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X-doped Graphene Interaction with Anodic Material LIBs

HAMID REZA JALILIAN, MAJID MONAJJEMI* and HOSSEIN AGHAEI

Department of Chemistry, Science and Research Branch, Islamic Azad University,Tehran, Iran.
*Corresponding author E-mail: m_monajjemi@srbiau.ac.ir

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ABSTRACT

The structures of graphite carbonadoes and hexagonal boron nitride or h-BN, parent materials for carbonadoes and boron nitride nano-compounds are quite similar. The measured reversible Li+ capacities of X-G// (h-BN)// X-G (X=Be, B, N) in theanode materials are extremely improved compared to the graphite structures in the based anodes. In this study Boron nitride sheet has been localized inside twoX-graphene electrodes as an option to enhance electrochemical ratio.Additionally, we have found the structure of G-X/(h-BN)n/X-G can beforimproving the capacities and electrical transports in the C-BN sheets of LIBs. In addition, the BN sheet modified and designed of X-G/ (h-BN)/X-G structures provide a strategyto improvethe yields of BN-G-sheet of anodes. X-G/h-BN/X-G could also be assembled into free standing electrode of any binder (current collector), which will causes for increasing specific energies and densities for the batteries design.

Keyword: Graphene, Doping, Anode lithium, Ion battery, LIBs.

INTRODUCTION

The carbona does such as graphite are layered materials composed of hexagonal lattices sheets; graphite[1,2] is including of carbon atoms at all direction in the lattice points, while the h-BN is consist of alternating atoms from boron and nitrogen respectively. The lattice constants for graphite and h-BN are 2.46 Å and 2.50 Å repectively[1,2]. In other side, layered BN is transparent and is an insulator[2,3] compare to graphite.The layers of h-BN are arranged as boron atoms in one layer which are located directly[2] on the top of nitrogen[2] atoms in a neighboring section and vice versa[3]. In graphite structures, stacking[3] is slightly different[2] whilehexagons are offset[2] and cannot lie on the top of each other so interlayer distances can be consider similar: 3.35 Å for graphite[1] and 3.33 Å for h-BN respectively Figure.1.

Recently, the theoretical approaches have been presented the band structures[3] of alone layer of graphite and h-BN whilefor a layer of graphite which called graphene, 2 bands cross each other at the Fermi[3] energies. For this matter, graphene is a semimetal[4]. In contrast graphene, for a alayer of the h-BN, equivalent[4] bands cannot cross each other and amount 4.5 eV band gap forms. Via an

experiment, h-BN has been calculated to have a band gap around 5.8 eV[4]. Crystallographic of BN is classified into four polymorphic[3] forms: Hexagonal[4] BN (h-BN) (Fig 1(a); rhombohedral[3,4] BN (r--BN); cubic B-N (c--BN); and wurtzite[4] BN (w--BN).

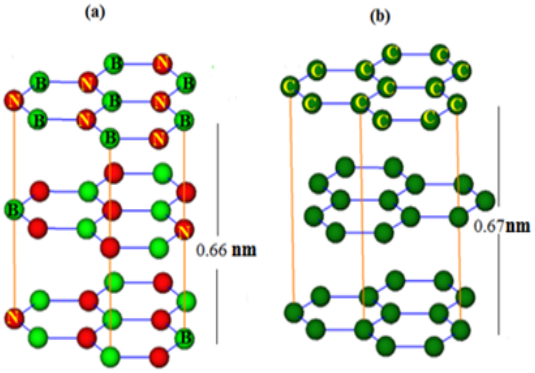

Fig.1. Crystal structures of (a) graphite; (b) hexagonal boron nitride

In 1842, Balmain[5] sensitized- BN as reaction products via boric-oxide and potassium cyanide[5] through1 atmosphere pressure. Then, various methods have been reported through h-BN and r-BN which formed under ambient[5] pressure and c-BN has been synthesized from h-BN via high pressure and high temperatures. It is notable that w-BN is prepared from h-BN via high pressure at room temperature[6].

The discovery of amazing reversible, low-voltage[7] Li-intercalation carbonaceous[8] materials, Sony Company realized the commercialization[7] of xC6/Li $_{1-x}$ CoO2 cells in 1991[7]. Lithium ion batteries (LIBs) are widely used in small gridstorage systems.

LIBs generally consist of positive and negative electrodes including a conducting electrolytewhere store electrical energy in the two electrodes[8] in the form of Li-intercalation[8] compounds. Electrodes, separator, and electrolyte are the main components of the LIB where the anode plays an essential role in the performance of these devices.

In the charging mechanism of the LIBs, Li^+ released from the negative electrode and move inside the electrolyte then inserted into the positive electrode. In the discharging mechanism,Li^+ are extracted[8] from the (+) electrode and move back to the (-) electrode. Although the electrolyte establishes high ionic conductivity[9] between two electrodes, the electrolytes[9] are not responsible[8,9] for the conduction of free-electrons . So the electrons complete the 1/2 reaction will move in the way of an extra[9] external wire.

Various experiments have accomplished for confirming the utilization of graphene in the forms of nano-sheets or nano-ribbons for enhancing lithium storage[9] capacities and for improving recharge performance[9-11]. Furthermore in this study, semi-empirical MM calculations have been donefor investigatingLi + storage between two graphene[11] sheets[12], as well as a few heteroatom-substituted[11]carbon materials[13].

Dis-charging or charging of Li+ in carbonadoes iswell established and arrangedup to now[18-21]. It has also been exhibitedthe mechanism of the repulsive forces[13] in the mixed stages which can result in the pure stages during intercalation[19,23]. In this study, chargingand discharging of Li-ions has investigated in h-BN with the positive electrode reaction as:$LiCoO2 \rightleftarrows Li1\text{-}x\ CoO2 + x\ Li+ + x\ e$ and the negative electrode reaction as: $x\ B_3N_3 + x\ Li^+ + x\ e \rightleftarrows LiB_3N_3$, while the whole reaction is:$LiCoO2 + xB_3N_3\ Li_{1-x}CoO2 + x\ LiB_3N_3$. It has been suggested[22] that lithium atoms are stored[23] via two mechanisms: intercalation and alloying[24].

Recently many works has been established for describing the intercalation and diffusion of Li^+ at different sites on carbonadoes graphite and many studies have been performed in order to explain the mechanism by which Li^+ s are stored in electrodes, including theoretical works[13-24].

The electrical conductivities for the Li+-Graphene increases[25] via increasing intercalation levels due to the donor[26] nature of electronsfor the lithium. This is in contrast of ionic conduction[26] in which diffusivity[27] decreases[26] due to the insertion of Li ions[27]. In the case of amorphous[26] carbon as thedisorder[28] increases electrical conductivity[28] significantly decreases[29]. Recently, Fisher group fabricated[29-30] a tube-in-tube structure with Li^+ intercalation capacities[2] times higher than that of the template-synthesized[30,40] Carbon-NTs, as the inner tubules provided more electrochemical[40,43] active sites for intercalation of Li ions[28,51].

Boron nitride tubes(BN-NT), which firstly predicted and synthesized by Rubio and Chopra respectively[40,48], has a structural similar to Carbon-NTs but,in contrast to the Carbon-NTs being metallic 40(semiconductor) depending on chirality[42,46]. BNNTs are usually can be an insulator regardless of their helicity, tube diameters and number of tube walls[42-49].

Experimental results have exhibited that small SW-Carbon-NTs are usually found inside multi-walled Carbon-NTs[40-51]. There is, therefore49, also a strong motivation to study in detail the stability and interaction of small Boron-Nitride-NTs inside a larger one (viewpoint of diameters), which makes easier to understandthe experimental results. Besides, the study on double-walled Boron-Nitride-NTs (DBN-NTs) has demonstrated an interesting variation in their electronic50 properties when compared with those of freestanding49 component of BNNTs[48-51]. So it is also important to see the inter-wall coupling behavior and interaction energies associated with the small Boron-Nitride-NTs.

In summary, Graphene and h-BN compounds as one kind of classical materials 42 with a mature studied history will play asignificant role in the battery market of the near future,but how to combine hybrid materials together to obtainsafe, stable, and high-capacity electrodes has always beenthe radical problem that many researchers are trying tosolve.

Theoretical background

Diffusion properties[45,51] of Li ion cell deter mines some of the keys performance metrics of Li^+ ion batteries cells, consist fo the charges and discharges rate, practical capacities and cycling stabilities. The governing equation describing the diffusion process is known as Fick' slaw as:

$j_i = -D_i \Delta C_i$ (1) And $\frac{\sigma c_i}{\sigma_t} = \nabla.(D \nabla C_i)$ (2)

where "j_i" is ionic flux, mol cm^{-2} s^{-1}, D_i is diffusivity of solute (i =1, 2), cm2 $s^{-1}$and C_i is concentration of species i , (mol cm3).The proportionality[40-50]. factor D is the diffusivity or diffusion coefficient as

$$D_i = \frac{K_B T}{6\pi\mu R_0} \quad (3)$$

Li^+ ion cells consist of, all Keyes phenomena involves conducting charged particles as a primary cell from cathodes to anode or vice versa as a secondarycell from anode to cathodes. Typical commercially used lithium-ion battery consists of several interconnected electrochemical cells, where each cell is composed of a graphite anode (such as Meso-carbon microbeads), a cathode formed by lithium metal oxide (such as LiCoO2) and electrolyte (such as LiPF6 dissolved in ethylene carbonate/dimethyl carbonate mixture) embedded in a separator felt.

Anode materials

In the case of anode, Li metal is found to be the most electropositive (-3.04 V versus standard hydrogen electrode) with large reversible capacity (≈ 4000 A h kg-1). However, due to safety considerations (explosion hazards as a result of dendrite growth during cycling), metallic Li has been substituted by various carbonaceous materials.

During discharge, Li^+ ions are extracted from the layered graphite, they pass[55] through the electrolytes and intercalate among the LiCoO2 layers (Fig.2.).

Density and energy of lithium in diffusion model

The electron densities has been defined as [52,54]. Where η_i is occupational number of orbitals (i), φ are orbitals wave functions, χ is basis function and C is coefficient matrix, the element of i_{th} row j_{th} column[52] corresponds to the expansion coefficient of orbital j respect to basis function i. Atomic unit for electron density can be explicitly[54] written as e/Bohr^3.Electron localization and chemical reactivityies[55] have been built by Bader[55].

$$\rho(r) = \eta_i |\varphi_i(r)|^2 = \sum_i \eta_i |\sum_l C_{l,i}\chi_i(r)|^2 \quad (5)$$

$$\nabla\rho(r) = [(\frac{\partial\rho(r)}{\partial(x)})^2+(\frac{\partial\rho(r)}{\partial(y)})^2+(\frac{\partial\rho(r)}{\partial(z)})^2]^{\frac{1}{2}} \quad (6)$$

$$\nabla^2\rho(r) = \frac{\partial^2\rho(r)}{\partial x^2} + \frac{\partial^2\rho(r)}{\partial y^2} + \frac{\partial^2\rho(r)}{\partial z^2} \quad (7)[52,54]$$

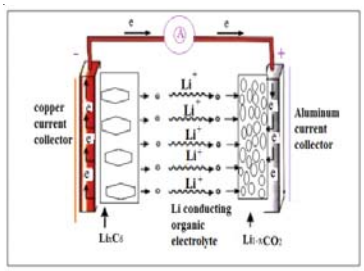

Fig. 2 a typical commercial lithium-ion battery

The Hamiltonian kinetics energies densities K(r)

The kinetic energies densities are not defined, since it has been expected value for kinetic energies operators $<\varphi - \left(\frac{1}{2}\right)\nabla^2\varphi >$ (8) has been recovered via integrating kinetic energies densities from an alternative definition. One of general used definition can be demonstrated as:

$k(r) = -\frac{1}{2}\sum_i \eta_i \varphi_i^*(r)\nabla^2\varphi_i(r)$ (9) "G(r)" is famous as positive definite kinetic energies densities.

$G(r) = \frac{1}{2}\sum_i \eta_i \nabla(\varphi_i)^2 = \frac{1}{2}\sum_i \eta_i\{[(\frac{\partial\varphi_i(r)}{\partial(x)})^2+(\frac{\partial\varphi_i(r)}{\partial(y)})^2+(\frac{\partial\varphi_i(r)}{\partial(z)})^2]\}$ (10) $K(\mathbf{r})$ and $G(\mathbf{r})$ are directly related by Laplacian of electron density.

$\frac{1}{4}\nabla^2\rho(r) = G(r) - K(r)$ (11)

Electron localization function (ELF)

Becke and Edgecombe noted that spherically averaged likespin conditional pair probability has direct correlation with the Fermi hole and then suggested electron localization function (ELF)[53-54].

$ELF(r)=\frac{1}{1+[D(r)/D_{0(r)}]^2}$ (12) where $D(r)=\frac{1}{2}\sum_i \eta_i \nabla\varphi_i^2 - \frac{1}{8}[\frac{\nabla\rho_\alpha^2}{\rho_\alpha(r)} + \frac{\nabla\rho_\beta^2}{\beta(r)}]$ (13)

and $D_{0(r)} = \frac{3}{10}(6\pi^2)^{\frac{2}{3}}[\rho_\alpha(r)^{\frac{5}{3}} + \rho_\beta(r)^{\frac{5}{3}}]$ (14) for close-shell system, sinece $\rho_\alpha(r) = \rho_\beta(r) = \frac{1}{2}\rho$ D and D_o terms can be simplified as $D(r)=\frac{1}{2}\sum_i \eta_i \nabla\varphi_i^2 - \frac{1}{8}[\frac{\nabla\rho^2}{\rho(r)}]$ (15)

$D_{0(r)} = \frac{3}{10}(3\pi^2)^{\frac{2}{3}}\rho(r)^{\frac{5}{3}}$ (16) Savin, has reinterpreted the ELF[52] in the view of kinetics energies[52-58].

$LOL(r) = \frac{\tau(r)}{1+\tau(r)}$ (17) where $(r) = \frac{D_o(r)}{\frac{1}{2}\sum_i \eta_i \nabla\varphi_i^2}$ (18) $D_0(r)$ for spin-polarized system and close-shell system are defined in the same way as in ELF[53].

Local Entropies

Local information entropiesare quantification of information, which was proposed by Shannonto decompose di-atomic and tri-atomic molecules into space by a minimized information entropy[52,57].Parr *has* discussed the relationship between information entropies and atom partition as well as molecular[54] similarity[54]. Noorizadeh and Shakerzadeh suggested using information entropy to study aromaticity. probability function is $s=-\int P(\chi) InP(\chi)d\chi$ (19). If $P(x)$ is replaced by $\frac{P(r)}{N}$ then the integrand can be called LIE of electrons.$S(r)=-\frac{P(r)}{N} in\frac{P(r)}{N}$(20)Where, N is the total number of electrons in current system.

At each inter-tube configuration, a single-point calculation is carried out and the total energy is recorded.The resulting sliding-rotation energy surfaces are used to fix our model in better position. $(E_{total}E_{xLi}+E_{h\text{-}BNsheets})\}+E_{BSSE}$ Where the ΔE_s is the stability energy of system.The contour line map has drawn via Multiwfn software[52-54]. The graph sareex habited on interactive interfaces and the methods in this work has based on our previous work[59-99].

RESULT AND DISCUSSION

We have listed the data of density, energy, electron localization function (ELF), localized orbital locator (LOL) and local entropy, gap energy, charge from ESP, electrostatic potential ,ionization energy,the charges of two doped graphene electrodes and the stability energy of X-G-(h-BN) -X-G and dielectric in 4 tables (tables1-6) and these data have plotted in 10 the (Figures.1-10)

We have calculated the gradient norm and the Laplacianof electron density via equals7 and 8 for the lithium diffused in the X-G/(h-BN)/X-G system respectively and the data are listed in table1. For calculation the electron spin density from the difference between alpha and beta density, we have Used $p^s(r)=p^\alpha(r)-p\beta(r)$ then the spin polarization parameter function will be returned instead of spin density $=\xi(r)=\frac{\rho^\alpha(r)-\rho^\beta(r)}{\rho^\alpha(r)+\rho^\beta(r)}$.The absolute value of going from zero to unity corresponds to the local region going from un-polarized case to completely polarized case Table1.In this work it has been calculated the local Information entropies for each of Li atoms via eqs. 19-20 and the integrating of those functions over whole spaces yield the information entropies. The data of local Information entropies are listed in Tables 1-5.

Weak interaction (equals 20 and 21) has significant influence on conformation of macro-molecules, however reproduction of electron densities by *ab initio* and grids data calculation of reduced density gradient (RDG) for such huge systems are always too time-consuming.In this work it has been exhibited the complex of X-G/(h-BN)/X-G which demonstrate a high electrical conductivity and a good mechanical strength, excellentflexibility, great chemical stabilities and high specific surfaces area. Thoseare especially noticeable when the graphene are chemically converted via greater proportion of functional groups, proving that they are suited for using as the basecomposite

electrodes materials as wellas enhancing the electrode's mechanical stabilities. As a result, X-G/(h-BN)/X-G containing electrode materials have high capacity and good rate performance. X-G/(h-BN)/X-Gflexibilities makes thoseas an idealmaterial for buffering metal electrode's volume expansionand contraction during the charge or discharge phenomenon.Further, the excellent electrical properties of X-G/(h-BN)/X-Gcan enhance the conductivity of metal electrodematerial. Finally, the lithium storage capacity for mostmetal oxide composite materials with X-G/(h-BN)/X-Gcan be useful greatly.

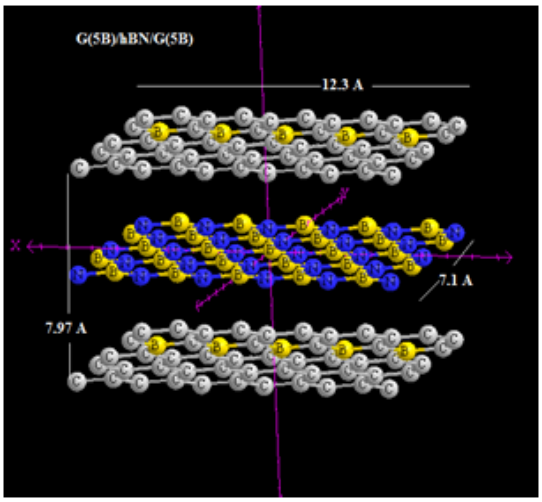

Fig. 3. h-BN sandwich inside two boron graphene doped as two electrodes of B-G/h-BN/B-G and Be-G/h-BN/Be-G capacitors.

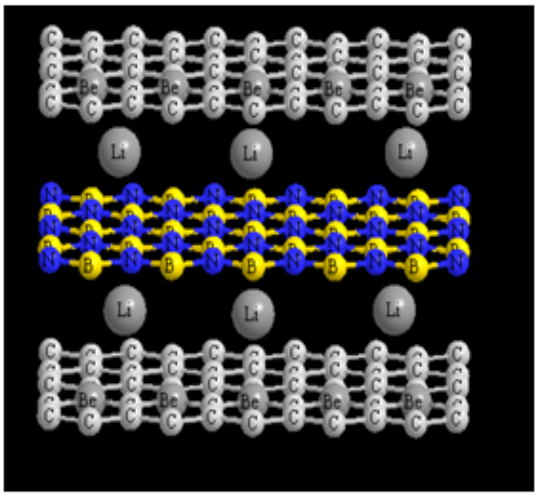

Fig. 4. Six diffused ion lithium between h-BN and B& Be doped graphene sheet layers

Table.1: Density, energy, Electron localization function (ELF), Localized orbital locator (LOL) and Local Entropy for each Li of 6 lithium diffused on X-G/(h-BN)/X-G (X=B,N and Be) mixed layers

Lithium No	Density of all electron x(10^{-4})	Density of α electron (10^{-4})	Density of β electron (10^{-4})	Spin density of electron	Potential energy density (10^{-3}J)	Hamiltonian kineti Energy (10^{-4}J)	LOL x10^{-3})	Local Entropy x10^{-6}	Ellipticity	ELF 10^{-7}	Eta index
					x=B						
Li+(2)	0.30	0.15	0.15	0.0	-0.23	-0.15	0.16	0.50	-0.15	0.31	0.16
Li+(4)	0.26	0.13	0.13	0.0	-0.29	-0.15	0.18	0.52	-0.30	0.32	0.14
Li+(6)	0.38	0.19	0.19	0.0	-0.27	-0.12	0.17	0.53	-0.22	0.31	0.17
					X=Be						
Li+(2)	0.22	0.11	0.11	0.0	-0.28	-0.14	0.21	0.50	-0.19	0.38	0.17
Li+(4)	0.26	0.13	0.13	0.0	-0.27	-0.13	0.18	0.54	-0.12	0.35	0.13
Li+(6)	0.34	0.17	0.17	0.0	-0.25	-0.15	0.19	0.51	-0.41	0.36	0.16

Table. 2: The Charges of two doped graphene electrodes and the stability energy of x-G/(h-BN)/x-G.

		X= 6 atoms of Be, B and N			
Li_xG-(h-BN) -G	***½Dielectric thichness(A)***	**ΔE_s(ev)=**	**$q^+_{m\text{-}G}$**	**$q^-_{m\text{-}G}$**	**$q_{(h\text{-}BN)2}$**
		X=B			
Li_2G-(h-BN)-G	3.98	-14.55	+0.19	-0.15	-0.04
Li_4G-$(h\text{-}BN)_2$-G	4.02	-30.32	+0.007	-0.004	-0.003
Li_6G-$(h\text{-}BN)_2$-G	3.99	-49.29	+0.14	-0.10	-0.02
		X=Be			
Li_6G-$(h\text{-}BN)_2$-G	4.03	-33.49	+0.13	-0.010	-0.120

Table. 3: The dielectric of X-G/(h-BN) /X-G modeled in various Lithium number.

Li_nX-G/(h-BN)/X -G	***½Dielectric thickness(A)***	$\Delta(V^{(1)}_{B-G} - V^{(2)}_{B-G})$ **(a.u.)**	κ
Li_2N-G/(h-BN)/N-G	3.97	3.6	1.89
Li_2 G-$(h\text{-}BN)_2$-G	4.01	2.2	1.83

Table. 4: Nucleor list and HOMO/LUMO and Gap energy for the B-C/h-BN/B-G.

```
125(C ) --> Charge:   4.000000   x,y,z(Bohr):    6.976609   -6.869205    3.400056
126(C ) --> Charge:   4.000000   x,y,z(Bohr):    4.651075   -5.976403    4.402859
127(B ) --> Charge:   3.000000   x,y,z(Bohr):    4.651075   -4.190800    6.408467
128(C ) --> Charge:   4.000000   x,y,z(Bohr):    6.976610   -3.297999    7.411271
129(C ) --> Charge:   4.000000   x,y,z(Bohr):    6.976610   -1.512396    9.416879
130(C ) --> Charge:   4.000000   x,y,z(Bohr):    4.651075   -0.619594   10.419683
131(C ) --> Charge:   4.000000   x,y,z(Bohr):    2.325540  -12.226014   -2.616768
132(C ) --> Charge:   4.000000   x,y,z(Bohr):    0.000005  -11.333212   -1.613964
133(C ) --> Charge:   4.000000   x,y,z(Bohr):    0.000005   -9.547609    0.391644
134(C ) --> Charge:   4.000000   x,y,z(Bohr):    2.325540   -8.654808    1.394448
135(C ) --> Charge:   4.000000   x,y,z(Bohr):    2.325540   -6.869205    3.400056
136(C ) --> Charge:   4.000000   x,y,z(Bohr):    0.000005   -5.976403    4.402859
137(B ) --> Charge:   3.000000   x,y,z(Bohr):    0.000005   -4.190800    6.408467
138(C ) --> Charge:   4.000000   x,y,z(Bohr):    2.325540   -3.297999    7.411271
139(C ) --> Charge:   4.000000   x,y,z(Bohr):    2.325540   -1.512396    9.416879
140(C ) --> Charge:   4.000000   x,y,z(Bohr):    0.000005   -0.619594   10.419683
141(C ) --> Charge:   4.000000   x,y,z(Bohr):   -2.325549  -12.226014   -2.616768
142(C ) --> Charge:   4.000000   x,y,z(Bohr):   -4.651083  -11.333212   -1.613964
143(C ) --> Charge:   4.000000   x,y,z(Bohr):   -4.651083   -9.547609    0.391644
144(C ) --> Charge:   4.000000   x,y,z(Bohr):   -2.325549   -8.654808    1.394448
145(C ) --> Charge:   4.000000   x,y,z(Bohr):   -2.325549   -6.869205    3.400056
146(C ) --> Charge:   4.000000   x,y,z(Bohr):   -4.651083   -5.976403    4.402859
147(B ) --> Charge:   3.000000   x,y,z(Bohr):   -4.651083   -4.190800    6.408467
148(C ) --> Charge:   4.000000   x,y,z(Bohr):   -2.325548   -3.297999    7.411271
149(C ) --> Charge:   4.000000   x,y,z(Bohr):   -2.325548   -1.512396    9.416879
150(C ) --> Charge:   4.000000   x,y,z(Bohr):   -4.651083   -0.619594   10.419683
151(C ) --> Charge:   4.000000   x,y,z(Bohr):   -6.976618  -12.226014   -2.616768
152(C ) --> Charge:   4.000000   x,y,z(Bohr):   -9.302153  -11.333212   -1.613964
153(C ) --> Charge:   4.000000   x,y,z(Bohr):   -9.302153   -9.547609    0.391644
154(C ) --> Charge:   4.000000   x,y,z(Bohr):   -6.976618   -8.654808    1.394448
155(C ) --> Charge:   4.000000   x,y,z(Bohr):   -6.976618   -6.869205    3.400056
156(C ) --> Charge:   4.000000   x,y,z(Bohr):   -9.302153   -5.976403    4.402859
157(B ) --> Charge:   3.000000   x,y,z(Bohr):   -9.302153   -4.190800    6.408467
158(C ) --> Charge:   4.000000   x,y,z(Bohr):   -6.976618   -3.297999    7.411271
159(C ) --> Charge:   4.000000   x,y,z(Bohr):   -6.976618   -1.512396    9.416879
160(C ) --> Charge:   4.000000   x,y,z(Bohr):   -9.302153   -0.619594   10.419683
161(C ) --> Charge:   4.000000   x,y,z(Bohr):  -11.627688  -12.226014   -2.616767
162(C ) --> Charge:   4.000000   x,y,z(Bohr):  -11.627688   -8.654808    1.394448
163(C ) --> Charge:   4.000000   x,y,z(Bohr):  -11.627688   -6.869205    3.400056
164(C ) --> Charge:   4.000000   x,y,z(Bohr):  -11.627688   -3.297999    7.411271
165(C ) --> Charge:   4.000000   x,y,z(Bohr):  -11.627688   -1.512396    9.416879
Note: Orbital   326 is HOMO of alpha spin, orbital   985 is HOMO of beta spin
      LUMO/HOMO gap of alpha orbitals:     0.000289 a.u.    0.007873 eV
      LUMO/HOMO gap of beta orbitals:      0.000011 a.u.    0.000307 eV
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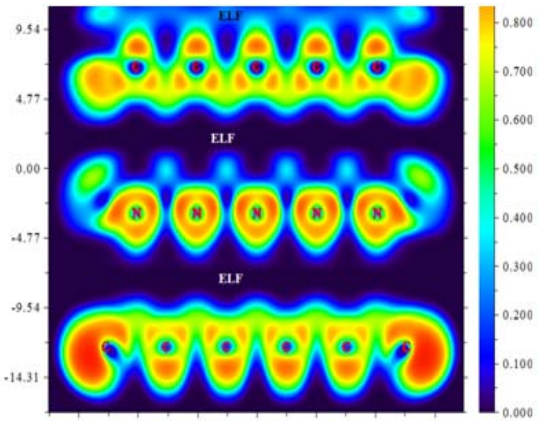

Fig. 5.ELF of B-G/h-BN/B-G for

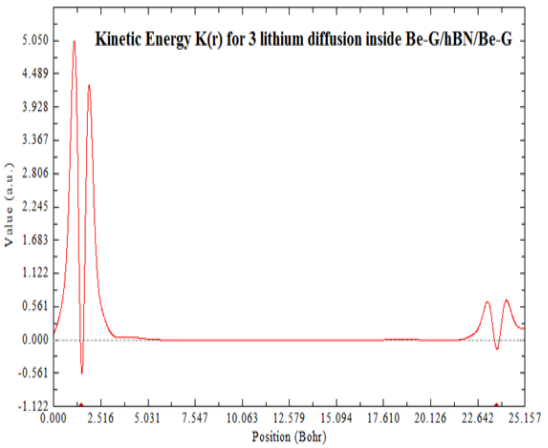

Fig. 6. K(r)of 3 lithium diffusion inside Be-G/h-BN/Be-G

CONCLUSION

The structure of G-X/(h-BN)n/X-G can be for improving the capacities and electrical transports in the C-BN sheets of LIBs. In addition, the BN sheet modified and designed of X-G/ (h-BN)/X-G structures provide a strategy to improve the yields of BN-G-sheet of anodes. X-G/h-BN/X-G could also be assembled into free standing electrode of any binder (current collector), which will causes for increasing specific energies and densities for the batteries design.

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REFERENCES

1. Tatar,R.C.;Rabii, S, *Physical Review B.***1982,** *25*4126-41.
2. Sichel, E. K.; Miller, R. E.; Abrahams, M. S.;Buiocchi,C. J. *Physical Review B*, **1976,** *13*, 4607-11
3. Hyun,K.Y.; Chang, K.J.; Louie,S.G. *Physical Review B*, **2001**, *63*, 205408 4. A. Zunger, Katzir, A.; Halperin,A. *Physical Review*,**1976**, B *13,* 5560-73
5. W. H. Balmain, *J. Prakt. Chem*. **1842,***27*, 422
6. Sato,T.;*Report of National Institute for Research in Inorganic Materials, Tsukuba, Japan.,* **1987**.
7. Yang,Z. G.; Zhang,J. L.;Kintner-Meyer,M .C .W.; Lu,X. C.; Choi,D.W. Lemmon,J. P.; Liu,J.; *Chem. Rev.***2011**,*111*, 3577–3613.
8. Guerard,D.;Herold,A.; **1975,***13*, 337-345.
9. Yoo,E. J.; Kim,J.; Hosono, E.; Zhou, H. S.;Kudo ,T.; *Nano Lett*, **2008**, *8,* 2277-2282.
10. Wang,G.;Shen,X. P.; Yao,J.; Park,J.;*Carbon*, **2009**, *47*, 2049-2053.
11. Bhardwaj ,T.; Antic, A.;Pavan, B.; Barone,V.; Fahiman, B. D.; *JACS*, **2010**, *132*, 12556-12558
12. Suzuki,T.; Hasegawa,T.; Mukai,S. R.; Tamon, H.; *Carbon*, **2003**, *41*, 1933-1939.
13. Hasegawa,T.; Suzuki, T.; Mukai, S. R.; Tamon, H.; *Carbon*, **2004**, *42*, 2195-2200.
14. Noel,M.; Suryanarayanan,V. *Journal of Power Sources,* **2002**, *111* , 193–209.
15. Tirado,J.L.; *Materials Science and Engineering* R , **2003**, *40*, 103–136.
16. Fu, L.J.; Liu, H.; Li, C.Wu, Y.P.; Rahm, E.; Holze, R.; Wu, H.Q. *Solid State Sciences*, **2006**, *8*, 113–128
17. Frackowiak, E.; Béguin,F.;*Carbon*, **2002**, *40*, 1775–1787
18. Whittingham,M. S.; Jacobson (Eds.), A.J.;*Intercalation, Chemistry, Academic Press.* **1982**
19. Safran,S.A.;Hamann,D.R.;*Physical Review Letters.***1979**, *42* (21), 1410–1413
20. Levi,M.D.; Aurbach,D.; Maier,J. *Journal of*

Electroanalytical Chemistry, **2008**, *624* 251–261.
21. Zabel,H.; Solin (Eds.),S. A.; *Graphite Intercalation Compound I, Springer-Verlag*, **1990.**
22. Wu,Y.P.; Rahm,E.; Holze, R. *Journal of Power Sources*, **2003**,*114*, 228–236
23. Lee,J.K.; An,K.W.; Ju,J.B.; Cho,B.W.; Cho,W.I.; Park,D.; Yun,K.S.; *Carbon*, **2001**, *39,* 1299–1305
24. C. De las Casas, and W.Z. Li, *J. Power Sources*, **2012**, *208*, 74–85
25. Z. H. Yang, and H. Q. Wu, Mater. *Chem. Phys.*, **2001**, *71*, 7–11
26. K.S. Novoselov, A.K. Geim, S.V. Morozov, D. Jiang, Y. Zhang, S.V. Dubonos, I.V.Grigorieva, and A.A. Firsov, *Science*,**2004**, *306* , 666–669
27. B. Partoens, and F.M. Peeters, *Physical Review B*, **2006**, *74*, 075404-1–075404-11
28. H. Tachikawa, and A. Shimizu, *Journal of Physical Chemistry B*, **2006**,*110*, 20445–20450
29. K. Naoi, N. Ogihara, Y. Igarashi, A. Kamakura, Kusachi, K. Utsugi, *Journal of the electrochemical Society*, **2005**,*152*(6) , A1047–A1053.
30. H. Groult, B. Kaplan, S. Komaba, N. Kumagai, V. Gupta, T. Nakajima, and B. Simon, *Journal of the Electrochemical Society*, **2003**,*150* (2), G67–G75
31. M. Endo, Y. Nishimura, T. Takahashi, K. Takeuchi, M.S. Dresselhaus, *Journal of Physics and Chemistry of Solids*,**1996**,*57 (*6–8), 725–728
32. T. Ohzuku, R.J. Brodd, *Journal of Power Sources*, **2007**,*174*, 449–456.
33. Monajjemi,M.; Boggs,J.E.;*J. Phys. Chem. A*, **2013**,*117,*1670-1684.
34. Monajjemi,M.; Lee,V.S. Khaleghian, M.;Honarparvar,B.;Mollaamin,F.;*J. Phys. Chem. C*. **2010**,*114,* 15315.
35. Monajjemi.M.;*Journal of Molecular Modeling*, **2014**, *20,* 2507.
36. Monajjemi, M. *TheorChemAcc*, **2015**, *134*:77 DOI 10.1007/s00214-015-1668-9.
37. Monajjemi,M.;*Struct. Chem*, **2012**, *23*., 551
38. Monajjemi.M.;Jafari Azan,M.;Mollaamin,F. *Fullerenes, Nanotubes, and Carbon Nanostructures*., **2013**, 21(6), 503–515.
39. Monajjemi,M.;*Chemical Physics*. **2013**, 425, 29-45
40. Novoselov, K.S.;Geim,A.K.;Morozov,S.V.; Jiang,D.; Zhang,Y.; Dubonos,S.V.; Grigorieva,I.V. Firsov,A.A. *Science*, **2004**,*306*, 666–669
41. B. Partoens, and F.M. Peeters, *Physical Review B*, **2006**, *74* 075404-1–075404-11
42. Monajjemi,M.;Mollaamin,F.;*Journal of Cluster Science*, **2012**, *23*(2), 259-272.
43. L. Ravagnan, P. Piseri, M. Bruzzi, S. Miglio, G. Bongiorno, A. Baserga, C.S. Casari, A. Li Bassi, C. Lenardi, Y. Yamaguchi, T. Wakabayashi, C.E. Bottani, and P. Milani, *Physical Review Letters* , **2007**, *98,* 216103-1–216103-4
44. Wu,G.T.; *Journal of Power Sources*, **1998,** *75*,175
45. Jalilian,H.;Monajjemi,M.;*Japanese Journal of Applied Physics*. **2015**, *54*, 085101.
46. Chew,S.Y.; et al., *Carbon*, **2009**,*47*, 2976.
47. Monajjemi, M.; Khaleghian, M, *Journal of Cluster Science*. **2011**, *22*(4),673-692
48. E. Frackowiak, S. Gautier, H. Gaucher, S. Bonnamy, F. Beguin, *Carbon*, **1999**, *37* (1999) 61.
49. Monajjemi, M.; Wayne Jr, Robert.; Boggs, J.E. *Chemical. Physics*. **2014**, *433*, 1-11
50. *S. Y. Chew,* S. H. Ng, J .Wang, P. Novak, F. Krumeich,S. L. Chou, J. Chen, and H . K. Liu. *Carbon*, **2009**, *47, 2976*
51. E. Frackowiak, S. Gautier, H. Gaucher, S. Bonnamy, and F. Beguin, *Carbon,***1999**,*37* 61 Joseph, Doninger, Z. Vyacheslav, Barsukov (Eds.), *New Carbon Based Materials for Electrochemical Energy Storage Systems, Springer*, **2006**, 269–276.
52. T. Lu, F. Chen, *ActaChim. Sinica*, **2011**, *69*, 2393-2406.
53. T. Lu, F. Chen, *J. Mol. Graph. Model*, **2012**, (38): 314-323.
54. T. Lu, F.ChenMultiwfn: A Multifunctional Wavefunction Analyzer, *J. Comp. Chem.* **2012**, (33) 580-592.
55. R.F.W. Bader, atoms in Molecule: A quantum Theory (Oxford Univ. press, Oxford, **1990**.
56. Becke and Edgecombe *J. Chem. Phys*., **1990.** *92*, 5397.
57. *A.* Savin, Angew. Chem. Int. Ed.Engl., **1992,** *31,* 187.
58. J.P. Perdew, K.Burke ,Ernzerhof, *Phys. Rev. Lett*. *77*, 3865-3868.,**1996**.
59. Chegini, H.; Mollaamin, F.; Farahani, P. *Fullerenes, Nanotubes, and Carbon Nanostructures*., **2011**, 19, 469–482
60. Baei, M.T.;Mollaamin, F. *Russian Journal of Inorganic Chemistry.* **2008,** *53 (9)*,1430-1437

61. Mollaamin, F.; Monajjemi, M, *Journal of Computational and Theoretical Nanoscience***. 2012**, *9 (4)* 597-601
62. Mollaamin, F.; Varmaghani, Z.; Monajjemi, M, *Physics and Chemistry of Liquids.* **2011**, *49,* 318
63. Razavian, M.H.; Mollaamin,F.; Naderi,F.; Honarparvar,B.; *Russian Journal of Physical Chemistry A* , **2008** , *82 (13),* 2277-2285.
64. Monajjemi, M.; Faham, R.; Mollaamin, F. *Fullerenes, Nanotubes, and Carbon Nanostructures,* **2012** *20*, 163–169.
65. Monajjemi, M.;Honarparvar, B. H. ; Haeri, H. ; Heshmat ,M.; *Russian Journal of Physical Chemistry C*. **2006**, 80(1), S40-S44.
66. Monajjemi, M.; Mollaamin, F. *Journal of Computational and Theoretical Nanoscience*, **2012**, 9 *(12),* 2208-2214.
67. Monajjemi, M.; Honarparvar, B.; Nasseri, S. M. .; Khaleghian M. *Journal of Structural Chemistry*. **2009**, *50*, 1, 67-77.
68. Ardalan, T.; Ardalan, P.; Monajjemi, M. *Fullerenes, Nanotubes, and Carbon Nanostructures*, **2014**, *22*: 687–708.
69. Monajjemi, M.; Najafpour, J.; Mollaamin, F. *Fullerenes, Nanotubes, and Carbon Nanostructures*. **2013**, *21*(3), 213–232
70. Monajjemi, M. Falahati, M.; Mollaamin, F.; *Ionics,* **2013**, *19*, 155–164
71. Tahan, A.; Monajjemi, M. *Acta Biotheor,* **2011,** *59*, 291–312.
72. Lee, V.S.; Nimmanpipug, P.; Mollaamin, F.; Kungwan, N.; Thanasanvorakun, S..; Monajjemi, M. *Russian Journal of Physical Chemistry A,* **2009***,* 83, 13, 2288–2296.
73. Monajjemi, M.; Heshmat, M.; Haeri, HH, *Biochemistry (Moscow),* **2006,** *71* (1), S113-S122
74. Monajjemi, M.; Yamola, H.; Mollaamin, F. *Fullerenes, Nanotubes, and Carbon Nanostructures*, **2014***, 22*, 595–603.
75. Monajjemi, M.; Ahmadianarog, M. *Journal of Computational and Theoretical Nanoscience*. **2014**,*11*(6), 1465-1471.
76. Mollaamin, F.; Monajjemi, M. *Physics and Chemistry of Liquids* . **2012**, *50*(5). 596–604.
77. Monajjemi, M.; Khosravi, M.; Honarparvar, B.; Mollaamin, F.; *International Journal of Quantum Chemistry***, 2011**, *111,* 2771–2777
78. Monajjemi, M.; Baheri, H.; Mollaamin, F. *Journal of Structural Chemistry*. **2011,** *52*(1), 54-59
79. Mahdavian, L.; Monajjemi, M.; Mangkorntong, N. Fullerenes*, Nanotubes and Carbon Nanostructures*, **2009**, *17 (5)*, 484-495
80. Monajjemi, M.; Farahani, N.; Mollaamin, F. *Physics and Chemistry of Liquids*, **2012**, *50(2)* 161–172
81. Monajjemi, M.; Khaleghian, M.; Mollaamin, F. *Molecular Simulation*. **2010**, *36*, 11, 865–
82. Monajjemi, M. *Biophysical Chemistry*. **2015,** *207*, 114 –127
83. Mahdavian, L.; Monajjemi, M. *Microelectronics Journal*. **2010**,*41*(2-3), 142-149.
84. Monajjemi, M.; *Journal of Molecular Liquids*, **2017**, *230,* 461–472.
85. Monajjemi, M*.; Macedonian Journal of Chemistry and Chemical Engineering,* **2017**, *36*, 1, 101–118.