List of Tables

Table 3.1	Calculated HOMO energies, LUMO energies, energy band gap (E_g) , adsorption energy (E_{ad}) , Fermi level energies (E_F) and distance of the molecules over BNNT (d) .	47
Table 4.1	Calculated Lattice 'a' (Å), Bond length (Å), Bond angle (°), Energy band gap E_g (eV), Fermi level energies E_F (eV) of haeck-BN.	69
Table 4.2	Calculated total energy of nucleobase adsorbed haeck-BN system. Red color represents minimum energy.	78
Table 4.3	Calculated total energy of nucleobase adsorbed haeck-BN system with different orientation. Red color represents minimum energy.	79
Table 4.4	Adsorption energy $E_{ad}(eV)$, vertical distance d (Å) of nucleobases from haeck-BN, bandgap E_g (eV) and Fermi energy E_F (eV).	80
Table 5.1	Calculated Bond length (\mathring{A}) and Bond angle ($^{\circ}$) between B-N-B in BNNRs.	106
Table 5.2	Calculated energy gap (E_g) , difference in band gap (ΔE_g) , adsorption energy (E_{ad}) , distance between neurotransmitter and BNNRs, Fermi energy (E_F) and work function (Φ) .	111