) is "the Fermi distribution function" referred to as[30].

$$f(E,T) = [e^{B(E-E_f)} + 1]^{-1} \qquad (3)$$

"where $\beta=1/K_BT$ where K_B $=8.6x10^{-5}$ ev/k is Boltzmann's constant", and T is the temperature[31].

Results and discussion

The fundamental quantity "transport coefficient T(E)", which shows how electrons flow from the left to the right gold or graphene electrodes like they are part of a single molecule, must first be determined before we can investigate "the electrical and thermal" properties of a graphene gas sensor. This is shown in Figure 1,



Figures:2(A, B, C) . A :Transmission coefficient for Linked Electrodes Au With The doped graphene of NH3. B: Transmission coefficient for Linked Electrodes Gr With The doped graphene of NH3. C: Transmission coefficient for Linked Electrodes Gr With The doped Pt-graphene of Gr-P1, P2, P3 and P4

Figures 2(A and B) show the transmission coefficient of a pristine graphene gas sensor for NH3 with gold and graphene electrodes, as we can see there is no effect on the T(E) when increasing the NH3 gas concentrations on the surface of graphene. In case graphene is doped by Pt atom by replacing one carbon atom with a Pt atom see Figure 1.

where P1 represents Gr(Pt)+Gr, P2 is Gr(Pt)+NH3_1, P3is Gr(Pt)+NH3_2, and P4 is Gr(Pt)+NH3_3. No charge was transferred from the gas molecules onto the graphene sheet due to the homogeneity of the graphene structure [24].

Afterward, we looked into what happened when NH3 came into contact with the Pt-coated graphene. We re-examined the adsorption of several NH3 molecules on Pt-coated graphene using graphene electrodes. Broken uniformity and the interaction between Pt and gas are more effective on the T(E) when NH3 concentration increases [25]. As we can see from Figure 2C the T(E) decreases with an increase in the number of NH3 molecules. Since the NH3 molecules adsorbed on the graphene surface will act as a donor-like (n-type). These findings are consistent with those of other research [26].

It's important to take into account the various in-situ configurations of NH3 adsorption on pure graphene, however previous studies have shown that the adsorption energy values are extremely low regardless of the configuration used[27-28].

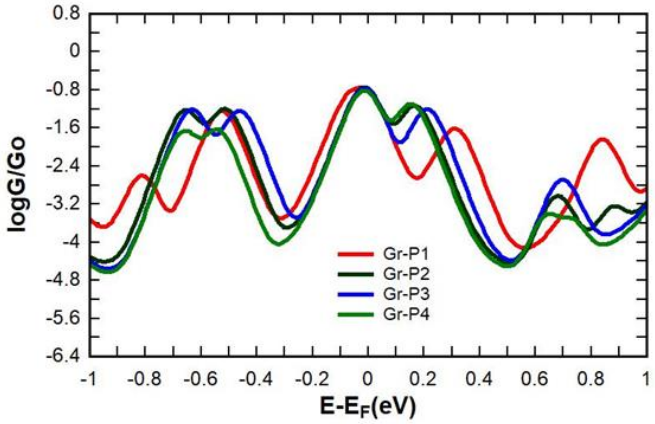
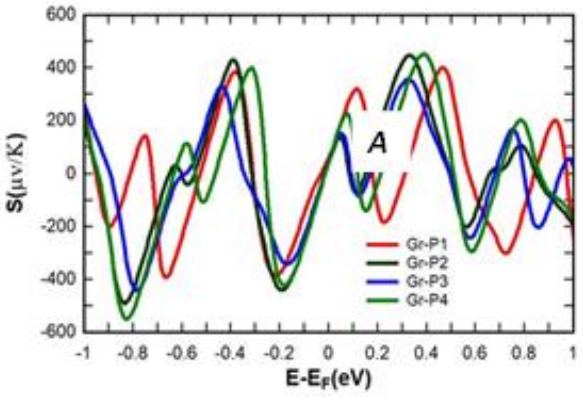
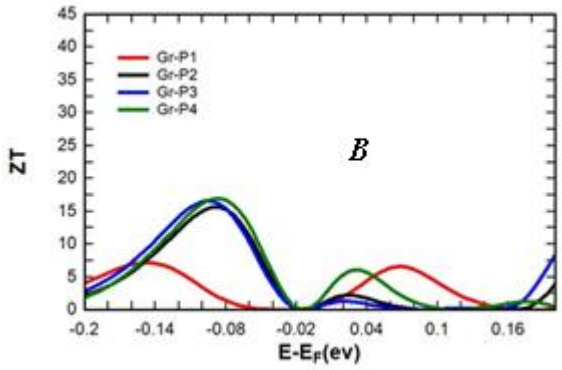


Figure 3:Graphene energy-based electrical conductance values at room temperature.

To see how much of an effect this has on conductance, we need to know the value of E_f, Hence, E_f can take any value within the range of the energy gap between "the HOMO and the LUMO" [32]. as demonstrated in figure3. The trend of electrical conduction is similar to the behaviour of T(E) at the range of energy between -0.5 to 0.6 eV.





Figures :4 (A, B) "the thermopower or Seebeck coefficient (S)" and "the thermoelectric figure of merit (ZT)" for graphene molecules as a result of energy.

The quantum thermal efficiency ZT is calculated by implying the following equation[33].

$$ZT_e = \frac{S^2 GT}{k_e} \qquad (4)$$

"Where G represents the electrical conductance", "K_e thermal conductance","T is the temperature", and S "represents the Seebeck coefficient"."The Seebeck coefficient(S)" [34-35]. is defined as the induced thermoelectric voltage ratio to the temperature gradient. Figure 4(A) shows the S which is ,varied between either "positive (p-type) or negative (n-type)"[36-37].

Figure 4(B)shows"the figure of merit (ZT)"versus energy for the system from P1 to P4. The value varies between 0.54 and 1.50 depending on the number of gas in the system; The P4 molecule has a greater value1.5, and as a result, it is considered a promising candidate for the conversion of thermal energy into electrical energy with high efficiency, as shown in Table 1.

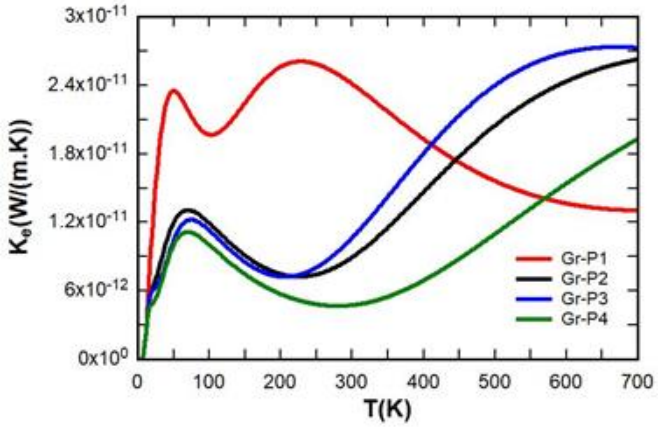


Figure5. Thermal conductance of various molecules.

"The thermal conductivity K_e"was calculated for all the system from P1 to P4 at T=300 ˚K, as we can see from figure 5 the-K_e decrease with an increase in the number of NH_3 gas.

TABLE 1:The values of "the conductance log G/G$_o$" as well as"the Seebeck (S)"and "ZT at E_f = 0", and "K_e at the temperature 300˚K".

Molecules	LOG(G/G$_o$)	S(μv/k)	ZT	K$_e$(w/k.m)
Gr -P1	- 0.81	60.87	0.54	2.41×10^{-11}
Gr-P2	- 0.77	41.86	0.77	8.95×10^{-11}
Gr -P3	- 0.84	42.25	0.55	1.06×10^{-12}
Gr -P4	- 0.79	43.76	1.50	4.76×10^{-12}

CONCLUSION

The present study compared pure graphene bonded to gold electrodes and graphene electrodes doped with NH_3, as well as platinum-doped graphene bonded to graphene electrodes with graphene (Pt).

We studied the concentration-dependent adsorption of ammonia molecules on Pt-decorated graphene surfaces. As a result, the graphene sheets, the electrical conductivity of the graphene sheets doped with Pt are more sensitive to the NH_3 gases' which is enhanced by the sensitivity of the electrical conductance and thermal conductance,

Based on our simulations, we find that natural graphene has a weak contact with NH_3 gas molecules. The addition of a Pt atom to graphene greatly improves its ability to interact with molecules with an increase in the number of molecules due to the uniformity and

broken interaction between Pt and gas. Figure of merit (ZT) versus particle energy from P1 to P4. The value varies between 0.54 and 1.50 depending on the number of particles in the system; The P4 molecule has a greater value and as a result is a promising candidate for the highly efficient conversion of thermal energy into electrical energy. The conductivity values of all molecules decrease with increasing number of NH_3 molecules. Our results indicate that Pt-decorated graphene is better than native graphene for gas sensing applications.

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تأثير تركيز غاز NH_3 الممتص على لوح الجرافين على الخواص الكهربائية والحرارية:دراسة نظرية

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الخلاصة

للتمييز بين إمكانات مستشعرات الجرافين ، يعد التحقيق في كيفية تفاعل الجسيمات المطعمة مع ورقة الجرافين أمرًا ضروريًا . لقد أستخدمنا حسابات تستند الى نظرية الكثافة الوظيفية DFT ، لتحليل خصائص صفائح الجرافين الاصلية والمطعمة بـ Pt مع امتزاز غاز NH3 على سطحها هدفنا هو تحديد كيفية عمل المادة كمستشعر للغاز . شوهدت زيادة في نقل الشحنة بعد امتزاز جزيئات غاز NH3 على سطح الجرافين المزين بـ Pt والذي كان أكبر بكثير ، وله مسافة له مسافة أصغر بين الجسيمات ، وكان له تهجين مداري أعلى مقارنة مع الجرافين الأصلي. كما أظهروا حساسية ممتازة للأمونيا NH3 في درجة حرارة الغرفة .

الكلمات المفتاحية : المواد ثنائية الأبعاد ، مستشعر الغاز ، DFT ، الجرافين المخدر Pt