

Functionalization of Bilayer Graphene-like AlN Material for Li-Ion Battery Applications; an Ab Initio Study

Rasool Akhtar¹, Irfan Ahmed², Muhammad Rafique³, Abdul Latif Abro⁴

¹⁻⁴Department of Electrical Engineering, Mehran University of Engineering and Technology, SZAB, Campus, Khairpur Mirs', Pakistan

¹Rasool.akhtar@muetkhp.edu.pk, ²Irfanahmed@muetkhp.edu.pk, ³Rafique.naich@muetkhp.edu.pk

Abstract– In recent times, graphene is seen as a prospective "wonder material" that may adjust the Li-molecule battery (LIB) field and can make basic development in the field of LIB. Notwithstanding, regardless of colossal proportion of work being finished every year in this field, handy plans of graphene like 2D materials-based batteries are in their evolving state without having commercial scale creation as of not long ago. In this assessment, starting is made with a description of arrangement of Li-molecule batteries' working and noteworthy thoughts, for instance, the solid electrolyte interface (SEI), trailed by the assessments on graphene and graphene composites (i.e., Boron and Nitrogen excited) as anode materials, highlighting the massiveness of graphene-like 2D materials as another approach towards the combination of different materials, the focal points and impediments of such materials. Consequently, this assessment may convey a suitable way out for arranging viable cathode materials reliant on graphene-like 2D materials to be utilized in Li-molecule batteries.

Keywords– Li-ion Batteries, B and N Intercalation and Graphene-like 2D Materials

I. INTRODUCTION

Along with the development of renewable energy technology, such as solar, wind and tidal energy, how to effectively store these kinds of energy becomes one of the major concerns. [3] Since 1990s, lithium ion batteries have been developing rapidly, widely used in portable electronic devices [4].

Lithium-Ion batteries (LIBs) are one of the leading broadly utilized vitality stockpiling gadgets today. Contrasted with different sorts of batteries, LIBs have various significant points of interest, including high vitality thickness, high Columbic and vitality productivity, moderately long life cycle and adaptability in plan, which make LIBs attractive for a wide scope of items, for example, advanced mobile phones, smart phones control stations. LIBs are likewise viewed as the most promising and encouraging force hotspot for vehicles operating on Electricity, mostly as of now monetarily accessible batteries; thus a lot of work and speculation has been set up to create LIBs through better execution in a more cost-proficient way.

While in comparison to other economically accessible batteries, LIBs have been assuming a significant job as the versatile power supply with higher volumetric and gravimetric densities, just as in the quick developing electric automobile industry. Right now, monetarily accessible LIBs are optional that utilize lithium stockpiling mixes for anode and cathode terminals. The working standards of Li-molecule batteries are displayed in Fig. 1. LIBs are frequently alluded to as an armchair battery in light of the fact that when the battery is in charging state or released, the Li particles move to and fro between the anode and cathode terminals [1].

Appearance of single layered two-dimensional (2D) honeycomb sorted out graphene material in 2004 [2] began another field of concentrate for materials known as "Flat Land" structuring. This epic 2D monolayer graphene material conveys with itself some enchanting and wondrous intrinsic properties [3], [4]. These as of late risen physical and substance set of properties further strengthened standard scientists to discover and mix novel 2D materials, for instance,

hexagonal boron nitride (h-BN), Aluminum Nitride (AlN), Arsenene, Germanene, Phosphorene and other change metal oxide (TMOs) monolayer structures, along these lines adding indisputable composition to the field of Flat Land planning. Consistently, piles of research papers have been appropriated on these 2D materials, to make them functionalize for down to earth building contraction applications [5]-[8].

As referenced by Geim [9] that, the assessment work submitted only to graphene has expanded unpredicted raised level and its applications are increasing bit by bit in applied sciences. Since its disclosure, around 23,945 research dispersions have been made on age of graphene on greater scale and proportion of generation is growing exponentially. Along these lines, a great deal of work has been finished on some other graphene-like 2D materials additionally [7], [8], [10].

Fig. 2 shows a couple of age courses through graphite & transforming into rGO, the most conventionally utilized grapheme family member in exploring LIB. It has been represented that expandable graphite in the wake of being thermally broadened can be stripped by methods for ultrasonication to get rGO layered sheets [13], while the graphite oxide shedding is the normal strategy used for rGO

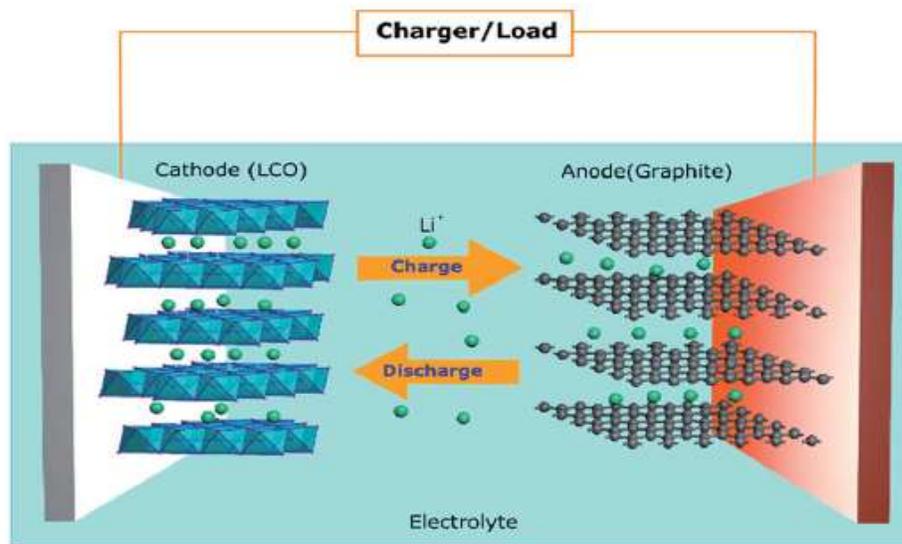


Fig. 1: Graphical representation of an LCO–graphite cell. Adopted from Ref. [1]

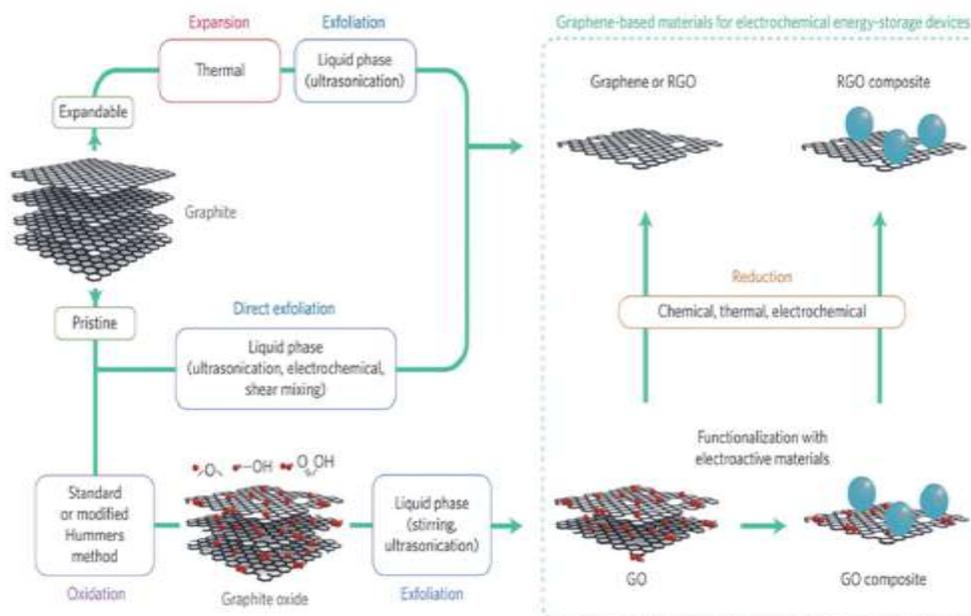


Fig. 2: Typical Flow Chart to produce GO, G-O, rGO, and rGO based nano-composite materials for applications of storing energy. Adopted from Ref. [1]

creation in the LIB field [14]. This plan of rGO creation is generally started through utilization of an oxidant and strong destructive, which oxidized the graphite, which fabricates the interlayer partitioning among the sheets and deteriorates the van der Waals controls with nearby GO layers. Afterwards, it is stripped to outline G-O. It can be mind boggling interest not similarly as a widely appealing thing to shape graphene, yet furthermore as a material in solitude. Graphene is different from G-O, as it contains hydroxyl, epoxy and carboxyl social events externally and progressively fundamental

imperfections. The physico-chemical properties of G-O varies with the level of oxidation and disarraying the cross area. The oxygen containing functional social occasions in GO give endless goals for securing electro dynamic materials to outline composites comprising G-O [15]. Abatement is consistently expected to recreate the sp² structure and the incredible electrical properties can be achieved which is ensured by G-O [16]. Essential composing is starting at now available on LIB field, while graphene and composite graphene structures doped with various contaminations to be utilized in LIB are

hardly analyzed. Accordingly, this work would grow the B and N molecule substitution technique to the graphene structures and the utilization of such systems in LIB field.

This paper work is regarding electrical parameters of AlN layer in low electron energy range i.e., 0–12 eV energy to improve the performance and efficiency of a LIB. B and N intercalation improved Li ion capturing capability of layered AlN system, making it a suitable material for storage applications.

II. COMPUTATIONAL DETAILS AND GEOMETRY MODELS

The study is done using First principles system DFT (FP-DFT) computation technique in combination with approximation of generalized gradient (GGA) and VASP software package is utilized for calculation, that is accurate and efficient computational tool [24], [25]. Through this study computations are done by utilizing plane-wave basis set in combination with ultrasoft pseudopotentials [23], [25] and 450 eV cut-off energy on 4×3 supercell arrangement for bilayer AlN having 15 Å vacuum thickness in the Z-direction [20], [26]. For avoiding the interference among neighboring layers, vacuum thickness is added. Different configuration of B & N is made and the effect of intercalation on the electronic and structural properties of bilayer AlN are investigated. BN-intercalated graphene like AlN systems were optimized until the Hellmann-Feynman force parameter gained 0.02 eV/Å value and the total energy value reached 10⁻⁷ eV limit. Partial occupancy problem is solved through Gaussian smearing method. For obtaining the electronic structures with fine quality, 40 points are adopted along Γ -M-K- Γ path in the Irreducible Brillouin zone (IBZ).

Main focus of our work regarding electric parameters is to manipulate and improve the aforementioned parameters of AlN layer in low electron energy range i.e., 0–12 eV energy. Main theme of this work is to tailor and improve the energy storage capability of Li-ions by surface activation of layered AlN system by intercalating B & N to form anode/cathode material. B/N atoms enhanced electronic band gap and reduced conduction so that charge can be stored rather than flow of electrons on the surface.

III. RESULTS AND DISCUSSION

For handling electrical, electronic and charge transport properties of graphene bilayer AlN system, first-gauges estimations reliant on thickness utilitarian speculation system are utilized. All of the calculations are performed using Materials Studio and Vienna Ab initio re-enactment pack (VASP) with plane wave premise set. In addition, for geometry improvement fundamentally Materials studio 7.1 programming pack is used. Both programming groups are using thickness utilitarian speculation system.

Recently referenced research establishment and reviewing completes the manner in which that assessment organize is looking for after changed systems to make capable Li-Ion batteries which can satisfy the growing needs of back and forth movement century. In any case, by no and incomprehensive composing work is done on graphene and

composite graphene-like 2D structures to be utilized in LIB field. Since Li-molecule batteries are a noteworthy bit of our consistently utilization of electrical power, subsequently it gets fundamental to devise innovative procedures to convey profitable and prudent batteries. This work can clear another route in the field of LIB, by organizing B and N doped intercalated graphene layered 2D systems to be considered as anode/cathode materials in LIB field.

Major outcomes of this work and related analysis and discussions are given below:

A) Structure diagrams of B & N doped monolayer Li-Ion Anode

Structures and some important electronic parameters are investigated for different combinations and are compared with each other using FPS-DFP technique. The structure diagrams of different combinations of B-N doped AlN layers are shown in Fig. 3(a) - Fig. 3(d).

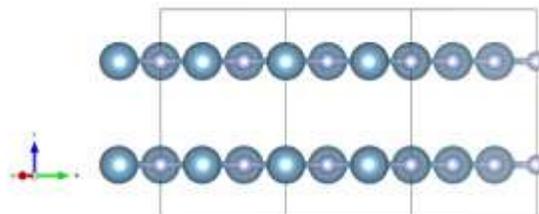


Fig. 3(a): Structural diagram (side view) of pure bilayer

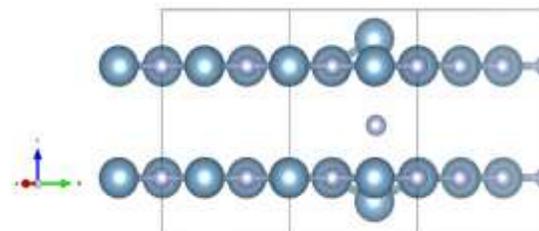


Fig. 3(b): Structural diagram (side view) of AlN with 1N (Grey colored at center of two layers)

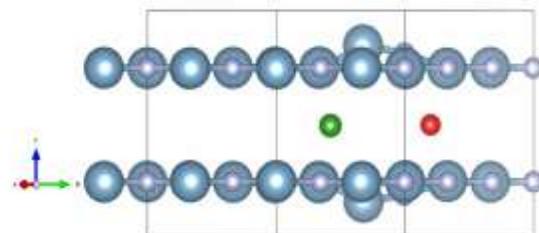


Fig. 3(c): Structural diagram (side view) of AlN 1N (Red colored) & 1B (Green colored)

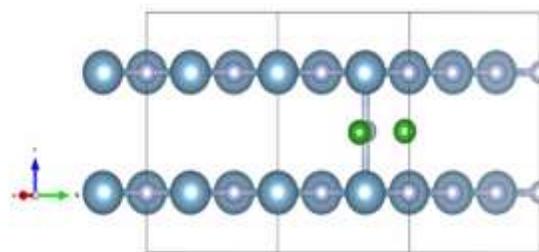


Fig. 3(d): Structural diagram (side view) of AlN with 1N (Grey colored) 2B (Green Colored)

Addition of 1N intercalated in between the two layers of AlN layered system causes the disturbance in bonding of original layer. Further addition of 1B will cause extended disturbance in the layers and may lead to bond redistribution or shifting of electrons. In next step another layer of B is intercalated. Formation of bond can be easily visualized in Fig. 3(d) which indicates that the addition of both elements has improved the bond structure of anode and may help in greater energy storage.

B) Band Structure of B & N intercalated AlN layered system

The electronic structure of pure bilayer AlN is shown in Fig. 4(a), purple dotted line indicates the Fermi level. After the intercalation of N the gap is reduced from 2eV to 0.5eV. Red lines indicate the band structures of N in combination with parent band structures. Energy step from E_f level approximately 1.2~1.5 eV. By further addition of B atom in between the layers further reduces the band gap and the bands nearly overlap each other above the Fermi level. The band gap become approximately 0.2eV and may reduce to a negligible value and electrons can easily shift from valence band to conduction band. Energy step from E_f level becomes approximately 0.2~0.3 eV.

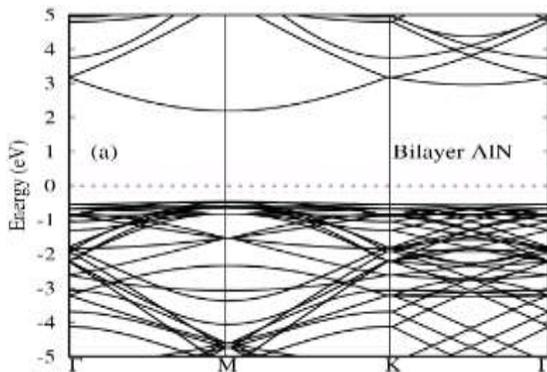


Fig. 4(a): Band structure of pure bilayer AlN

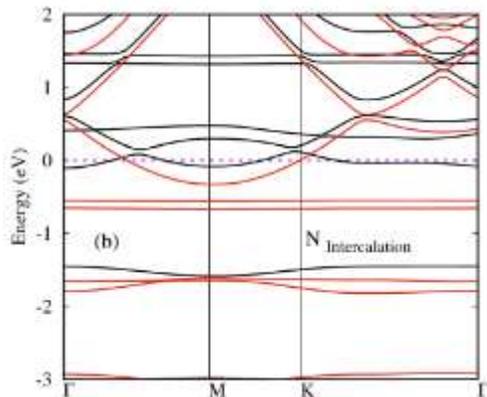


Fig. 4(b): Band structure of AlN with N intercalation

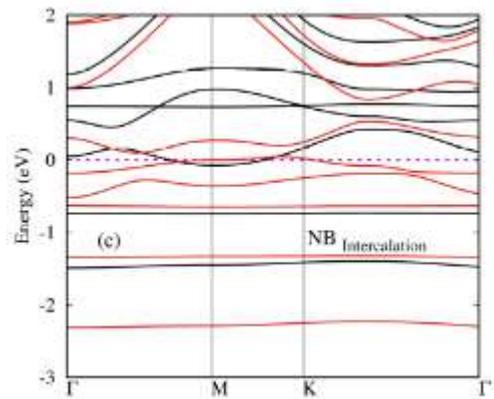


Fig. 4 (c): Band structure of AlN with N & B intercalation

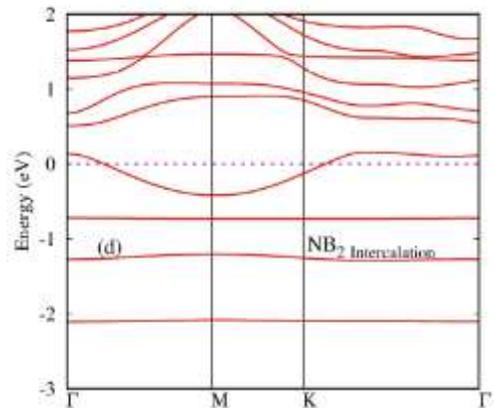


Fig. 4(d): Band structure of AlN with NB₂ intercalation

By increasing the atom of B in N-B intercalated anode material, the band gap remains constant and no significant change in band structure can be depicted as clearly shown in the Fig. 4(d). The band gap remains constant at 0.2~0.3 eV.

C) Charge Storage Capacity of B & N monolayer Li-Ion Anode

Here, we investigate the charge storage capacity of different combination of B-N intercalated AlN material. It is specified in q/cm and the comparison among BL/AlN, N, NB & NB₂ is shown in Fig. 5(a).

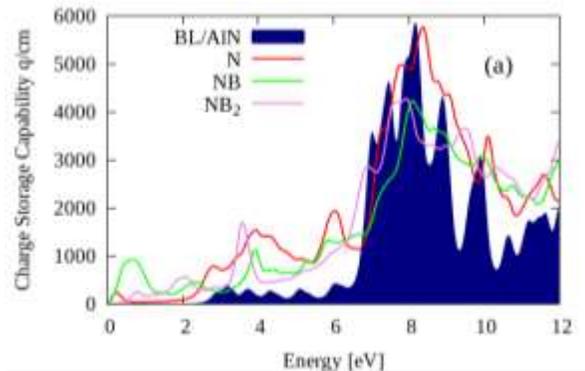


Fig. 5 (a): Charge Storage Capacity comparison of BL/AlN with N & B doping

It clearly indicates that the storage capacity of N intercalated anode material is much greater than other configurations. At lower eV values i.e. 0.5 eV, storage capacity of NB combination is approximately 1000 q/cm, whereas at 3.5 eV NB₂ has greater storage capacity 1800 q/cm. At 6 eV the storage capacity of N based anode is greater than other combinations which is 2000 q/cm. But at 7~9 values of eV values, N doped anode material and pure bilayer AlN has almost equal attributes of charge storage. At almost 10 eV, N doped material exhibits far greater charge carrying capacity than others. At 12 eV NB₂ remain dominant in charge storage capability.

D) Conductivity of B & N monolayer Li-Ion Anode

Here, we investigate the conductivity of B & N based AlN layered system, the comparison is shown in the Fig. 5(b).

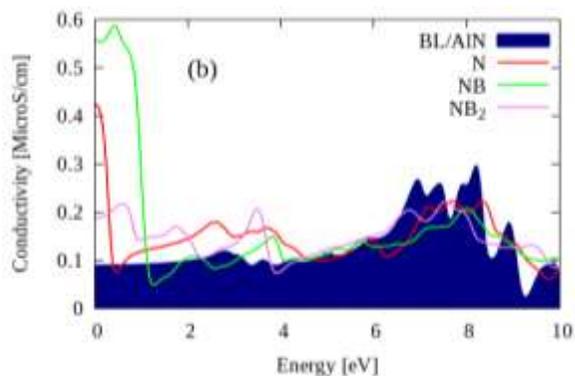


Fig. 5(b): Conductivity comparison of BL/AlN with N & B doping

It is clear from the figure that for smaller energy ranges of fewer eV values the conductivity of N-B and N alone with AlN has dominant conductivity properties, the spike in the start is about 0.58 μ S/cm and 0.43 μ S/cm respectively. From 2 eV to 4 eV there is consistency in conductivity of N intercalated AlN and is approximately of 0.15~0.12 μ S/cm. For the energy range 6~8 eV the conductivity remains dominant. Similarly, conductivity of N-B based material varies throughout the range of eV, it is maximum up to 0.1 eV having value of 0.58 μ S/cm. But it remains lower than other combination in remaining interval of eV. Conductivity of NB₂ attains maximum value at 3.8 eV energy range and has linear growth in conductivity from 4.2 to 6.2 eV and then remain lower than other combinations and attains second peak value at 9.5 eV.

E) Charge Density difference of B&N intercalated AlN layered system

To completely analyze the effect of B & N intercalation on charge difference maintenance, charge distribution is investigated which is shown in the Fig. 6(a) - Fig. 6(c). Fig. 6(a) shows the N based AlN where, yellow colour indicates electron gain, cyan colour indicates electron loss configuration. From the charge difference diagrams it can be suggested that N and B intercalation causes the variation in the electron cloud of interlayer space, as electrons are trapped

in between, thus suggesting charge holding capability of layered AlN system.

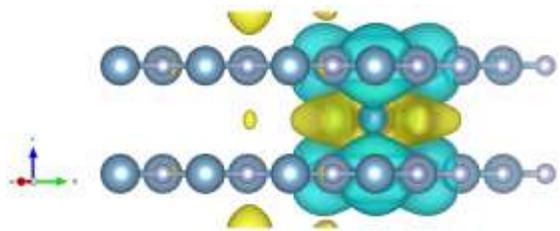


Fig. 6(a): AlN 1N Charge Density

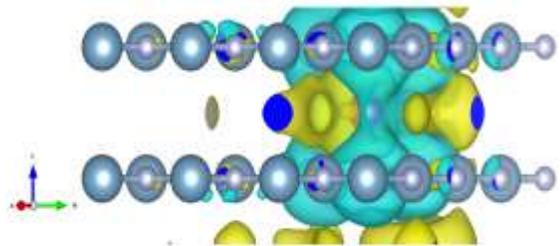


Fig. 6(b): AlN 1N 1B Charge Density

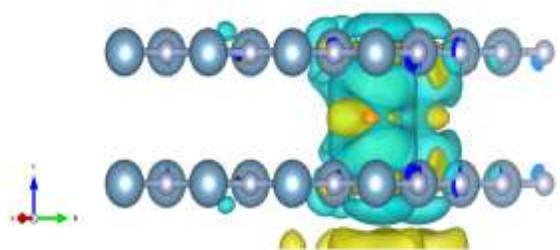


Fig. 6(c): AlN 1N 2B Charge Density

IV. CONCLUSIONS

At last by performing ab initio electronic structures are investigated with intercalated B & N with different concentrations. Band gap is investigated after chemical doping method and investigation is made for varying concentration of B and N intercalation techniques. It can be suggested that, obtained calculations are promising and can laid foundation for further research and investigations.

As per our results, the doped B-N AlN anode for Li-Ion battery exhibits better electronic properties i.e., band gap voltage reduces to 0.2~0.3 eV, similarly the charge carrying capability, conductivity & charge distribution analysis is evident that among other configurations B-N anode combination in Li-Ion can be promising element and improve the energy storage capability of Li-Ion battery.

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