The work done in the present thesis is open ended and hence there are great possibility of further research on considered materials and properties. Throughout this thesis density functional theory (DFT) has been the methodology for the calculation of novel properties of novel materials. In the last few years DFT has become an important tool of research in materials science mainly due to the enhancement in computational facilities, effective numerical methods and emergence of various new exchange correlation functionals. First two chapters of the thesis, provide proper introduction to recent trends which are developed to shrink the dimensionality of materials for the access of desire unique material properties for their application in the novel field electronics, optical and biomedical applications. We also discussed briefly the two dimensional materials, graphene, other low dimensional carbon allotropes and boron nitride nanostructures (BNNs), BNNT, BNNR and haeckelite-BN a new member of low dimensional BN structures. The prediction of haeckelite-BN has been confirmed using energetics and phonon calculation. State-of-the-art dispersion corrected density functional theory is also used to provide accurate results for adsorption energy because it takes care of long range van der Waals interaction.

Chapter 3 is devoted to understand the underlying physics behind the interaction of biomolecules (caffeine and nicotine) with the boron nitride nanomaterials (BNNs) to use them practically as bio-nanomaterials. The investigation of the electronic structures and adsorption properties of alkaloids (Caffeine and Nicotine) over boron nitride nanotube (BNNT) and boron nitride nanoribbon (BNNR) is carried out under the frame work of density functional theory based first principles calculations. The study of density of states (DOS) along with partial density of states (PDOS) depicts major contributions of both molecules caffeine and nicotine

in top of the valance band. The PDOS reveals that the 's' orbital of nitrogen and boron do not contribute significantly. Suitability of BNNs as filtration or sensing of alkaloids is also checked by adsorption energy calculation of both molecules over BNNT and BNNR, and found BNNR as superior candidate than BNNT for the filtration/sensing.

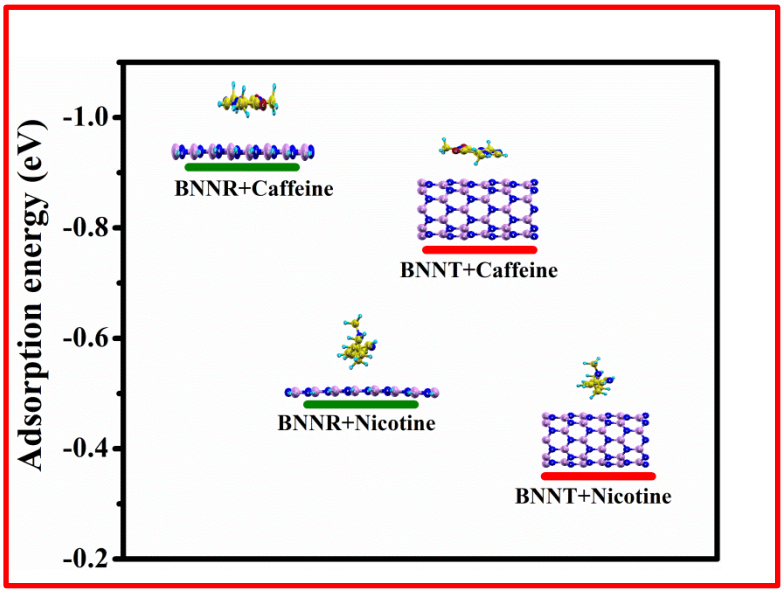

Figure 6.1: *Adsorption energy of alkaloids over BNNR and BNNT depicting superiority of BNNR than BNNT.*

For incorporating the dispersion correction in the calculation to consider proper long range van der Waals interaction, we used DFT-D2 with GGA-PBE scheme which increases the accuracy of adsorption energy calculation. Physisorption of both molecules over BNNs has been seen as the adsorption energy ranging between -0.35 and -0.76 eV, and -0.45 and -0.91 eV for caffeine and nicotine over BNNT and BNNR respectively. The most beneficial orientation of caffeine and nicotine over BNNT and BNNR is hetero atoms facing in-parallel for adsorption. Figure 6.1 clearly indicates the large adsorption energy of both alkaloids over BNNR than BNNT. Charge transfer analysis between BNNs and the adsorbed alkaloid molecules has also been checked by Lowdin charge analysis which depicts negligible charge

transfer between BNNs and alkaloid molecules. Both BNNT and BNNR are sensitive towards both alkaloids which are observed from density of states, electronic structure calculations and quantum conductance. Our analysis shows that the BNNR strongly interacts with both alkaloids. Absence of any covalent interactions between the considered alkaloids and BNNs species (BNNT/BNNR) confirms its superiority as sensing materials. From our study one may conclude that the boron nitride nanostructures may be useful in designing sensitive alkaloids sensing device.

In ***Chapter 4,*** we have systematically investigated structural, vibrational and electronic properties of newly predicted allotrope of BN with octagonal and square ring morphology, haeckelite BN (haeck-BN).

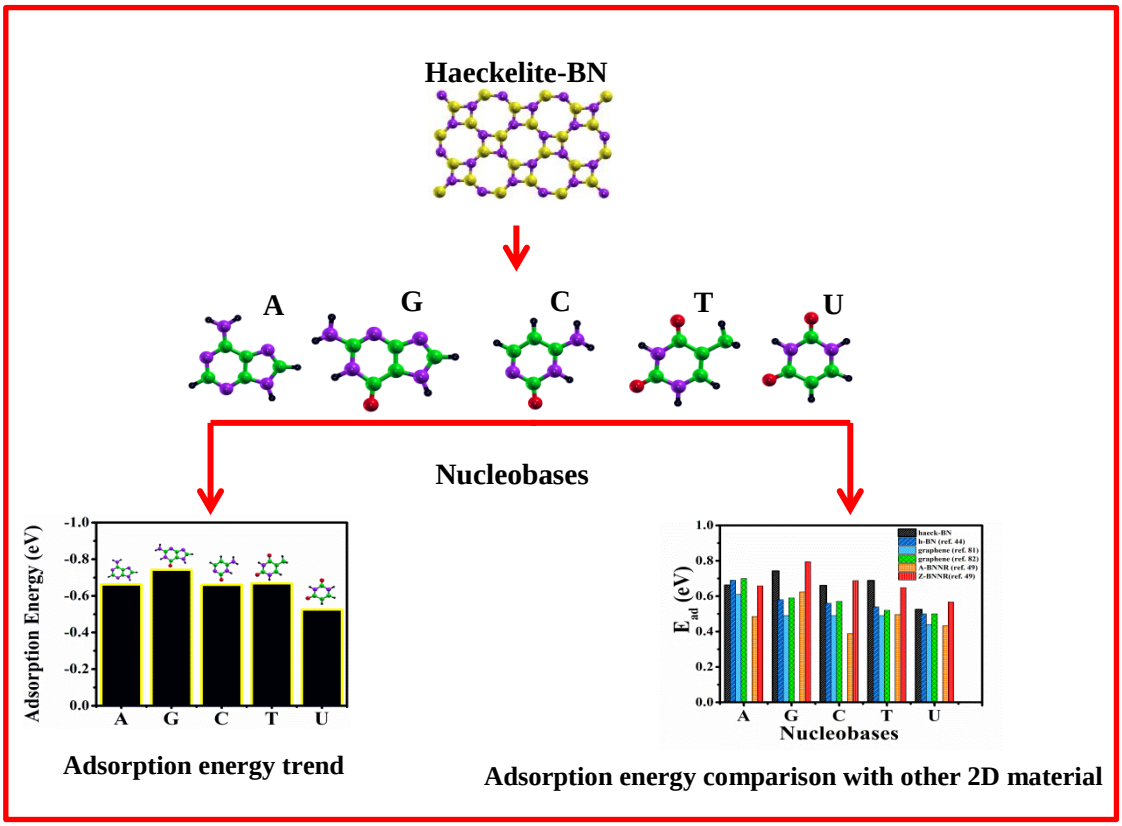

Figure 6.2: *Schematic of adsorption energy trend of nucleobases over haeck-BN and comparision with other 2D materials.*

We further explore its applicability as biosensor by investigating the adsorption mechanism of most important basic building block of DNA i.e. nucleobases adenine (A), guanine (G), cytosine (C), thymine (T) and uracil (U). For the appropriate consideration of long distance van der Waals interaction, dispersion correction (DFT-D2) is included in our calculation. The adsorption energy over haeck-BN for all five nucleobases has the following order: G > T > A ≈ C > U. The calculated adsorption energy for G, A, C, T and U is -0.742 eV, -0.662eV, -0.660eV, -0.668 eV and -0.525 eV respectively which is higher in comparison to h-BN, graphene and BNNT. The adsorption energy trend of nucleobases over haeck-BN and its comparison with other 2D material are illustrated in Figure 6.2. The adsorption of nucleobases is confirmed by the significant variation seen from the calculated values of electronic properties, density of states and work function. We have also calculated the recovery time because it confirms reusability of a sensor. The calculated recovery time depicts ultrafast recovery times (in millisecond) of 292 ms, 130 ms, 120 ms, 160 ms and 0.6 ms for G, A, C, T and U adsorbed haeck-BN systems respectively. Our finding suggests superiority of haeck-BN over boron nitride nanotubes, h-BN and graphene for the detection of nucleobases which makes it a good candidate to be utilized as an improved biosensor.

Chapter5 contains results of the structural and electronic properties of two significant neurotransmitters dopamine (DA) and adrenaline (AD) adsorbed over boron nitride nanoribbons (BNNRs) for investigating the feasibility of BNNRs as neurotransmitter carrier. A comparative study of adsorption mechanism is performed on armchair BNNR (ABNNR) and zigzag BNNR (ZBNNR) using dispersion corrected density functional theory to check the superiority in adrenaline and dopamine adsorption among both BNNRs.

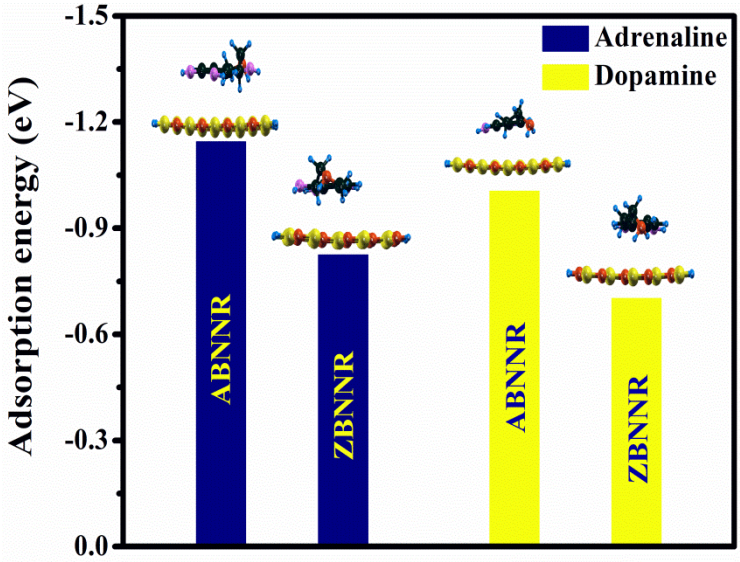

Figure 6.3: *Adsorption energy plot of neurotransmitter over ABNNR and ZBNNR.*

Both neurotransmitters adsorption effectively modulate the electronic structure of ZBNNR and ABNNR. Significant reduction of 0.992 eV and 1.135 eV in bandgap is observed in case of ABNNR adsorbed by DA and AD respectively while in case of ZBNNR reduction of 0.769 eV and 0.942 eV in the band gap is observed by DA and AD respectively. A strong interaction of neurotransmitters (DA and AD) is observed with BNNRs (ABNNR and ZBNNR). Adrenaline and dopamine have higher adsorption energy with ABNNR (-1.144 eV and-1.013eV) as compared to ZBNNR (-0.824eV and -0.701eV). Figure 6.3 shows the adsorption energy of both neurotransmitters have higher magnitude over ABNNR compared to ZBNNR Significant modulation in the work function is seen for dopamine and adrenaline adsorbed pristine BNNRs. The 32% (becomes 3.350eV) of reduction in the work function of ZBNNR (4.970eV) is observed after the adsorption of DA while it reduces up to 26 % (becomes 3.661eV) in case of AD adsorption. Moreover, 26 % (become 3.057eV) and 25 % (become 3.111 eV) reduction in work function in case of ABNNR (4.152 eV) after DA and AD

adsorption is observed. The present study helps in understanding the underline physics behind the interaction between BNNRs and neurotransmitters and possibility to explore BNNRs as a carrier for these neurological medicines. The present results will help researchers to design new sequencing material for human health as well as live cells.

Future Scope

One of the important aims of the present thesis is to comprehend the nature of boron nitride nanostructures at the atomic level along with its bioconjugation for the bio-applications. Over the past few years, boron nitride has become an interesting substitute to graphene based materials as far as the bio-applications are concerned. Boron nitride nanostructures grant possibilities of tuning the properties for chosen applications. In the present thesis, we have studied bio-conjugation of boron nitride nanostructures along with their interaction mechanism and electronic properties.

As a future plan to expand the current work, few objectives are highlighted. Unlike graphene based nanomaterials where the preparation method, their size and shape together with working conditions play significant role in concluding toxicity and bio-compatibility, the pristine boron nitride nano structures are bio-compatible in vitro and in vivo. To explore boron nitride nanostructures capability in drug delivery/DNA sequencing, molecular dynamics (MD) simulations can be done for huge proteins and DNA with boron nitride nanostructures. Further, one can see the possibilities of newly predicted haeckelite structured boron nitride in one dimension for sensing and sequencing of amino acids and nucleobases respectively. Moreover, its sensitivity towards hazardous gases for pollution free environment will be an interesting

and important investigation. Boron nitride nanostructures can be an excellent nominee for the electrocatalytic activities and many more. Boron nitride nanostructures have presented several attractive electrical and magnetic properties through different functionalizing strategies. However, a large band gap hinders them from achieving their full potential. By developing innovative strategies in structural designing their electronic properties can be modulated. Further, one can calculate the linear responses of the considered bioconjugated system. However, a word of caution here is that the linear response calculations require tremendous computational power.

"A Problem Well Stated is a Problem Half-Solved"

By Charles Kettering