

## List of Figures

<b>Figure 2.1</b>	Growth of research papers based on DFT calculation. (From web of science data <a href="http://www.webofknowledge.com">www.webofknowledge.com</a> ).	15
<b>Figure 2.2</b>	Schematic representation of first Hohenberg and Kohn theorem. Here, the HK theorem completes the circle, while other smaller arrow shows the solution of Schrödinger equation. Image adapted from ref. [13].	23
<b>Figure 2.3</b>	Same as Figure 2.2 but for Kohn – Sham ansatz. $HK_0$ defines Hohenberg and Kohn theorem applied to non-interacting system. The connection between many body and the independent particle systems provided by Kohn – Sham that labelled as double arr.	25
<b>Figure 2.4</b>	Schematic flow chart to find the solution of KS equation. [From Quantum Espresso Tutorial].	28
<b>Figure 3.1</b>	Optimized structure of (a) Caffeine (b) Nicotine (c) Pristine boron nitride nanotube and (d) Pristine boron nitride nanoribbon. The figure also shows the side view of optimized structures.	45
<b>Figure 3.2</b>	Equilibrium geometry of physisorbed Caffeine and Nicotine molecules on (a-b) BNNT and (c-d) BNNR. The figure also shows the side view of optimized structures of functionalized BN nanostructures with alkaloids	46
<b>Figure 3.3</b>	HOMO (red) and LUMO (blue) of (a) caffeine molecule and (b) nicotine molecule.	48
<b>Figure 3.4</b>	HOMO (red) and LUMO (blue) of functionalized BNNT (a-b) and BNNR (c-d) with caffeine molecule and nicotine molecule.	49
<b>Figure 3.5</b>	Total charge density plot of BNNT and BNNR conjugated with Caffeine and Nicotine (a) BNNT and (b) BNNR. Isosurface levels were set at $0.09 \text{ bohr}^{-3}$ .	52
<b>Figure 3.6</b>	Total DOS of (a) caffeine molecule, (b) nicotine molecule, (c) pristine and alkaloid (nicotine and caffeine) conjugated BNNT and (d) pristine and alkaloid (nicotine and caffeine) conjugated BNNR.	53

<b>Figure 3.7</b>	PDOS of (a) pristine BNNT, (b) conjugated BNNT with caffeine, (c) conjugated BNNT with nicotine, (d) pristine BNNR, (e) conjugated BNNR with caffeine, (f) conjugated BNNR with nicotine.	55
<b>Figure 3.8</b>	Quantum conductance plot of BNNT and BNNR (a) conjugated with Nicotine and (b) conjugated with Caffeine.	57
<b>Figure 4.1</b>	(a) Optimized structure of haeck-BN monolayer in addition with the enlarge view having bond length and bond angle, (b-c) Structure of bulk h-BN and 2D h-BN. Yellow and purple ball represents boron and nitrogen respectively.	68
<b>Figure 4.2</b>	Calculated band dispersion curve of haeck-BN. Along with total DOS and PDOS of haeck-BN at the right panel.	70
<b>Figure 4.3</b>	Total charge density plot of haeck-BN. The blue colour represents the large value of electron charge density while red colour shows relatively low charge density	71
<b>Figure 4.4</b>	Phonon dispersion curve along with the phonon density of states (PHDOS).	73
<b>Figure 4.5</b>	Optimized structures of five nucleobases A, G, C, T and U. Red, green, black and purple ball corresponds to oxygen, carbon, hydrogen and nitrogen atoms respectively.	76
<b>Figure 4.6</b>	Optimized structures of (a) pristine haeck-BN and nucleobases adsorbed haeck-BN (b) Adenine (c) Guanine (d) Cytosine (e) Thymine (f) Uracil (top and side view).	76
<b>Figure 4.7</b>	Different parallel orientation of haeck-BN adsorbed by nucleobases (a) Adenine, (b) Cytosine, (c) Guanine, (d) Thymine, (e) Uracil.	77
<b>Figure 4.8</b>	Comparative adsorption energies plot of nucleobases with different nanostructures.	81
<b>Figure 4.9</b>	Band structure plots of haeck-BN (a) pristine and nucleobase adsorbed (b) Adenine (c) Guanine (d) Cytosine (e) Thymine (f) Uracil.	82

<b>Figure 4.10</b>	Charge density plot of (a) haeck-BN and haeck-BN adsorb by nucleobases (b) Adenine, (c) Cytosine, (d) Guanine, (e) Thymine, (f) Uracil.	84
<b>Figure 4.11</b>	HOMO and LUMO of (a) haeck-BN and (b-f) nucleobase adsorbed haeck-BN system; (b) Adenine, (c) Cytosine, (d) Guanine, (e) Thymine, (f) Uracil.	85
<b>Figure 4.12</b>	Electronic density of states (DOS) plot of pristine haeck-BN along with nucleobase adsorbed nucleobases.	86
<b>Figure 4.13</b>	Partial density of states (PDOS) plot of nucleobases adsorbed haeck-BN system (a) Adenine, (b) Guanine, (c) Cytosine, (d) Thymine and (e) Uracil.	87
<b>Figure 4.14</b>	Work function plot of pristine and nucleobases adsorbed haeck-BN system (a) Pristine, (b) Adenine, (c) Guanine, (d) Cytosine, (e) Thymine and (f) Uracil.	91
<b>Figure 5.1</b>	Optimized structure of (a) adrenaline (b) dopamine (c) ABNNR and (d) ZBNNR. Oxygen, carbon, hydrogen boron and nitrogen are represented as pink, black, blue, yellow and orange ball respectively. W shows the width of both nanoribbons.	105
<b>Figure 5.2</b>	Optimized structure of ABNNR adsorbed with (a) adrenaline and (b) dopamine. The distance between the molecules and BNNRs, is represented by d.	107
<b>Figure 5.3</b>	Optimized structure of ZBNNR adsorbed with (a) dopamine and (b) adrenaline. The distance between the molecules and BNNRs, is represented by d.	108
<b>Figure 5.4</b>	Molecular orbitals of (a) dopamine and (b) adrenaline.	109
<b>Figure 5.5</b>	Total and partial DOS of (a) ABNNR and (b) ZBNNR.	110
<b>Figure 5.6</b>	Density of states of (a) ABNNR adsorbed neurotransmitter and (b) ZBNNR adsorbed neurotransmitter.	112
<b>Figure 5.7</b>	Partial density of states of ABNNR adsorbed with (a) Adrenaline and (b) Dopamine.	113

<b>Figure 5.8</b>	Charge density plots (a-b) ABNNR/ZBNNR, (c-d) DA adsorbed ABNNR and AD adsorbed ABNNR and (e-f) DA adsorbed ZBNNR and AD adsorbed ZBNNR.	114
<b>Figure 5.9</b>	Charge density plots (a-b) ABNNR/ZBNNR, (c-d) DA adsorbed ABNNR and AD adsorbed ABNNR and (e-f) DA adsorbed ZBNNR and AD adsorbed ZBNNR.	115
<b>Figure 5.10</b>	Work function of BNNR and neurotransmitter adsorbed (a) ABNNR and (b) ZBNNR.	117
<b>Figure 6.1</b>	Adsorption energy of alkaloids over BNNR and BNNT depicting superiority of BNNR than BNNT	124
<b>Figure 6.2</b>	Schematic of adsorption energy trend of nucleobases over haecck-BN and comparison with other 2D materials.	125
<b>Figure 6.3</b>	Adsorption energy plot of neurotransmitter over ABNNR and ZBNNR.	127