1 Electronic Supplementary Information (ESI)

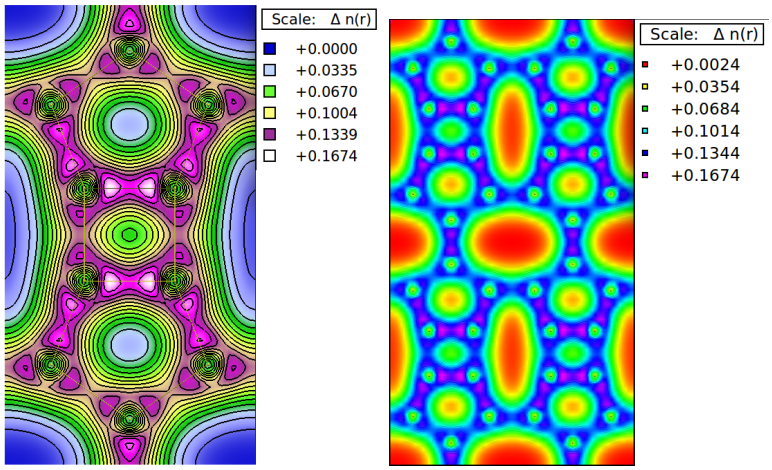

Figure S.1: Charge density for unit cell (left) and that for a 2x2x1 supercell (right)

Table S.1: Table to show the formation energy of different structures.

System	N	B	C	Formation energy (eV)
C10	10	0	0	-8.5773429
4N4B2C	4	4	2	-6.8251887
4N2tB4C	4	2	4	-6.6635473
2N4B4C	2	4	4	-7.2402774
4N2aB4C	4	2	4	-6.8675997
9C1Bp	0	1	9	-8.2283812
9C1Bt	0	1	9	-8.1808443
9C1Np	1	0	9	-8.0380544
9C1Nt	1	0	9	-8.1088692
2tN8C	2	0	8	-7.8113438
2aN8C	2	0	8	-7.5329196
4taN6C	4	0	6	-6.8986084
6N2B2C	6	2	2	-5.8872227

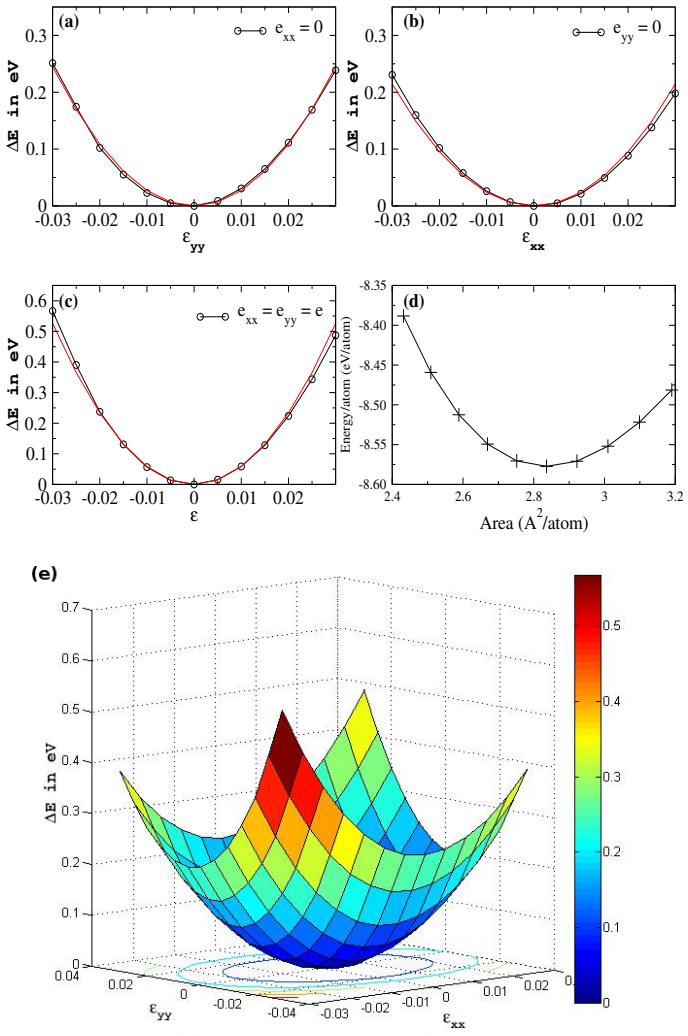

Figure S.2: (a) Strain energy for uniaxial strain along $\vec{b}$ direction, (b) Strain energy for uniaxial strain along $\vec{a}$ direction, (c) Strain energy graph for equal strain along both directions. Red curves show parabollic fit on the data. (d) Formation energy vs area per atom curve. (e) Strain energy surface under strain in both directions including uniaxial tensile, uniaxial compressive, biaxial tensile, biaxial compressive and asymmetric biaxial strains.

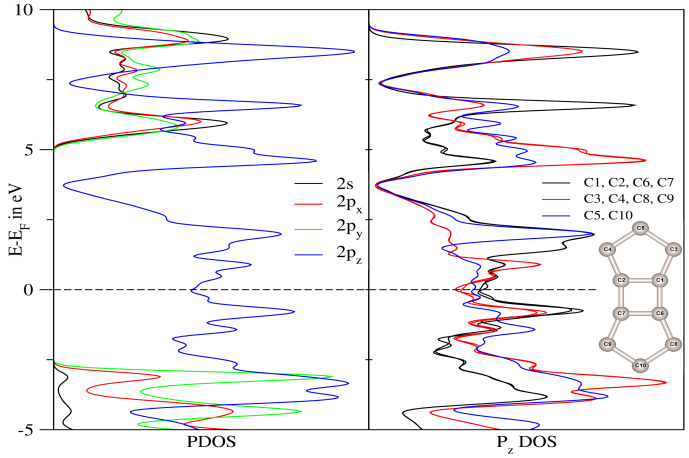

Figure S.3: Projected density of state (left). Partial density for p_z orbital for all ten carbon atoms classified in three bunches of similarity (right)

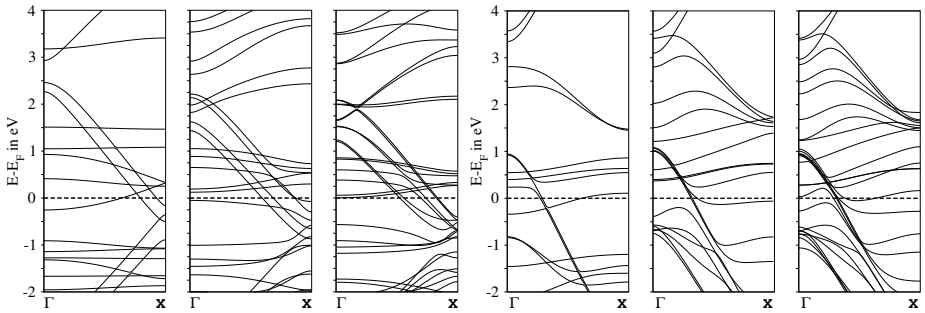

Figure S.4: Band structure for nano ribbons of larger width. (Left) Bands of NR1 for n = 1, 2 & 3. (Right) Bands of NR2 for n = 1, 2 & 3

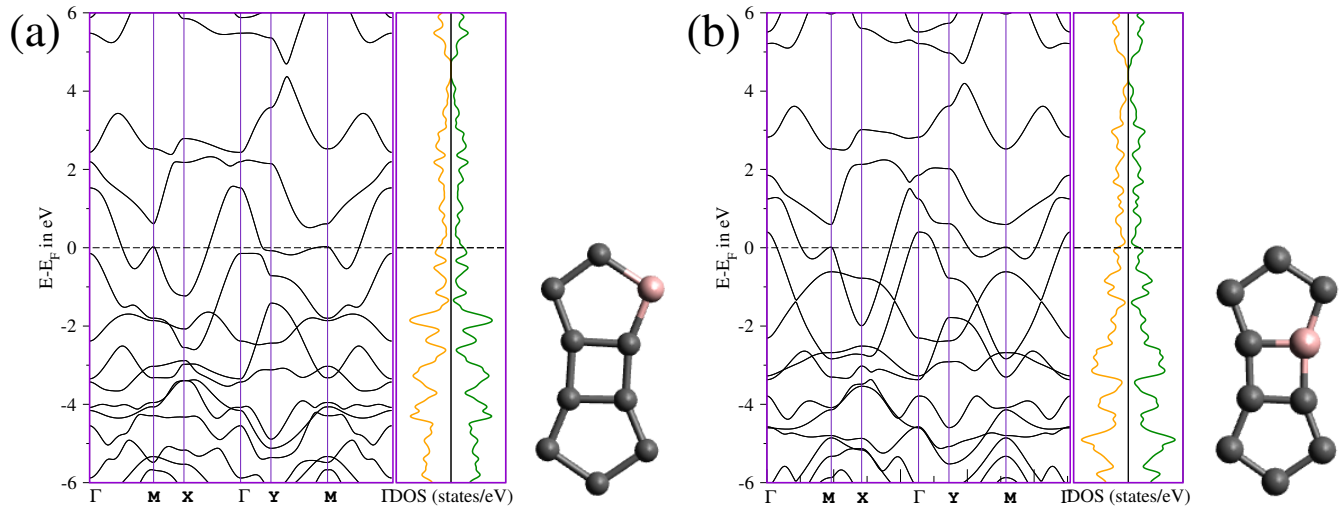

Figure S.5: (a) Boron doping in pentagon-octagon site. (b) Boron doping in tetragon-pentagon-octagon site.

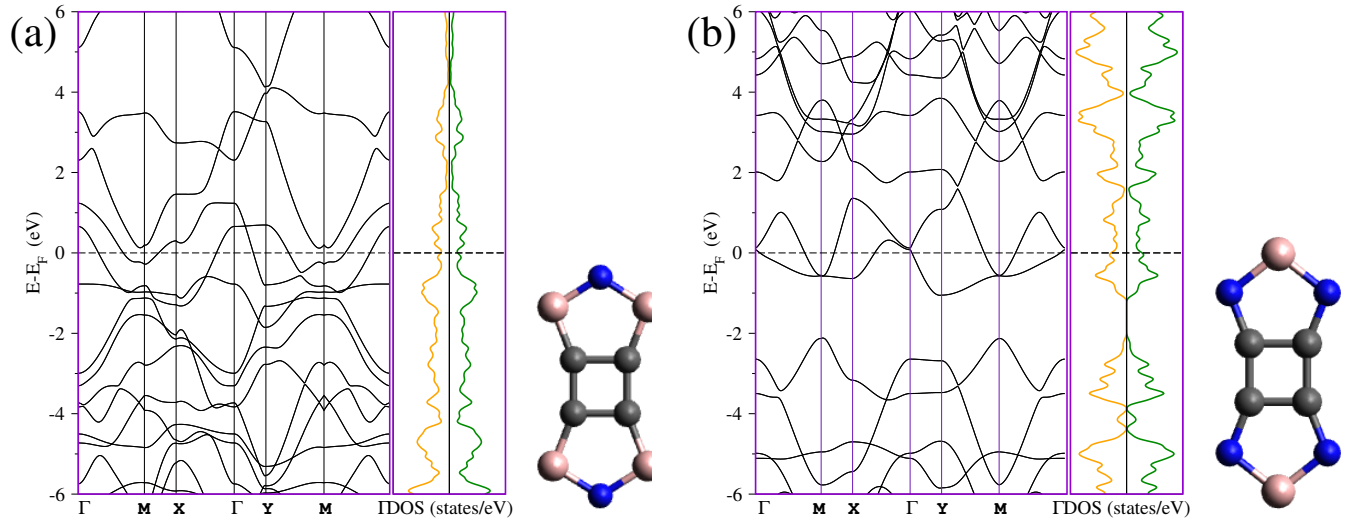

Figure S.6: (a) $C_4B_4N_2$ system. (b) $C_4B_2N_4$ system. Nitrogen-Boron co-doping keeping the carbon tetragonal ring unaltered.

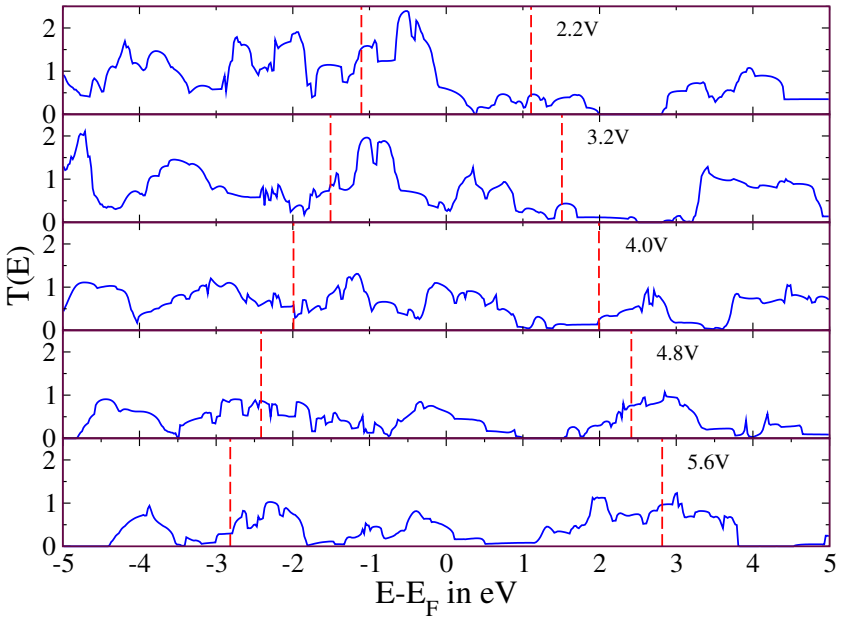

Figure S.7: The transmission function plotted with Fermi level shifted energy at different bias for device 1. The red dotted lines indicate the electrode Fermi levels

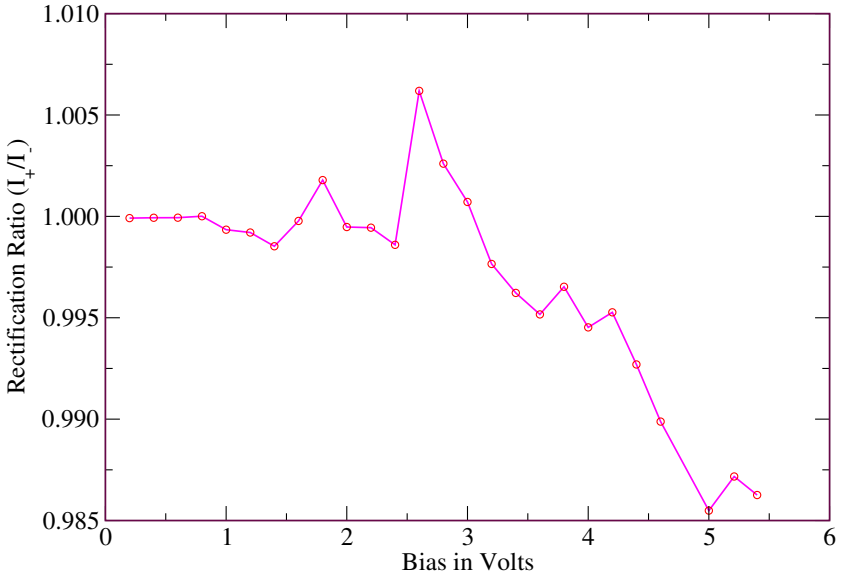

Figure S.8: Rectification ratio of device 1.

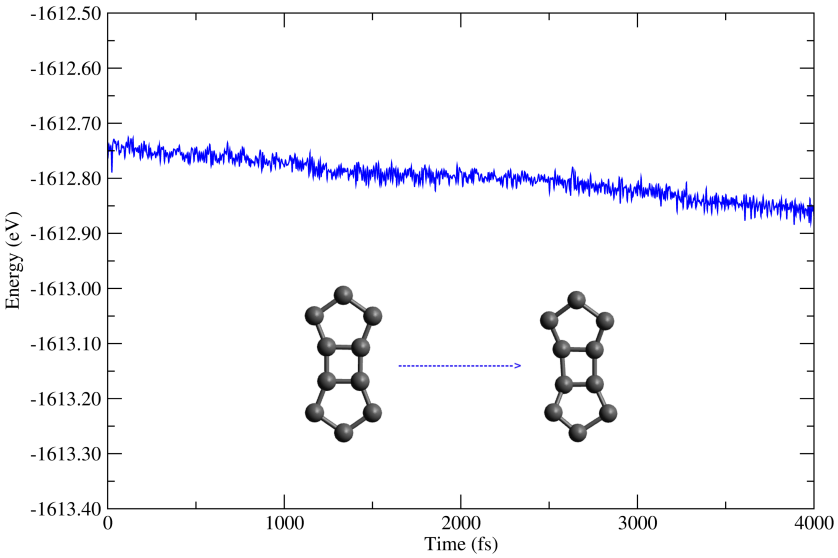

Figure S.9: E-t curve for AIMD simulation of TPO-graphene at 2000K with initial and final structures.

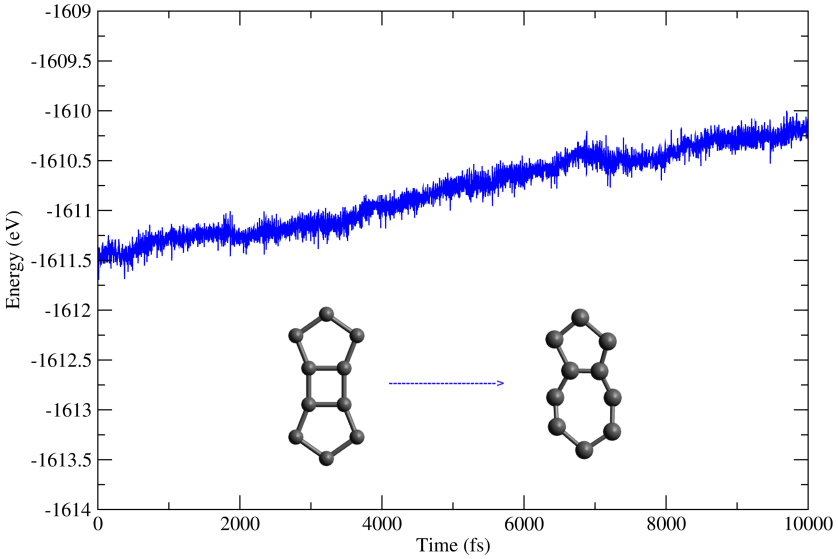

Figure S.10: E-t curve for AIMD simulation of TPO-graphene at 3000K with initial and final structures.

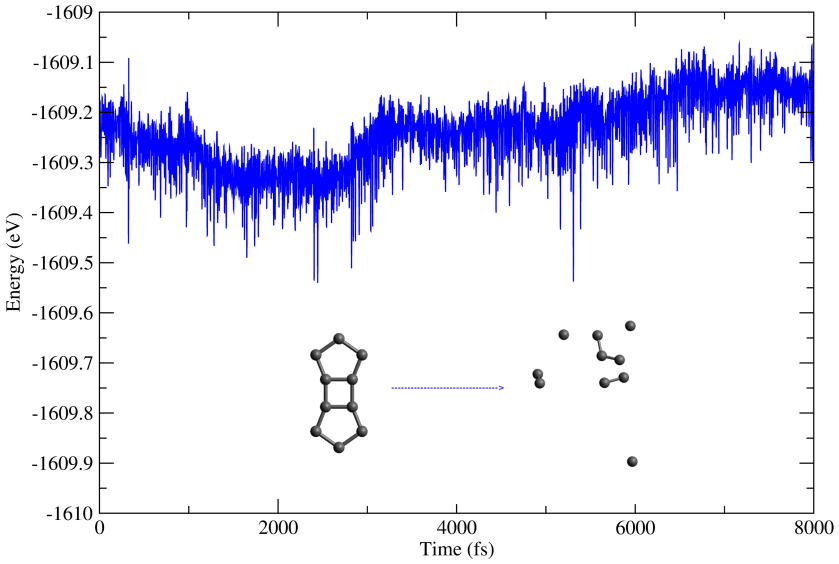

Figure S.11: E-t curve for AIMD simulation of TPO-graphene at 5000K with initial and final structures.

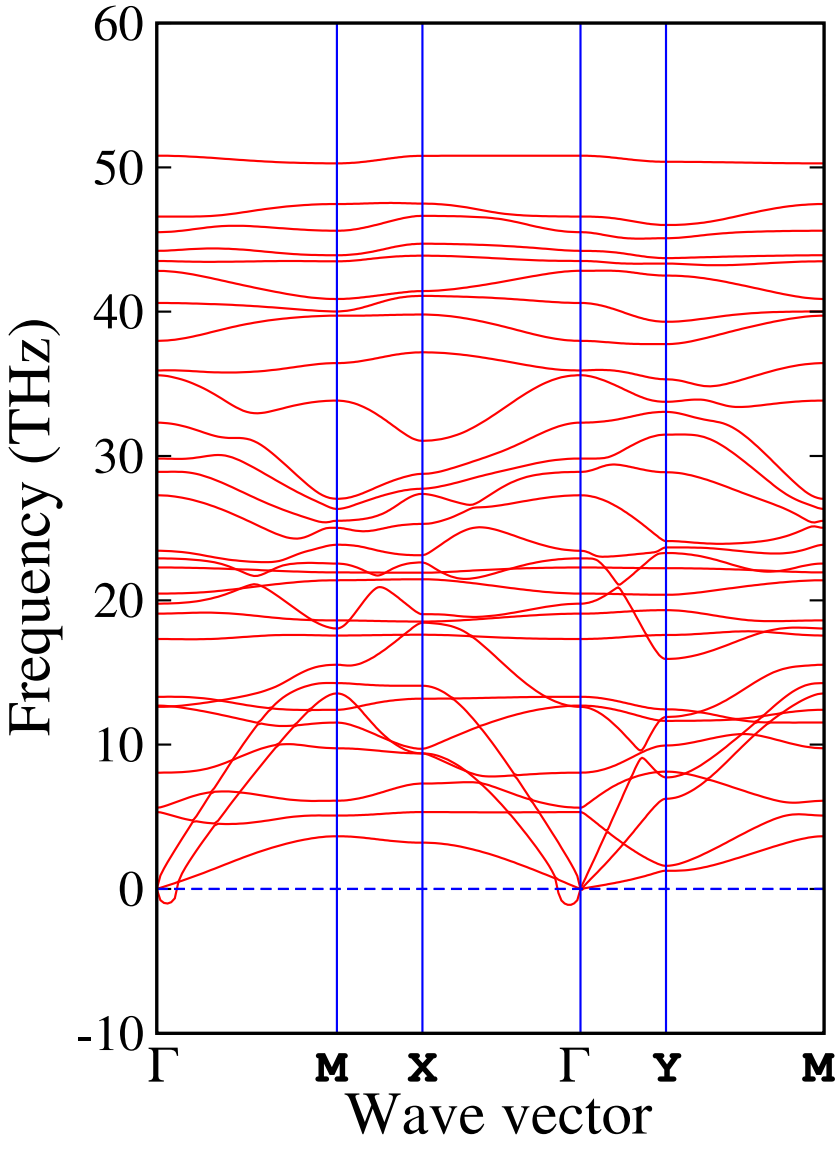

Figure S.12: Phonon spectra for Nitrogen doped at PO site structure. Ref. Fig.8(a)

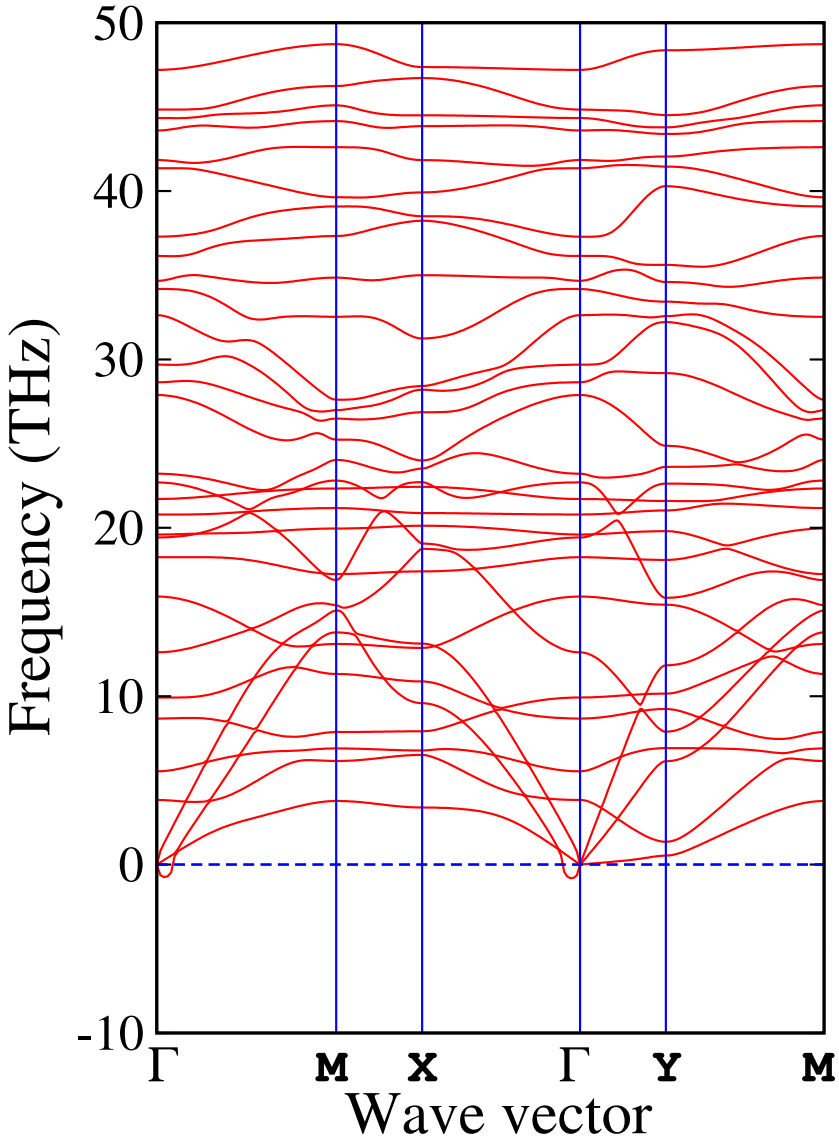

Figure S.13: Phonon spectra for Nitrogen doped at TPO site structure. Ref. Fig.8(b)

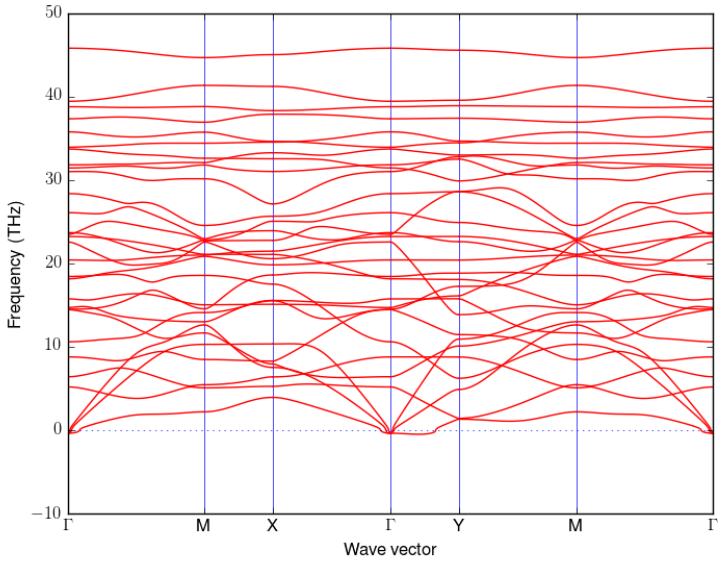

Figure S.14: Phonon spectra for $C_4B_4N_{2a}$ structure. Ref. Fig.S.6(a)

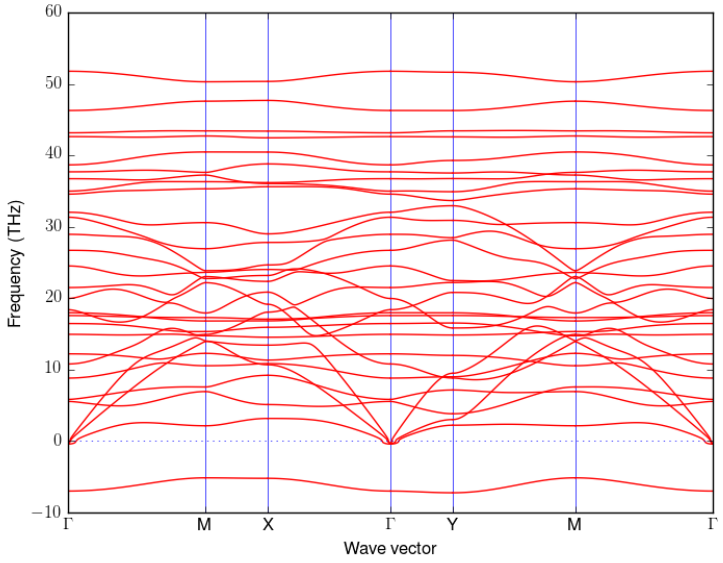

Figure S.15: Phonon spectra for $C_4B_{2a}N_4$ structure. Ref. Fig.S.6(b)

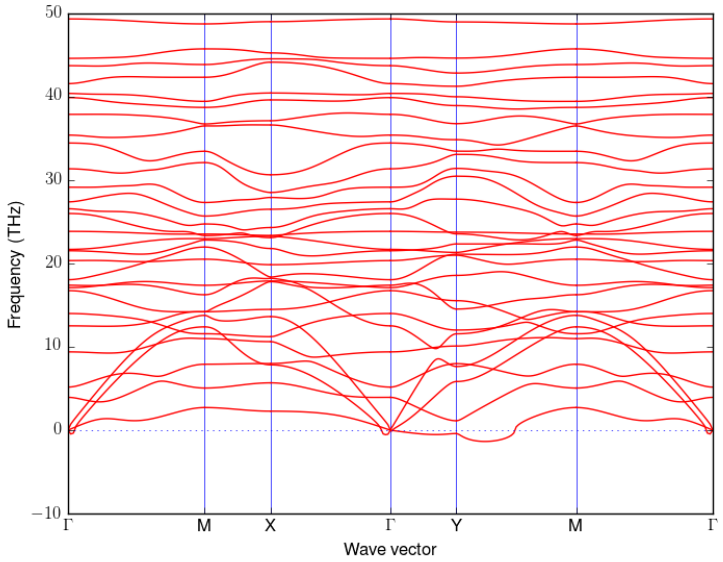

Figure S.16: Phonon spectra for C_9B_{1p} structure. Ref. Fig.S.5(a)

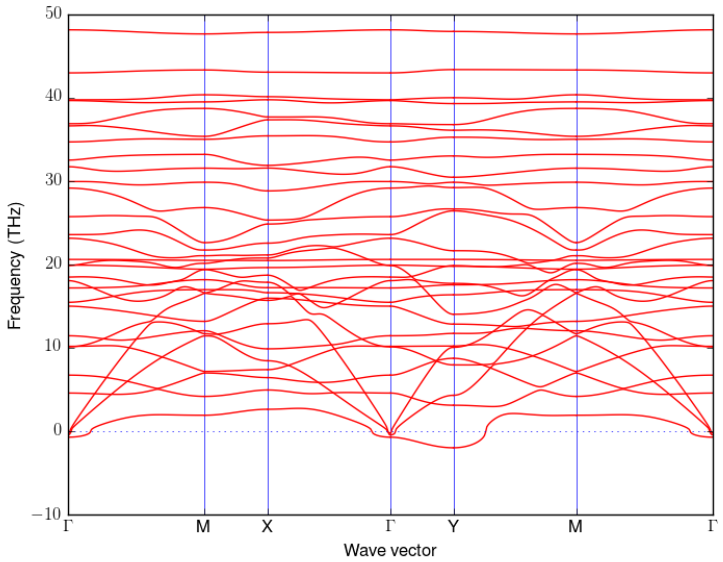

Figure S.17: Phonon spectra for $C_2B_4N_4$ structure. Ref. Fig.9(b)