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REACTIVITY PARAMETERS OF BLACK GRAPHENE VS. WHITE GRAPHENE WITH DIMENSIONS OF 1.0 NM^2: A COMPUTATIONAL QUANTUM CHEMISTRY STUDY

Vianeis De Jesús Araujo Contreras[1]
Olga Lucía Castellano[2]
Samuel Eligio Sambrano Rojas[3]
Ramón De Jesús Bertel Palencia[4]

ABSTRACT

This study calculated reactivity parameters of extended graphene (black graphene with D_2h symmetry) and boron nitride (h-BN) (white graphene with C_2v symmetry), both with dimensions of 1.0 nm^2, using the density functional theory (DFT) combined with an HCTH/GGA/DNP methodology. For structural stability, we considered the criterion of obtaining positive eigenvalues in the Hessian matrix. For reactivity parameters (chemical potential, chemical hardness, gap, and electrophilic index), the HOMO and LUMO molecular orbitals were considered. Furthermore, the molecular density of states (DOS) and electrical and electronic properties were reported. The results indicate that white graphene is much more stable, but also more reactive than black graphene. This is due to the values obtained for chemical hardness (1.157 eV and 0.329 eV, respectively), chemical potential (2.39 eV and 3.85 eV, respectively), and gap (2.313 eV and 0.657 eV, respectively). The electrophilic index values indicate that black graphene could adsorb molecules on its surface preferentially through physisorption ($\varepsilon = 0.0$ eV), while white graphene could be more suitable for chemisorption given the observed non-zero values ($\varepsilon = 0.28$ eV).

KEYWORDS: Graphene, boron nitride, density functional theory, molecular orbitals, reactivity parameters.

PARÁMETROS DE REACTIVIDAD DEL GRAFENO NEGRO VS. GRAFENO BLANCO DE DIMENSIONES DE 1,0 NM2: ESTUDIO QUÍMICO CUÁNTICO COMPUTACIONAL

RESUMEN

Se investigaron los parámetros de reactividad del grafeno extendido (grafeno negro con simetría D_2h) y el nitruro de boro (h-BN) (grafeno blanco con simetría C_2v), ambos con dimensiones de 1.0 nm^2, usando la teoría del funcional de la densidad (DFT) combinada con la metodología HCTH/GGA/DNP. Para la estabilidad estructural se consideró el crite-

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[1] Degree in chemistry and biology, PhD in chemistry. Full-time teacher in Universidad de La Guajira. Member of the Research Group GIFES

[2] Degree in chemistry. PhD in chemistry and physics, Researcher at PDVSA-Intevep. El Tambor, Los Teques, Venezuela

[3] Degree in physics and mathematics, Magister in physical and applied sciences. Full-time teacher Universidad de La Guajira. Member of the research group GIFES

[4] Degree in mathematics, Magister in physical and applied sciences. Full-time teacher Universidad de La Guajira. Member of the research group GIFES

Correspondence author: Araujo Contreras, V.d.J. (*Vianeis De Jesús*): Universidad de la Guajira, Km 5 vía a Maicao. Tel.: (57) 3017359901 /
Email: varaujo@uniguajira.edu.co,

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rio de obtención de autovalores positivos de la matriz hessiana. Para obtener los parámetros de reactividad (potencial químico, dureza química, *gap* e índice electrofílico) se consideraron los orbitales moleculares HOMO y LUMO; además, se reportan la densidad de estados molecular (DOS) y las propiedades eléctricas y electrónicas. Los resultados indican que el grafeno blanco es mucho más estable, pero más reactivo que el grafeno negro, debido a los valores obtenidos para la dureza química (1,157 eV y 0,329 eV, respectivamente), el potencial químico (2,39 eV y 3,85 eV, respectivamente) y el *gap* (2,313 eV y 0,657 eV respectivamente). Los valores del índice electrofílico indican que el grafeno negro podría adsorber sobre su superficie alguna molécula prefiriendo el proceso de fisisorción (ε=0,0 eV), mientras que al grafeno blanco podría tener preferencia por la quimisorción dado que se observan valores diferentes de cero (ε=0,28 eV).

PALABRAS CLAVE: grafeno, nitruro de boro, teoría del funcional de la densidad, orbitales moleculares y parámetros de reactividad.

PARÂMETROS DE REACTIVIDADE DO GRAFENO PRETO VS. GRAFENO BLANCO DE DIMENSÕES DE 1,0 NM^2: ESTUDO QUÍMICO QUÂNTICO COMPUTACIONAL

RESUMO

Se pesquisaram parâmetros de reatividade do grafeno estendido (grafeno preto com simetria D_2h) e nitreto de boro (h-BN) (grafeno branco com simetria C_2v), ambos com dimensões de 1,0 nm^2, usando a teoria do funcional da densidade (DFT) combinada com a metodologia HCTH/GGA/DNP. Para a estabilidade estrutural se considerou o critério de obtenção de autovalores positivos da matriz Hessiana. Para obter os parâmetros de reatividade (potencial químico, dureza química, gap e índice electrofilico) se consideraram os orbitais moleculares HOMO e LUMO; Além disso, se reporta a densidade de estados moleculares (DOS) e as propriedades eléctricas e electrónicas. Os resultados indicam que o grafeno branco é muito mais estável, mas mais reativo do que o grafeno preto, isto devido aos valores obtidos para a dureza química (1,157 eVy 0,329 eV, respectivamente), o potencial químico (2,39 eV e 3,85 eV, respectivamente) e ogap (2,313 eV 0,657 eV, respectivamente). Os valores do índice eletrofílicos indicam que o grafeno preto pode adsorver sobre sua superfície alguma molécula preferindo o processo fisiossorção (ε = 0,0 eV), enquanto o grafeno branco poderia ter preferência por a quimissorção por que se observa valores diferentes de zero (ε = 0,28 eV).

PALAVRAS-CHAVE: Grafeno, nitreto de boro, a teoria do funcional da densidade, orbitais moleculares e parâmetros de reatividade.

1. INTRODUCTION

In order to understand the potential of nanotechnology, it is important to know that the physical and chemical properties of matter change on a nanometric scale given the dominance of quantum effects. Electrical conductivity, heat, resistance, elasticity, reactivity, and other properties of a material behave differently at different scales; Boddien and Junge (2011). Nanotechnology has had a significant impact on the field of chemistry, and the study of atom nanoclusters is a current topic of interest; Jacobser (2009), Maubert, *et al*. (2008), Whitesides (2005). Nanoclusters are important both for catalysis and for the development of new materials for various applications. On the nanometric scale, materials like graphene and boron nitride have been theoretically studied using molecular models which allow researchers to characterize these materials and thereby determine their potential applications, for example, their ability to adsorb molecules. The hexagonal structure of two-dimensional graphite, called graphene, was isolated by the group Novoselov *et al*. (2004), giving rise to a variety of materials with the same hexagonal structure as boron nitride; Novoselov, *et al*. (2005), graphane; Sofo, Chaudhari & Barber (2007), Elias *et al*. (2009). Recently, researchers were able to use exfoliation and chemical vapor deposition techniques to isolate monolayers of graphite with variable thicknesses, leading to a new type of tridimensional material known as graphene; Dresselhaus (2010), Nagashima, *et al* (1993). These structures have been confirmed by different experimental techniques, such as optical and atomic force microscopy, among others.

Since graphene was isolated, important properties and applications have been found for it, including its hardness, flexibility, optics, and its ability to absorb gaseous molecules; Schedin, *et al*. (2007), Lee, *et al*. (2008), Nair, *et al*. (2008). Since it was the first completely bidimensional type of material at the molecular level, graphene is considered to be a structural model for computational simulation studies related to graphite, fullerenes, and carbon nanotubes. Given its physical, chemical, and mechanical properties, such as hardness, high melting point, low dielectric constant, and large energy gap (6.0 eV), boron nitride is one of the most interesting compounds formed by atoms from groups II and IV of the periodic table; Arya & D'Amico (2002). Boron nitride forms different phases which are analogous to those of carbon. The hexagonal phase of boron nitride (h-BN) is similar to graphite, and the cubic phase of boron nitride (c-BN) is similar to diamond; Teghil, Marotta, & Di Palma (1998). Depending on the phase, different properties can be found. For example, boron nitride in the hexagonal phase forms sp^2 hybridization and is therefore a very useful material for lubricants compared to graphite; Xiaopeng, H. & Meiyan Y. (2002). h-BN is electrically insulating due to the lack of relocation of π bonds; Reisse & Weissmantel (1999). This material has a hardness of approximately 15 GPa and is also widely used for field emission devices, optoelectronic devices, and high-powered semi-conductors; Miyake & Wang (2005). Meanwhile, cubic boron nitride (c-BN) shows sp^3 hybridization, which allows it to have diverse properties such as high resistance to wear, resistance to oxidation, and a low coefficient of friction. It is also considered to be the second-hardest material after diamond with a hardness of 70GPa; Deng & Chen (2006). This material is a good candidate for coating tools that have been exposed to high-wear environments such as cutting tools. This hard coating depends highly on the thickness of the film. He & Li (2005). The research group that carried out this research has been interested in studying materials at the nanometric level with possible applications in different fields. Therefore, this study aims to use computational chemistry methods to examine the reactivity parameters of extended graphene and hexagonal boron nitride with dimensions of 1.0 nm^2.

2. MATERIALS AND METHODS (COMPUTATIONAL DETAILS)

This study used the density functional theory (DFT) Kohn, Becke & Parr (1996), Jones & Gunnarsson (1989), and Kohn (1999), developed by Walter Kohn in the 1960s, and the DMOL-3 code (version 4.3) made available by Accelrys Inc.; Delley (1990). The method was combined with the HCTH functional at the LDA level developed by Hamprecht, *et al*. (1998), which includes correction for the correlation gradient, and the polarized atomic base (including a p orbital for hydrogen and a d orbital for carbon, nitrogen, and boron) at the all-electron level for treatment of the core (DNP); Delley (1990) and Delley (2000). Multiplicity=1 (singlet) and charge=0 (neutral) were used for all structures. HOMOs (highest occupied molecular orbitals) and LUMOs (lowest unoccupied molecular orbitals) were considered to obtain reactivity parameters. Chemical hardness was represented as: n =(LUMO-HOMO)/2 Becke (1993). Chemical potential was represented as μ=(LUMO+HOMO)/2 Perdew, Burke & Wang (1992). The electrophilic index was represented as $\varepsilon = n^2/2u$ (considered as a parameter of electronic transference); Hehre, Dichfied & Pople (1972). The energy difference between the HOMO and LUMO is the gap energy; Fujita, *et al*. (1996). The convergence thresholds used with DFT/GGA/HCTH for energy variation, maximum force, and maximum atomic displacement between the optimization cycles were: 1×10-5 Hartree, 0,002 Hartree/Å and 0,005 Å, respectively. The maximum change allowed for any Cartesian coordinate was 0.3 Å. The criterion of having positive vibration frequencies was followed to find the minimum structure stability; Foresman & Frisch (1996).

3. RESULTS

As a preliminary step to studying the potential applications of graphene and h-BN, DFT calculations were used to theoretically describe the structural and reactivity properties of these materials using chemical and vibrational descriptors. According to the structural results obtained, we observed that both B-N, C-C, and C-H bonds and B-N-B and C-C-C angles are within the typical range of values for these atoms (see **Table 1**). In addition, analysis of the optimized geometrics Hessian matrix shows that the structure has a global minimum on the potential energy surface (real vibration frequencies) due to the absence of negative values on the Hessian matrix, with 198 vibration modes for the two materials. **Figures 2a** and **2b** of the HOMO molecular orbitals show contributions of only 2py from carbon for 1.0 nm^2 and 2pz for the nitrogen in 1.0 nm^2 h-BN (**Table 2**).

For the LUMO orbital (**Figures 3a** and **3b**), an atomic orbital contribution of 2pz from the boron in 1.0 nm^2 and 2py from the carbon in 1.0 nm^2 were observed. **Figures 2a** and **3a** show that when the graphene moves from the HOMO to the LUMO, there is a phase change in the wave function, which can be observed in the change of color on the right side of **Figure 3a** with regards to **Figure 2a**. In h-BN there is charge displacement since the charge distribution changes from the nitrogen atoms (HOMO) to the boron atoms (LUMO), and the charge density disappears from the center, increasing around the edges on the boron, that is, there is surface polarization. As was mentioned in the methodology section, these orbitals were used to ascertain the chemical reactivity of the systems. According to the results of the reactivity parameters (**Table 4**), these indicate that graphene shows a lower degree of reactivity than h-BN (according to chemical potential). This result does not agree with those reported by Chigo & Juárez, (2008). Likwise, graphene shows a lower resistance to electronic redistributions (according to chemical hardness) than does h-BN. In addition, graphene behaves as a semi-conductor (Graph 1a. DOS for graphene), and h-BN behaves as an insulator. (Graph 1b. DOS for h-BN).

The low numerical value of the electrophilic index (ε) indicates that graphene could be more stable when it accepts an additional electronic charge, with preference for the physisorption process (ε=0,0 eV), while h-BN may prefer chemisorption given that values other than zero were observed (ε=0,28 eV). Finally, there is a greater degree of covalence in graphene than in boron nitride, as is indicated by the dipole moment value.

Table 1. Structures for graphene and hexagonal boron nitride (h-BN) optimized with DFT/GGA/HCTH/DNP methodology

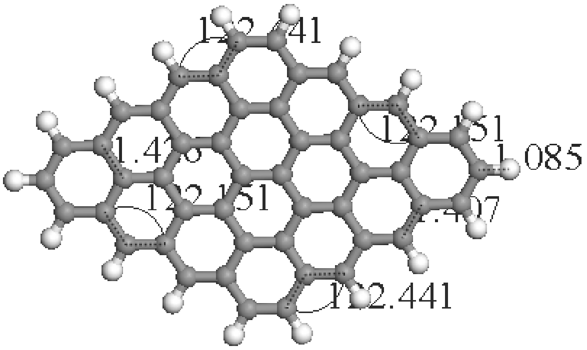


Figure 1a. Black graphene: C-C and C-H bonds, C-C-C angles.

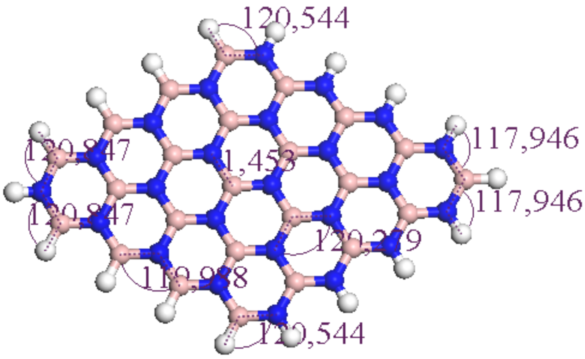


Figure 1b. h-BN: B-N bonds and N-B-N, H-N-B, and H-B-N angles.

C-C benzene: 1,4 Å; Pauling (1996); N-B graphite: 1.421 Å; Pauling (1996); C-C ferrocene / fullerene: 1.4 /1.46 Å; Seibold & Sutton (1965); nanotube-NB N-B: 1.45 Å; Rubio, Corkill, & Cohen (1994).

Table 2. HOMO molecular orbitals for 1.0 nm^2 graphene 1.0 nm^2 h-BN obtained using the DFT/GGA/HCTH/DNP methodology.

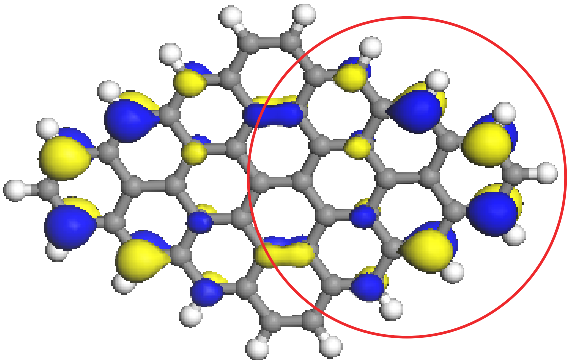


Figure 2a. HOMO molecular orbital of 1.0 nm^2 graphene with atomic distribution by 2py carbon atomic orbitals.

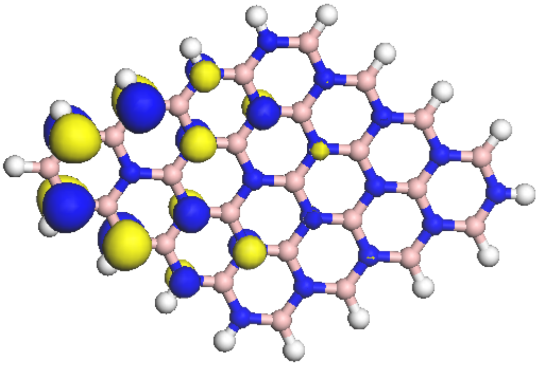


Figure 2b. HOMO molecular orbital of 1.0 nm^2 h-BN whose atomic contribution is due to 2pz nitrogen orbitals.

Table 3. LUMO molecular orbitals for 1.0 nm^2 graphene and 1.0 nm^2 h-BN obtained using DFT/GGA/HCTH/DNP methodology.

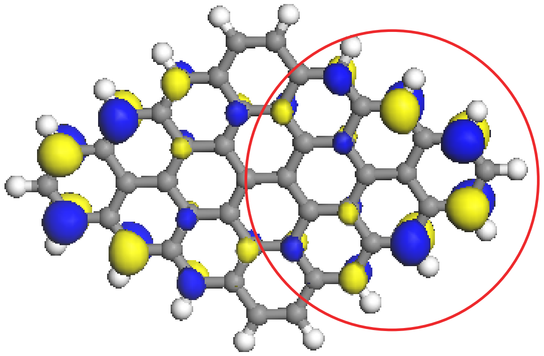


Figure 3a. LUMO molecular orbital of 1.0 nm^2 graphene with atomic contribution from 2py carbon atomic orbitals.

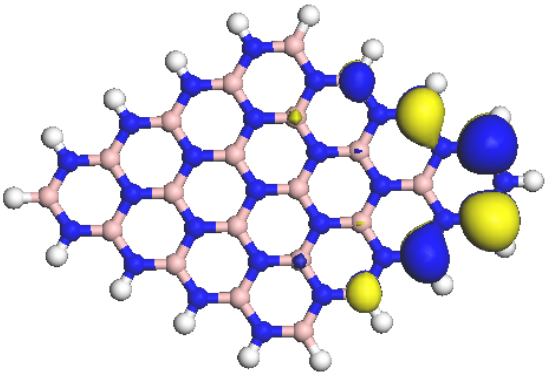


Figure 3b. LUMO molecular orbital of 1.0 nm^2 h-BN with atomic contribution from 2pz boron atomic orbitals.

Table 4. Chemical reactivity parameters calculated using HOMO and LUMO values and dipole moment for 1.0 nm^2 graphene and 1.0 nm^2 h-BN obtained using DFT/GGA/HCTH/DNP methodology.

MATERIAL	Dipole moment (Debye)	Chemical potential (μ) (eV)	Chemical hardness (n) (eV)	Electrophilic index (ε) (eV)	Gap (eV)
1.0 nm^2 graphene (D_6h symmetry)	0.0	-3.85	0.329	-0.01	-0.657
1.0 nm^2 h-BN (C_2v symmetry)	0.22	-2.39	1.157	-0.28	-2.313

Figure 1a. Graph 1a. DOS graph (electrons/Ha vs. energy in Ha) of 1.0 nm^2 graphene with gap = -0.657 eV .≈ -0.024 Ha.

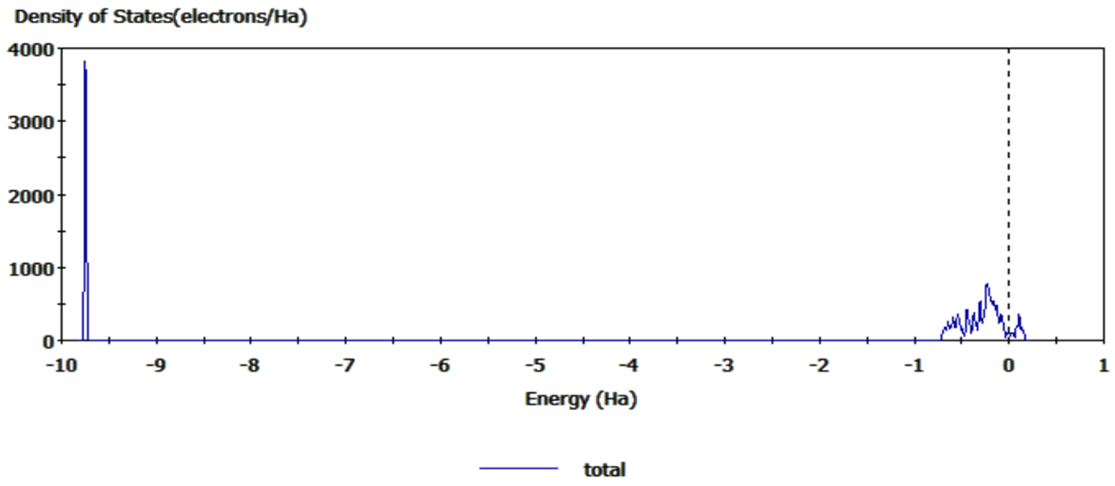
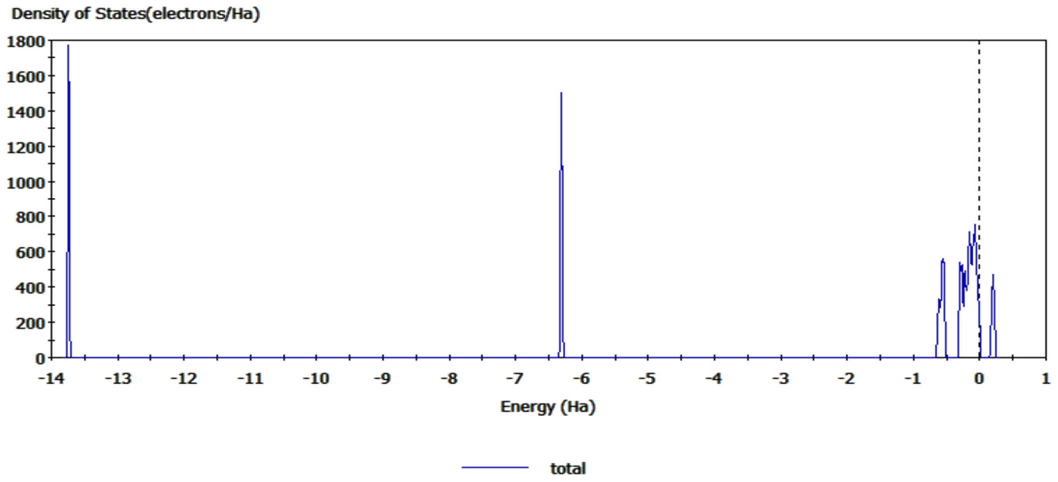


Figure 1b. Graph 1b. DOS graph (electrons/Ha vs. energy in Ha) of 1.0 nm^2 h-BN with gap = -2.313 eV ≈ - 0.084 Ha**.**



4. CONCLUSIONS

Computational molecular simulation was used in this study to provide results that are in agreement with those reported in the literature; Novoselov, *et al.* (2004) & Schedin, *et al.* (2007) regarding the existence of extended graphene and boron nitride under conditions of temperature and pressure. Said systems show semi-conductor electronic behavior for black graphene, and for boron nitride (white graphene) insulating electronic behavior was observed, but with greater chemical reactivity and a lower covalence than black graphene (indicated by dipole moment). Finally, we conclude that black graphene shows greater difficulty regarding the process of chemisorption than does h-NB, according to the numerical values for chemical reactivity parameters. This study is useful to better understand the process of atom and molecule adsorption on the surface of these materials, as well as to predict new structures.

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