ISSN NO. 2320-5407

Journal homepage: http://www.journalijar.com

INTERNATIONAL JOURNAL OF ADVANCED RESEARCH

RESEARCH ARTICLE

Influence of Doping on Electronic Properties to Graphene-Al/N Sheet by Using Density Function Theory

Ali S. Hasan ,Hamid I. Abbood
University of Babylon /College of Science

Manuscript Info

Manuscript History:

Received: 15 October 2015
Final Accepted: 18 November 2015
Published Online: December 2015

Key words:

Graphene Sheet, Energy gap, Ionization potentials, Electron affinity, Fermi energy, Electronegativity.

Corresponding Author

Ali S. Hasan

Abstract

In this research, we study Influence of Doping on Electronic Properties to Graphene-Al/N Sheet by Using Density Function Theory. The results of the ground state total energy, The total energy be the largest value at Pure Graphene Sheet and it was decreased with increasing the number of Al and N atoms in G-Al/N 3 Lines Sheet. The energy gap Eg are few, Pure Graphene Sheet (0.035ev). Fermi energy value increase for each of the Pure Graphene Sheet and G-Al/N 3 Lines Sheet, respectively, that means the electrons in these molecules have a large escaping tendency. The IP and EA are decrease with Adding the Al / N compound. Pure Graphene Sheet has the highest value for electronegativity, the reason goes back to the symmetrical distribution of the electrons.

INTRODUCTION

Graphene is a nanoscale allotrope of carbon. Unlike graphite, the most common allotrope, graphene is quasi-two-dimensional, since electrons can only move between carbon atoms in the 2D lattice. The extra quantum confinement of the electrons due to the lack of a third dimension gives graphene various novel properties. For example, electrons interact with carbon atoms in the lattice to create a system that acts like a single mobile charge carrier. The carrier moves ballistically over the graphene surface, enabling graphene sheets to conduct electricity very well [1,2]. Other complex interactions between electrons and the hexagonal lattice make graphene transparent, exible and strong [2,3]. These properties and others have compelled many researchers over the last half-decade to study graphene for a diverse array of uses. While graphite has been used for ages in a range of purposes from lubricant to pencils, researchers only began widely studying graphene around the year 1990. For the rst decade, research was hindered due to the diculty of producing it in an electrically isolated environment and without defects[4,5]. However, in 2004, two researchers named Andre Geim and Konstantin Novoselov at Manchester University discovered a new method for producing graphene through mechanical exfoliation [6,7].Graphene, an excellent conductor, is not a metal but rather a zero-gap semiconductor. While the valence and conduction bands do not overlap in graphene, they touch at the Fermi level [5,8,9].

Theoretical Methods and Computational Details

The electronic properties of the title compounds in have been calculated using Density functional theory LDA/SZ basis sets method, All calculations were carried out using the SIESTA – trunk - 462 program [10] , GOLLUM program " version 1.0 " [11] and Gaussian View 5.0.8 [12]. Fig.1 represents the molecules under study. All the computational studies were carried out using the density functional theory (DFT) methods implemented in the SIESTA – trunk - 462 of program (relaxation), and calculations of electronic and electrical properties by employing

the LDA/SZ density functional theory calculations using the Gollum program. Conformational analysis of the molecules has been performed to have an idea about the highest energy structures of the species. The LDA/SZ has shown to be highly successful for calculation the electronic properties such as ionization potentials, electron affinity, fermi energy, electrochemical hardness, electronic softness, electronegativity and energy gaps [16-18]. The DFT partitions the electronic energy are the electronic kinetic energy, the electron nuclear attraction and the electron-electron repulsion terms respectively.

The HOMO and LUMO energy was also used to estimate the IP and EA in the framework of Koopmans theorem:

$$IP = -\varepsilon_{HOMO} \text{ and } EA = -\varepsilon_{LUMO}$$

Within the framework of the density functional theory (DFT), one of the global quantities is chemical potential (μ), which is measures the escaping tendency of an electronic cloud, and equals the slope of the Energy versus N(number of electrons) curve at external potential v(r) [23]:

$$E_f = \left[\frac{\partial E}{\partial N}\right] v_{(\vec{r})}$$

Finite difference approximation to Fermi energy gives,

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

The theoretical definition of chemical hardness has been provided by the density functional theory as the second derivative of electronic energy with respect to the number of electrons N, for a constant external potential v(r) [23]:

$$\eta = \frac{1}{2}\left[\frac{\partial^2 E}{\partial N^2}\right]_{v(r)} = \frac{1}{2}\left[\frac{\partial \mu}{\partial N}\right]_{v(r)}$$

Finite difference approximation to Chemical hardness gives,

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

For Insulator and semiconductor, hardness is half of the energy gap (E_{HOMO} -E_{LUMO}) and the softness is given as [22] :

$$S = \frac{1}{2\eta} = \left(\frac{\partial^2 N}{\partial E^2}\right)_{V(r)} = \left(\frac{\partial N}{\partial \mu}\right)_{V(r)}$$

Results and Discussion

Table.1 shows the ground state calculations of the pure Graphene sheet and G-Al/N 3 Lines Sheet relax at the minimum energy. The results of the ground state total energy E_T in (ev), The total energy E_T be the largest value at Pure Graphene Sheet, It was decreased with increasing the number of Al, N atoms in G-Al/N 3 Lines Sheet, as we see in Fig.2, this result is a reflection of the binding energy of each structure [13]. This an indicates to that these structures have good relaxation. This leads us to be certain that the effect of adding atoms (Al,N) in Pure Graphene Sheet on the total energy of the molecule is effective. The energy gap Eg are few, Pure Graphene Sheet (0.035ev), and therefore the Graphene sheets have high conductivity and small energy gap, and less than the value of the energy gap by increasing the number of atoms added, as the energy gap of G-Al/N 3 Lines Sheet (0.079 ev), as we see in Fig.3, and the reason that the atoms are added (Al,N) have electronegative largest of electronegative (C). The Table.1 shows that the values of E_{LUMO} greater than the values E_{HOMO} for each of the Pure Graphene Sheet, G-Al/N Diagonal Sheet and G-Al/N 3 Lines Sheet. This change leads to reduce the gap between the LUMO and HOMO, as we see in Fig.4 and Fig.5[13,14]. In the Table.1 that the fermi energy value increase for each of the Pure Graphene Sheet and G-Al/N 3 Lines Sheet, Respectively, that means the electrons in these molecules have a large escaping tendency, Also, Indication of the decline in the value of HOMO and LUMO. as we see in Fig.6[14,15]. The ionization potential IP and electron affinity EA of the structures, where the IP and EA are decrease with Adding the Al / N compound, the IP and EA are Decreasing for each of the Pure Graphene Sheet and G-Al/N 3 Lines Sheet, respectively, as we see in Fig.7 and Fig.8, that means the doped Graphene Sheet has low ability to donating or accepting an electron to become cation or anion. As we see in Table.1. Fig.9) and Fig.10)showed that the Pure

Graphene Sheet and G-Al/N 3 Lines Sheet have high electrochemical hardness η and low electronic softness S. These results correspond to the result of energy gap that the species has, and indicate to the activity of the species in reaction with the surrounding species [13,14].
Electronegativity X of G-Al/N 3 Lines Sheet is less than that for Pure Graphene Sheet, as we see in Fig.11, which means that the electrons in G-Al/N 3 Lines Sheet have a large escaping tendency, While Pure Graphene Sheet has the highest value for electronegativity, The reason goes back to the symmetrical distribution of the electrons [14].

Table.1: Electronic Properties of Pure Graphene Sheet and and G-Al/N Lines

Species	ET(ev)	EHOMO (eV)	ELUMO (eV)	Eg(ev)	Ef(ev)	IP(ev)	EA(ev)	η(ev)	S(ev)	X(ev)
Pure Graphene Sheet	-32250.40852	-6.709	-6.675	0.035	-6.692	6.709	6.675	0.017	28.860	6.692
G-3 Lines Sheet	-77774.32129	-5.912	-5.834	0.079	-5.873	5.912	5.834	0.039	12.726	5.873

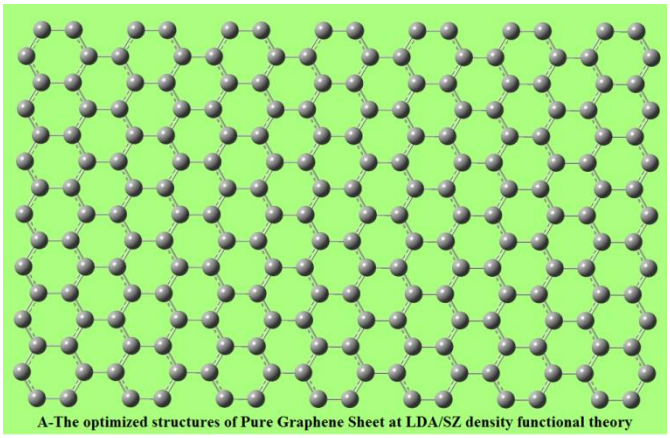

Fig.1: Structures of Graphene Sheets discussed in this work.
Nitrogen≡ blue, Carbon≡ gray, Aluminum ≡ violet .

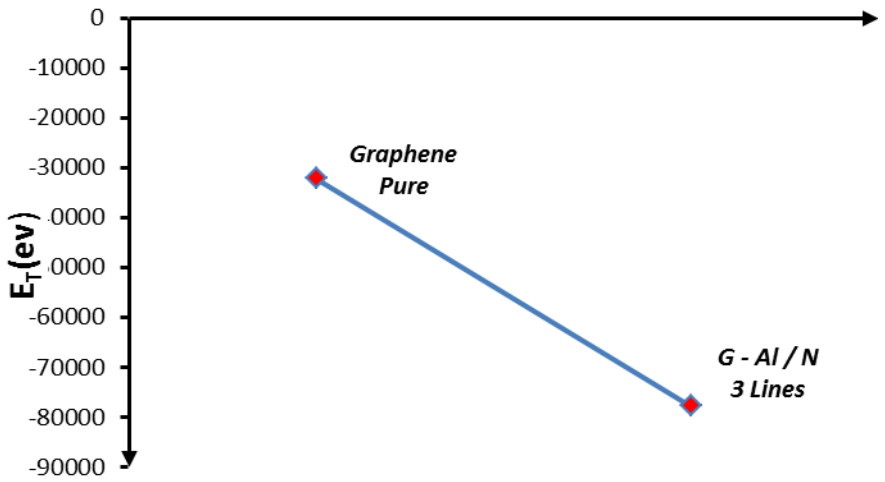

Fig.2: The total energy in ev of the Pure Graphene Sheet and G-Al/N 3 Lines Sheet

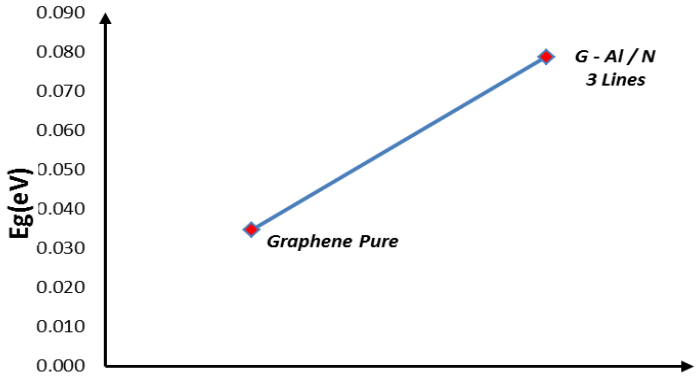

Fig.3: The forbidden energy gap in eV of the Pure Graphene Sheet and G-Al/N 3 Lines Sheet

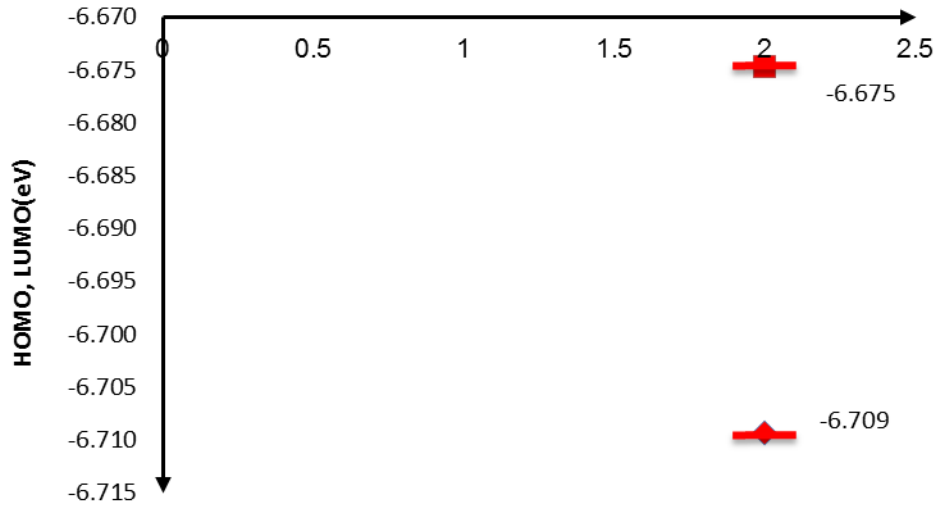

Fig.4: The LUMO –HOMO of Pure Graphene Sheet

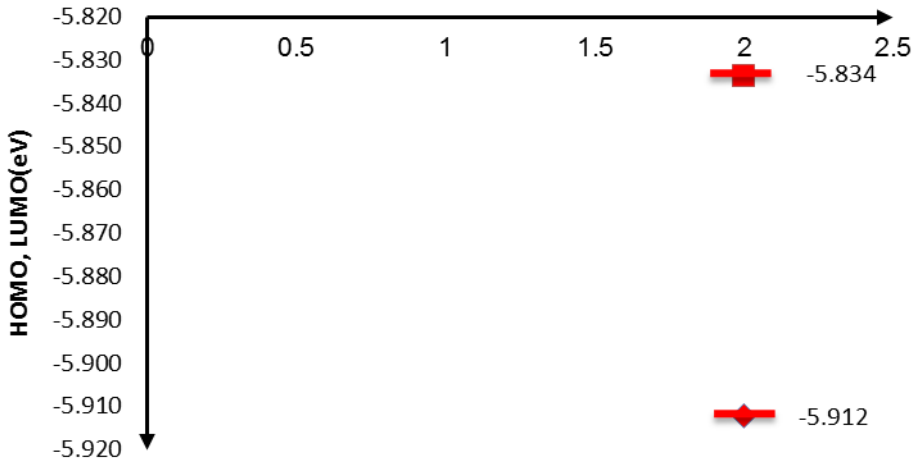

Fig.5: The LUMO –HOMO of G-Al/N 3 Lines Sheet

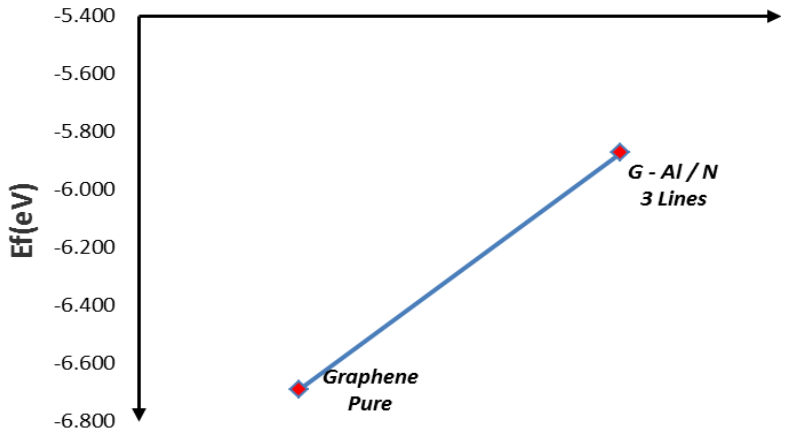

Fig.6: The fermi energy in eV of the Pure Graphene Sheet and G-Al/N 3 Lines Sheet

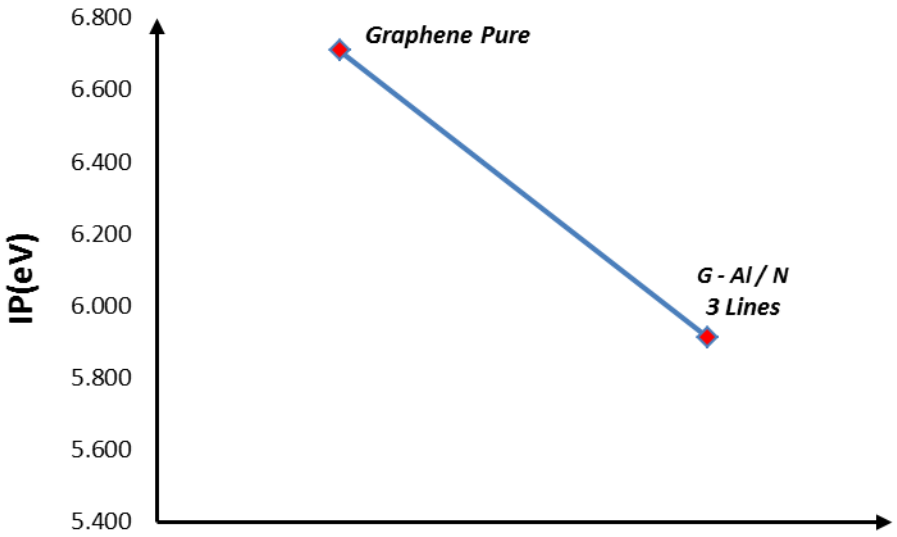

Fig.7: The ionization potential in eV of the Pure Graphene Sheet and G-Al/N 3 Lines Sheet

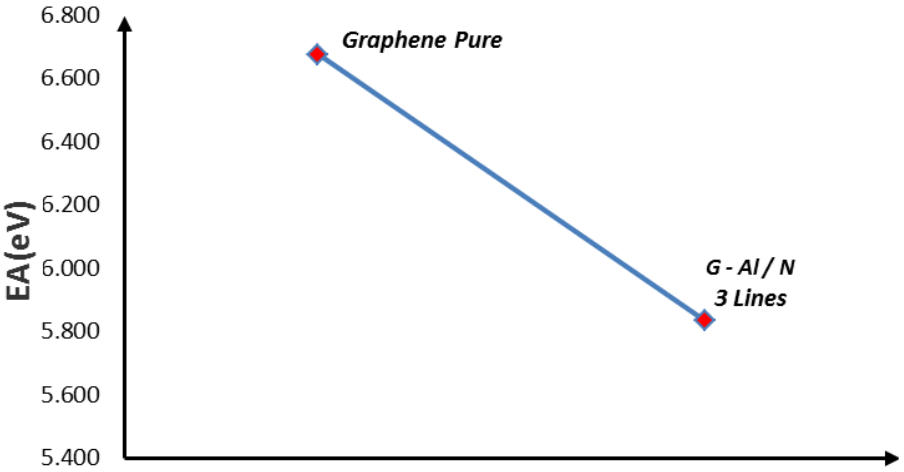

Fig.8: The electron affinity in eV of the Pure Graphene Sheet and G-Al/N 3 Lines Sheet

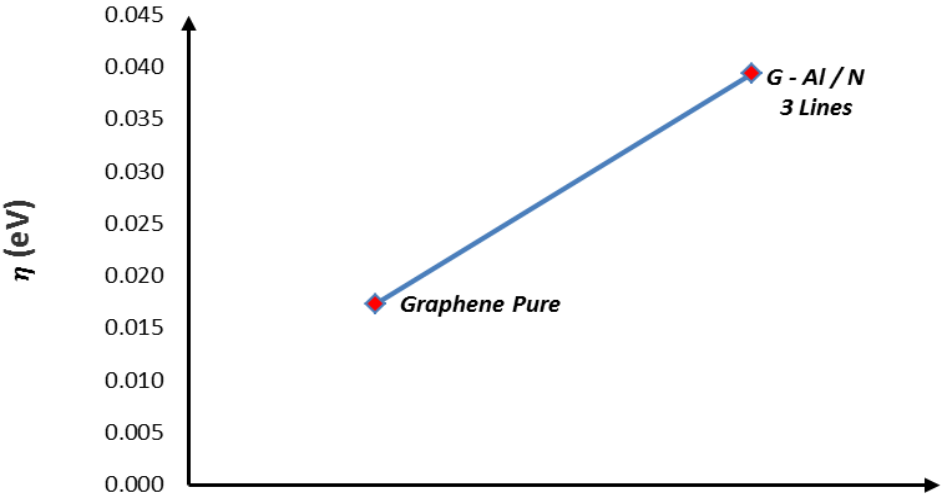

Fig.9: The electrochemical hardness in eV of the Pure Graphene Sheet and G-Al/N 3 Lines Sheet

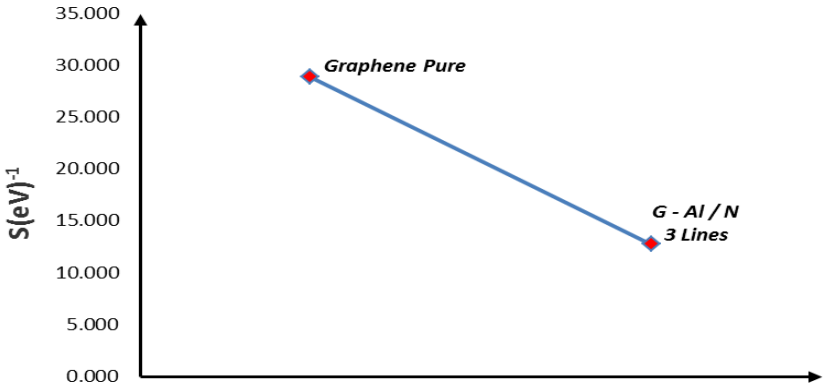

Fig.10: The electronic softness in $(eV)^{-1}$ of the Pure Graphene Sheet and G-Al/N 3 Lines Sheet

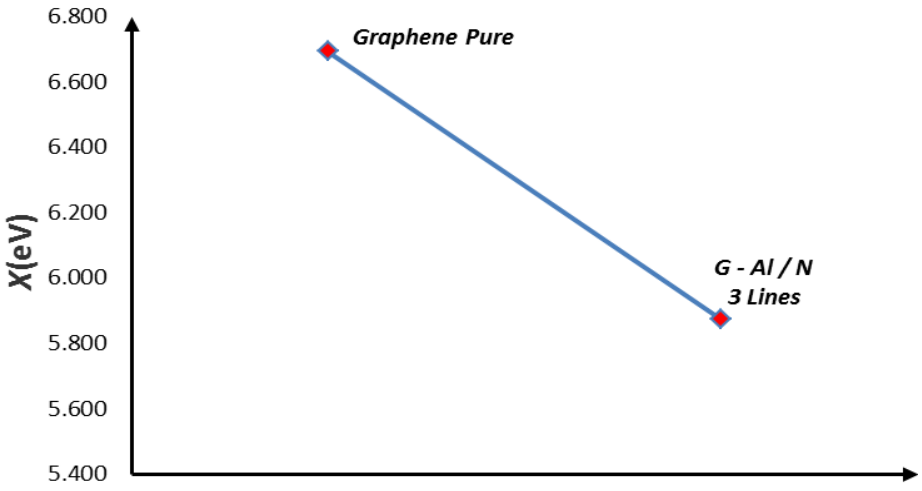

Fig.11: The electronegativity in (eV) of the Pure Graphene Sheet and G-Al/N 3 Lines Sheet

Conclusions

Graphene Sheet was design at Gauss View 5.0.8. and relax by employing the LDA/SZ Density functional theory at SIESTA – trunk - 462 of program, the electronic properties were calculated by employing the LDA/SZ calculations and carried out using the Gollum software. From the results, one can conclud:

1. The relax structure under study has geometrical parameters lie in the same range of the aromatic rings, that means the method we used in the relaxation is a suitable for these kinds of structures.
2. Geometry optimization for graphene sheet has been found in a good agreement with experimentalata, while for other studied molecules (1(A,B) it has not been found a reference data.
3. The total energy of the graphene sheet is decrease with increasing the number of Al / N atoms added in place of carbon atoms in the phenylene rings.
4. Number of Al / N atoms added in place of carbon atoms in the phenylene rings lead to increase forbidden energy gap, this is a sign to that the graphene sheet has high conductive than the graphene sheet.
5. Fermi energy value increase for each of the Pure Graphene Sheet and G-Al/N 3 Lines Sheet, Respectively, with adding the number of Al / N atoms.
6. The electronic properties (IP, EA, η, S, χ) was calculated by using energy-vertical method are a good agreement with experimental result and better than was calculated by using orbitalvertical method, thus Koopman's theorem is not satisfied accurately.

Refrences

[1] A. A. K. Geim. The rise of graphene. Nature materials, 6(3):183-191, 2007.
[2] J. S. Bunch, Scott S. Verbridge, Jonathan S. Alden, der Zande van, Jee-vak M. Parpia, Harold G. Craighead, and Paul L. McEuen. Impermeable atomic membranes from graphene sheets. Nano Letters, 8(8):2458-2462, 2008.
[3] Keun Soo Kim, Yue Zhao, Houk Jang, Sang Yoon Lee, Jong Min Kim, Kwang S. Kim, Jong-Hyun Ahn, Philip Kim, Jae-Young Choi, and Byung Hee Hong. Large-scale pattern growth of graphene _lms for stretch-able transparent electrodes. Nature, 457(7230):706-710,2009.
[4] Christian Schonenberger. Bandstructure of Graphene and Carbon Nan-otubes: An Exercise in Condensed Matter Physics.
[5] B. Pollard, Growing Graphene via Chemical Vapor Deposition, Department of Physics, Pomona College, 2011.
[6] Scott Berkley, Ian Frank, Arend van der Zande, David Tanenbaum, and Paul McEuen. Mechanical properties of suspended graphene sheets, 2008.
[7] Scott Berkley, Arend van der Zande, David Tanenbaum, and Paul McEuen. Gold nanoparticles on graphene surfaces, 2007.

[8] Anthony C. Fischer-Cripps. The materials physics companion. Taylor &Francis, New York, A.C. Fischer-Cripps.; Includes index, 2008.
[9] Ian Frank. Shaping graphene, an alternative approach. Undergraduate thesis, Pomona College Physics, 2008.
[10] E. Artacho, J. Gale, A.Garc, J. Junquera, P.Ordej, D. anchez-Portal and J. Soler, "SIESTA-trunk-462", Fundaci on General Universidad Aut onoma de Madrid, 2013.
[11] J. Ferrer, C. Lambert, V. García-Suarez, S. Bailey, S. Hatef, D. Manrique, "GOLLUM version 1.0", Lancaster University, 2014.
[12] R. Dennington, T. Keith and J. Millam, "Gauss View 5.0.8", Semichem Inc, 2008.
[13] S. Brun and M. Thomsen," Electronic and optical properties of graphene and graphene antidot structures", Aalborg Univers.
[14] R. Faccio, L.Fernández-Werner, H. Pardo, C. Goyenola, A. Denis and W. Mombrú," Mechanical and Electronic Properties of Graphene Nanostructures", University Campus STeP Ri.
[15] M. Topsakal, S. Cahangirov, and S. Ciraci, Appl. Phys. Lett. 96, 091912 (2010).