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Nano-capacitors as batteries including graphene electrodes and Ga-N mixed with bio-polymers as insulator

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ABSTRACT
Battery stores energy via a chemical process while a capacitor stores static electricity, therefore this generates when electric charges in a material are out of balance. Capacitors have several advantages than batteries because they charge and discharge faster, they don't use harmful chemicals, don't weigh as much and last longer. In this research, we have simulated one which is combined of a graphite layer that is separated through an insulating medium of polymerase's wurtzite Ga-N sheets. It has been shown that the alternate boron and nitrogen atoms instead of carbon are the suitable dopants for hetero-structures of the G// wurtzite Ga-N//G capacitors. We have shown that the Quantum effect has appeared in this capacitor due to the electropositive-electronegative coupled of wurtzite Ga-N and this effect cannot occur in the two electro negative or two electro positive elements layers. Therefore by this unique property our capacitor has been modeled to store a large capacity for green storage of energies in the new world of technologies.
Keywords: *graphene electrode, boron and nitrogen doping, nanoscale dielectric capacitors, wurtzite Ga-N dielectric.*

1. INTRODUCTION

Nanoscale capacitor has been developed for achieving the properties which are important to other systems of energy's storage and also they have been developed as one of the most significant energy storage mediums. Those capacitors are able to deliver higher quantities of charges at higher power limits. Their stable durability and quicker load periods select them beneficial in several subjects and equipment [1-5]. Recently; Graphene, h-BN, Ga-N and Nano capacitors including two electrodes and dielectric sheets have been developed in Nano biotechnology [5-7]. These nanoscale dielectric capacitors (NDC) consist of two metallic graphene layers separated through insulating N-Ga thin layer which has been applied for simulating in view point of structures and molecular designing. Experimentally and theoretically investigations on this system were focused for understanding the dielectric depended of these structures to form a unique capacitor including thin layers as charge holding mechanism [4-10].Furthermore it was explained that graphene might be preserve current densities five order of magnitude larger than the silver [6-12]. Since the major goal of using capacitors are for reserving energies through storing equal magnitude of electrical charges in both opposite sign of two electrodes (plates), the charged capacitors are in a static and non-equilibrium state. The energies stored are liberated when the electrodes are connected together via an external circuit, so that the discharged mechanism shifts into an equilibrium state. In this study, we consider the above mentioned of NDC model including graphene as two electrodes which combined with Ga-N plates as insulator using ab initio, density functional theory (DFT) and Extended-Huckel calculations. This nanoscale capacitor model consists of a few hexagonal Ga-N layers, which are stacked between two graphene plates (Fig.1) .

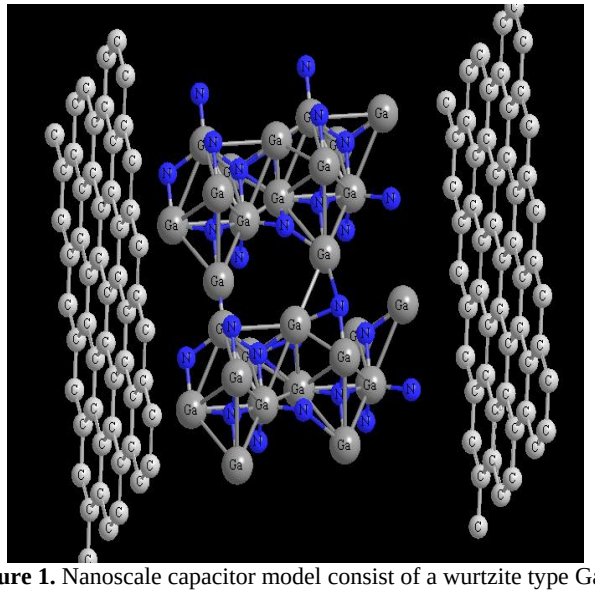

Figure 1. Nanoscale capacitor model consist of a wurtzite type Ga-N layer.

Gallium nitride (Ga-N) is a binary III/V direct bandgap. Semi-conductor usually applied in light-emitting diodes since the 1990s. These compounds are very hard material which has a Wurtzite crystal structure. Its wide band gap of 3.4 eV cause several special properties for using in optoelectronic or high -power and frequencies instruments. As forinstance, Ga-N is the substrate which makes violet (405 nm) laser diodes possible, withouttheuse of nonlinear optical frequency-doubling.

It is not sensitive to ionization with radiation therefore it is a suitable material for solar cell arrays for satellites and especially for militaries in spaces activities. Due to Ga-N transistors which operate at much higher temperatures and also work at much higher voltages is better material than gallium arsenide (GaAs) transistors.

Ga-N layer (Fig.2) has a suitable and wide band gap which can vail as an insulator dielectric material among the graphite layers. Since the distances between two electrodes and wall thickness of those insulators separation of these kind capacitors are less than 11 angstrom, the stored energy must be calculated from the first principles. In this work, the capacitance values have been obtained from the DFT and compared through an extended-Huckel method (QM/MM). Designing the spacing of capacitors between two electrode sheets at nanoscale is essential to achieve a high capacitance. So, the 3D combinations of those structures have been prepared via selected stacking of varying numbers of layers which can be enable us for offering number of options in constructing capacitors with different situations. Thus, in this kind capacitor model, considerable quantum size effects at small separations by varying the separation distances can be observed and must be evaluated.

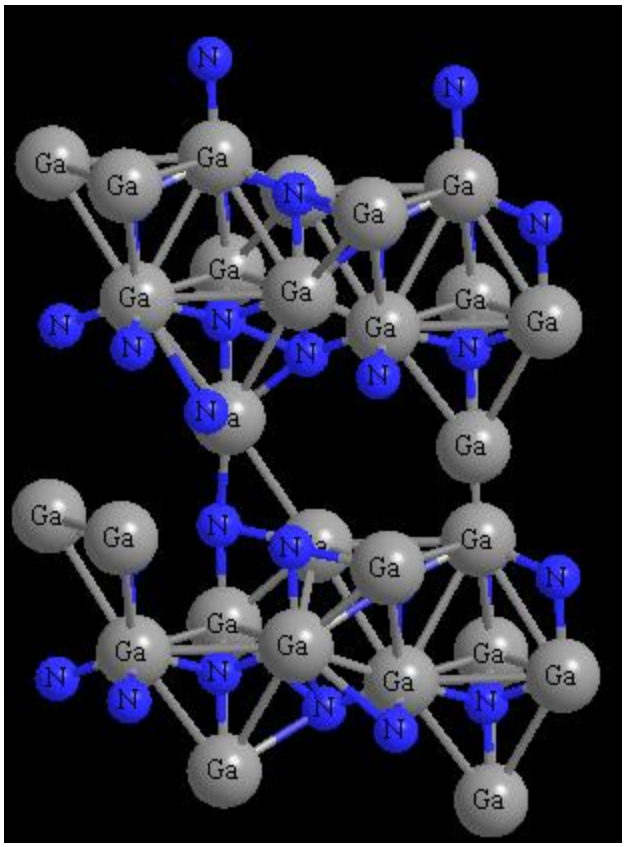

Figure 2. Ga-N layer has suitable and wide band gap.

In this investigation, a sample of a capacitor is made via creating a few insulating layers of (h-Ga-N) between two BN-doped graphene electrodes. It has been assumed that the electrodes field by $\pm Q$ charges from one of the electrodes toward the opposite electrode. By letting the electrons tunnel via the insulating layers from the (-) to the (+) terminals, thus the charges ($Q+\Delta q_e$) reside on the top sheet and ($-Q\ -\Delta q_e$) resides on the bottom sheet of electrodes. Therefore the stored energies in this position are now $E_f = \frac{(Q+\Delta q)^2}{2C}$ and the initial energies stored through an electrostatic field among the capacitor sheets and are given by equation $E_i = \frac{Q^2}{2C}$. These energies cannot be stored in the capacitor's sheets until an electron tunnels between insulator layers from the (-) to the (+) terminals.

Where the change in stored energy can be indicated as: $\Delta E_s = E_f - E_i = \frac{\Delta q(Q+\frac{\Delta q}{2})}{C}$ (1). in this mechanism the larger voltages are in the range of $-\frac{\Delta q}{2C} < \Delta V < +\frac{\Delta q}{2C}$, which are the tunneling currents and will only flow during sufficient voltages $|\Delta V| > |\frac{q_e}{2C}|$. This effect is known as the coulomb blockade.

Obviously, the capacitor plate's separation, "d", might be small for the tunneling effect for any taking places in the system. In the macroscopic systems for a small capacitor (in the range of C~10^{-13} F), it can be exhibited that amount of $|\Delta V| > 1.6\mu V$ are needed for any tunneling occurring. And meanwhile for nanoscale capacitors with capacitances in the ranges of C ~ 10^{-17} F and so on, the amount of $|\Delta V| > 1.6mV$ and for the nanoscale capacitor with C~10^{-19} F, the range of $|V| > 0.75$ are required for having the tunneling effects. Thus, coulomb block's effects are not appearing in the macro-sized circuits because of the low charging energies. However, it can be occur in the nanometers scales because of the charge quantization. For the small systems, the capacitances might be trivial that the charging energies "$\frac{e^2}{2C}$" is going to be great therefore the energy value for tunneling of the quantum position would then increase.

The tunneling resistances can also be assumed as: $R_{Tun} = \frac{\Delta V}{I}$ (2) that are not a normal resistance, however, theoretically allowing electrons for crossing the insulating junction as discrete occurrences where "I" is the resulting current due to the tunneling effect. Tunneling resistance is an imaginary one which allows the electrons for crossing the insulating junction during "t=$R_{Tun}C_Q$ (3) "and C_Q is the quantum capacitance. "t" is a time associated with tunneling events and is considered to be the approximate life-time for the energies states of each electron. The "R_{Tun}", have to be finite (not too big). Therefore in this condition, the charges are said to be well quantized and also the capacitors are evaluated to be a tunneling junction. When the quantum well descends below the Fermi's level, an electron start to be accommodated in the position of the quantum well and any further electrons (in the graphene layers) become sensitive for charging spilling into the vacuum spaces of the capacitors [12-27]. The hybrid capacitances and consequently the quantum capacitances are related to the net capacitances, C_{net}, via the equation of $\frac{1}{C_{net}} = \frac{1}{C_g} + \frac{2}{C_Q}$ (4). It is notable that C_Q is many orders of magnitude greater than the C_g.

2. MATERIALS AND METHODS

Computational details: Calculations were accomplished using Gaussian09 and GAMESS packages. In this investigation, it has been basically focused on the results from both DFT calculation and extended Huckel. For ab-initio the m06, m06-L methods have been applied and Extended-Huckel has been used for the non-bonded interaction of G/ (Ga-N)/ G, which are monotonous

through the comparison between different situations. The m062x, m06-L, and m06-HF are a novel ultra-hybrid density functional including a good reference in non-bonded interactions and are suitable for calculating the energies of the distances among the fragments of the capacitors, in medium (~3–6Å), and long ranges of dielectric thickness (≥6 Å)[28-32]. The double ζ-basis sets including polarization orbitals have been applied for doped graphene atoms. Meanwhile, single ζ-basis sets with polarization orbitals have been employed for the Ga-N layers. For the non-covalent interactions, B_3LYP and BLYP methods are unable for describing a van der Waals interaction between two plates of the capacitor system. In medium-range interaction, such as the interaction of two electrodes and also between dielectric and each electrode sheet meta- hybrid calculations are needed. In the lack of these kind abilities, most other popular functional describe medium-range of exchange and correlation energies limitation of their applicability for distant non-bonded systems between two electrodes and dielectric thickness. In addition, some recent works have been exhibited that in-accuracy for the medium-range exchange energies lead to large systematic errors for the prediction of molecular properties [33-36]. Geometry optimization and electronic structure evaluation have been carried out using the DFT approach which arebasedon an iterative solution of theKohn-Sham equationof the densityfunctional.The Perdew-Burke-Ernzerhof exchange correlation functional of the generalized gradient approximation (GGA) is adopted. In this simulation the two electrodes have doped through several percentages of boron atoms which are likely for adjusting to surrounding carbon host atoms. Therefore when graphene sheets are doped with one boron atom, this atom also undergoes sp^2 hybridization. Because of the nearly same size of C and B, no significant distortions in 2-D structure of graphene are expected, except for changing in adjoining bond length. As a result, the bond lengths are found for expanding to 1.48 Å. Using the computationalprocedure as mentioned, the electronic propertiesand band structures arepossible to be calculated.

The electron densities have been defined as $\rho(r) = \eta_i \left|\varphi_i(r)\right|^2 = \sum_i \eta_i \left|\sum_l C_{l,i}\,\chi_i(r)\right|^2$(5). [39] Where $\eta_i$is orbital (*i*), φ are orbital wave functions, χ are basis functions. Atomic unit for electron density can be explicitly written as e/Bohr^3. $\nabla\rho(r) = [(\frac{\partial\rho(r)}{\partial(x)})^2 + (\frac{\partial\rho(r)}{\partial(y)})^2 + (\frac{\partial\rho(r)}{\partial(z)})^2]^{\frac{1}{2}}$ (6) $\nabla^2\rho(r) = \frac{\partial^2\rho(r)}{\partial x^2} + \frac{\partial^2\rho(r)}{\partial y^2} + \frac{\partial^2\rho(r)}{\partial z^2}$(7) [39].

Through doping B atoms in graphite Fermi level shifts significantly below the Dirac point resulting intoa p-type doping. Therefore symmetry of graphite breaks into two graphene sub-lattices. The charge transfer and electrostatic potential-derived charge were also calculated using the Merz-Kollman-Singh, chelp, or chelpG which a detailed overview of this effect the charge distribution can be calculated. Although infinite graphite sheets are intrinsically metallic, our works indicate an increase in the metallic properties. The interaction energy for capacitor was calculated in all items as indicated in equation 9: $\Delta E_S(eV) = \{E_C - (2E_G + E_{GaN})\} + E_{BSSE}$ (8) where the "ΔE_S" is the stability energy of capacitor. Based on some previous work our calculation has been modeled and simulated [40-67].

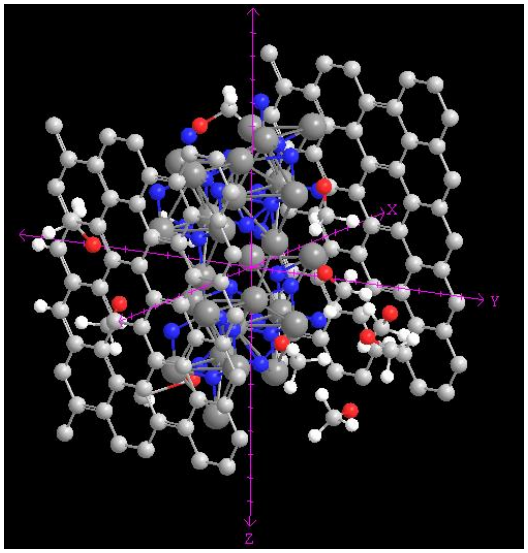

Figure 3. Nanoscale capacitor model consist of a wurtzite type Ga-N layer inside polymer' solvent.

3. RESULTS

In this investigation, Ga-N was selected as a capacitor sheet since it is suitable electrodes with excellent lattice constant near to that point of graphene. We specifically investigated the dielectric properties of graphene // $(Ga\text{-}N)_m$ // graphene, stacking for m= 1, 2 and 3 layers of dielectrics. The results are plotted in 6 Figures and the data are placed in two tables. Since the "BN" in nature is an ideal electrical chemical bond that can be polarized by applying an external electric field, the number of Ga-N between two plates of graphene has been calculated and optimized as a suitable simulation of dielectrics Table.1 and Figs 1-6.

Furthermore, graphene is well-known single layer honeycomb structure, so the proposed model can be easily fabricated. Similar to graphene, the anisotropic binding of G-BN allows for theformation of several layered structures. Long-range interlayer's interactions plays suitable dominant in characterizing the structural and mechanical properties of those systems.

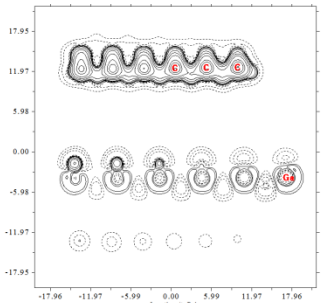

Figure 4. The situation of Kinetic Energy of Ga-N as G/ Ga-N/G capacitor

The values of the distances between Ga-N layers capping graphene layers, dielectric constants of the layered sheets (k),

magnitude of the charges on the graphene plates, electrostatic properties using the SCF density, fitting point charges to electrostatic potential charges from ESP fit, the stability energy of capacitor (eV), various capacitances including the net capacitance and the potential difference between two electrodes of graphene plates are listed in Tables1&2. Different numbers of dopants indicate proper situations for boron dopants in graphene electrodes .The potential energy difference between the two electrode layers, V $=\Delta_{EP}=\sum_{i=1}^{46}(EP_{GaNG_1}-EP_{GaNG_2})$(a.u.) are depicted in table2 and varies between 2.45 and 4.20 volts (Table.2), which leads to the accumulation of approximately identical amount of surface charges of the opposite sign.

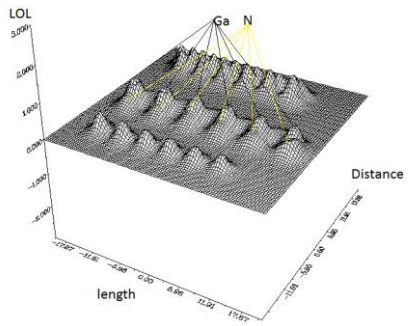

Figure 5. The situation of Density Energy of Ga-N as G/ Ga-N/G capacitor versus X, Y and Z-axis in Bohr.

Here we have considered the interlayer attraction using Extended-Huckel force field for G-BN to describe its interlayer interactions including wurtzite -Ga-N inter-layer potential, attractive components and the classical mono-polar electrostaticterm that takes intoaccount thepartially ionic character of h-Ga-N (Fig.4).

In this study, the number of h-Ga-N layers as a dielectric is 1, 2 and 3. For the nanoscale G/ $(Ga\text{-}N)_m$/ G and planar capacitor, the different voltages can be estimated from the band gap. For long distances of dielectric thickness, the classical capacitance rule of the "$C_g \propto \frac{1}{d}$" is adaptable. This adaptability does not go for short distances, which is attributed to the quantum size effect. We identified the dielectric permittivity as a function of dielectric size through ab-initio calculations Fig.5.

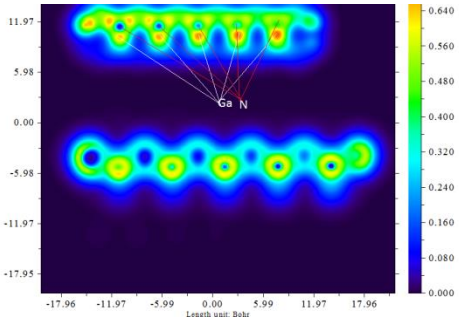

Figure 6. The color counter map of LOL Energies of Ga-N as G/ Ga-N/G capacitor

Table 2. The potential energy difference of modeled capacitors in various thicknesses

"Nano capacitor" Various sequence	Number of insulator layers	$\Delta V=\sum_{i=1}^{46}(EP_{G_1}-EP_{G_2})$		
	m	A	B	C
G/ (GaN)/G	1	2.453.10 2.70		
G/ (GaN)2/G	2	3.103.904.20		
G/ (GaN)3/G	3	3.252.152.30		

Table 1. The Charges of two G/ (GaN)/G and the stability energies.

"Nano capacitor" Various sequence	Number of insulator layers	$\frac{1}{2}Dielectric\ of\ thickness$			$\Delta E_S(eV)$			$\lvert\Delta q\rvert=\sum_{i=1}^{46}(q_{G_1}-q_{G_2})$		
	m	$A=d_1B=d_2C=d_3$			A	B	C	A	B	C
G/ (GaN)/G	1	7.158.35	6.78		0.240.310.88			0.58	0.450.46	
G/ (GaN)2/G	2	9.65	9.50	11.15	0.32	0.58	1.75	1.24	1.26	1.25
G/ (GaN)3/G	3	12.45	13.10	13.15	1.721.631.98			0.650.440.35		

4. CONCLUSIONS

In this study, we have shown the model of a nanoscale dielectric capacitor composed of a few dopant including metallic graphene layers separated by an insulating medium containing a few wurtzite -Ga-N layers. The capacitor with one layers of wurtzite -Ga-N has a high dielectric constant compared to other layers of wurtzite -Ga-N.

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6. ACKNOWLEDGEMENTS

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