Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

1 Electronic Supplementary Information (ESI)

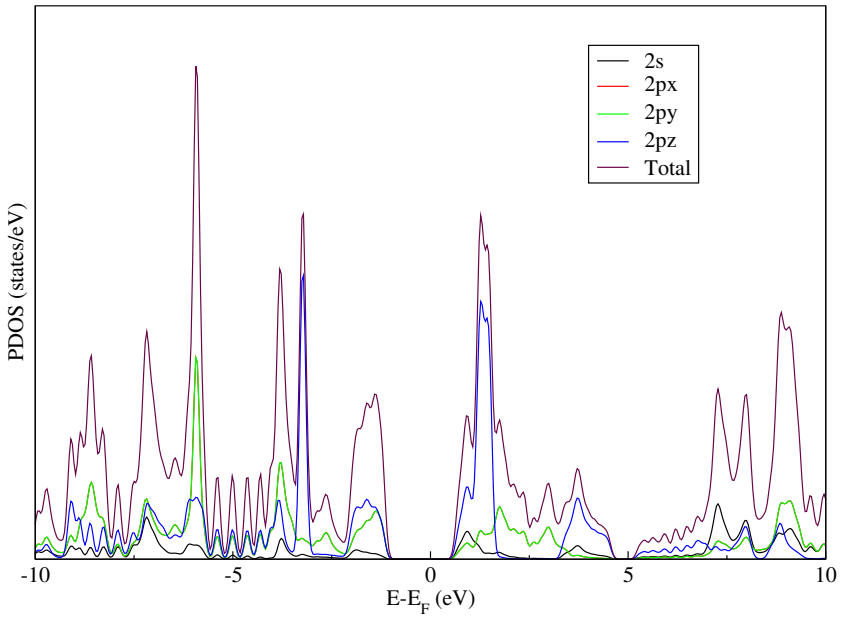

Figure S.1: PDOS for TTG.

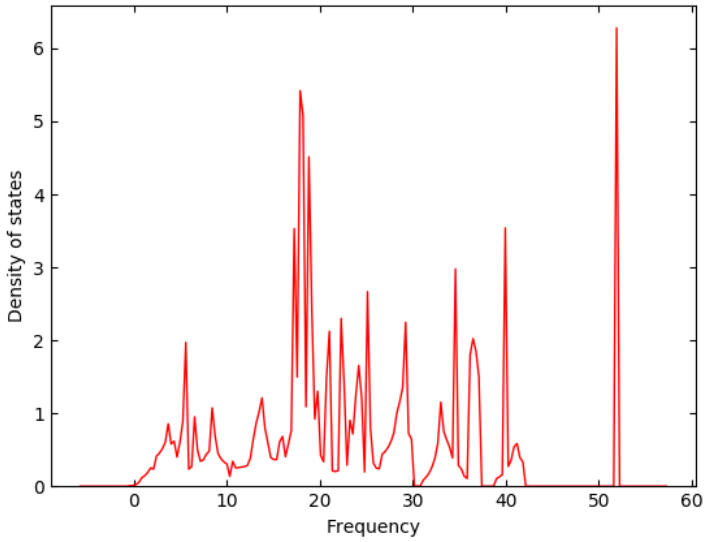

Figure S.2: Phonon DOS for TTG.

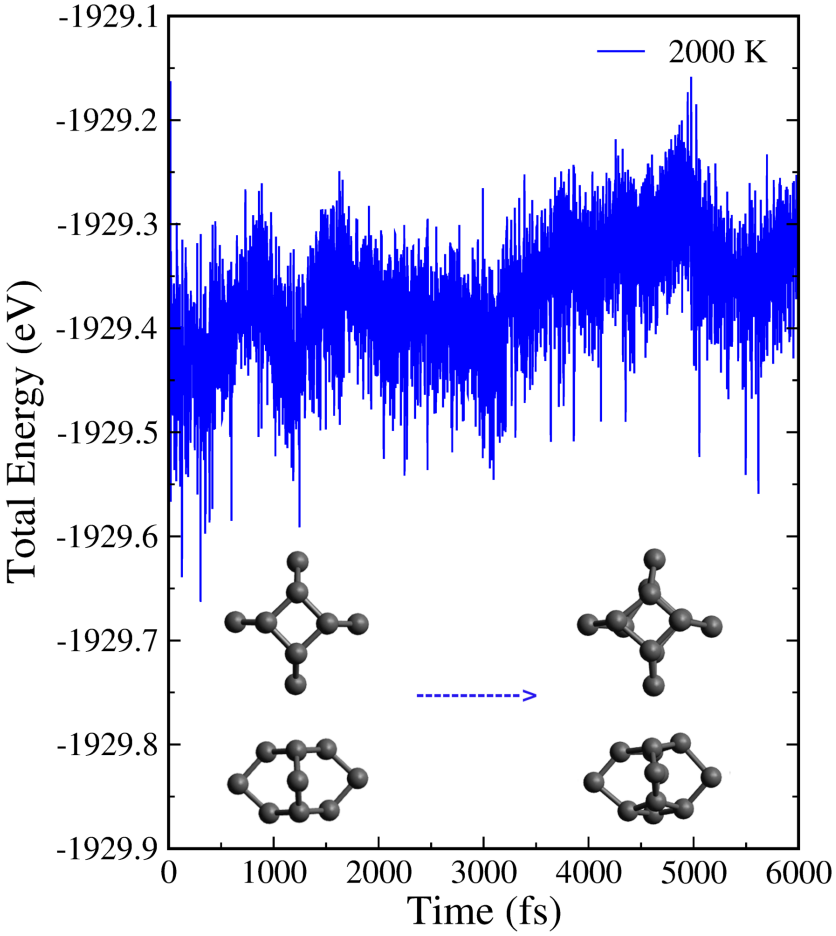

Figure S.3: AIMD data for TTG at 2000K.

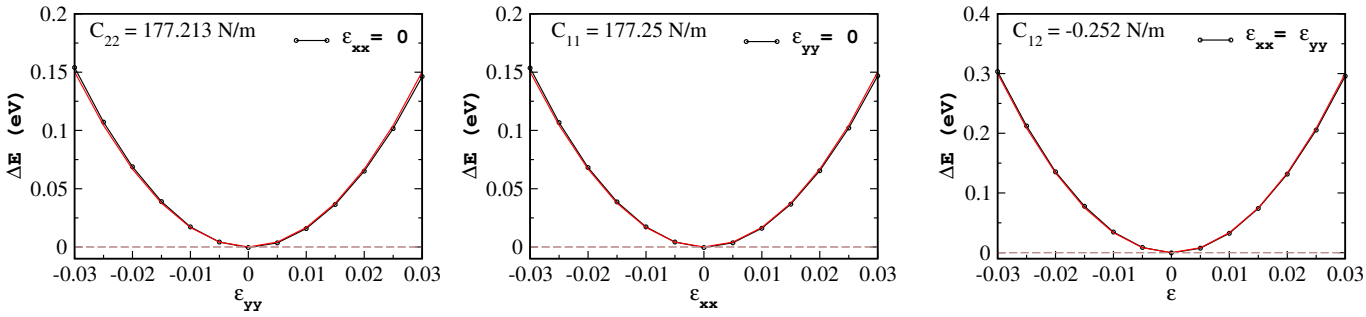

Figure S.4: Strain energy plot for different strain conditions.

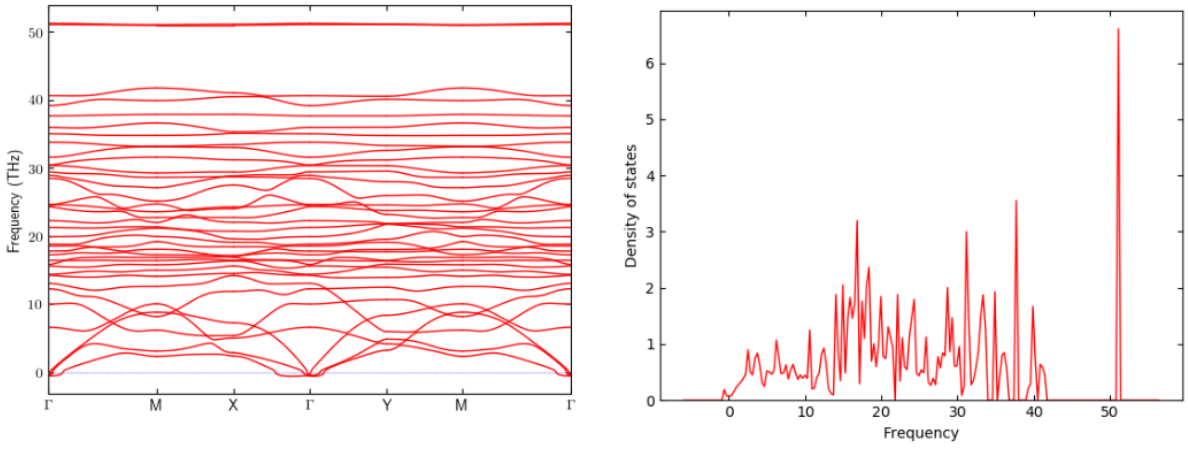

Figure S.5: Phonon band structure for single nitrogen doped TTG and its phonon DOS.

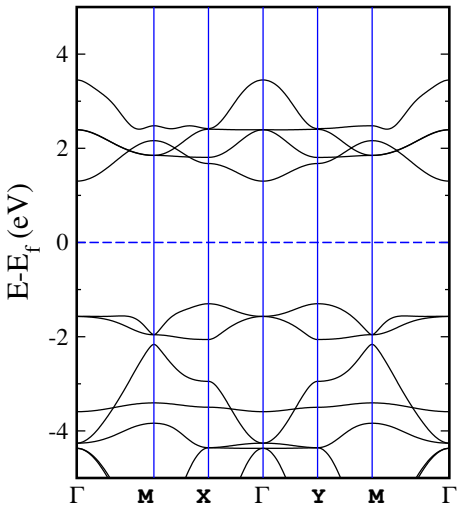

Figure S.6: The HSE06 electronic band structure of twin T-graphene.

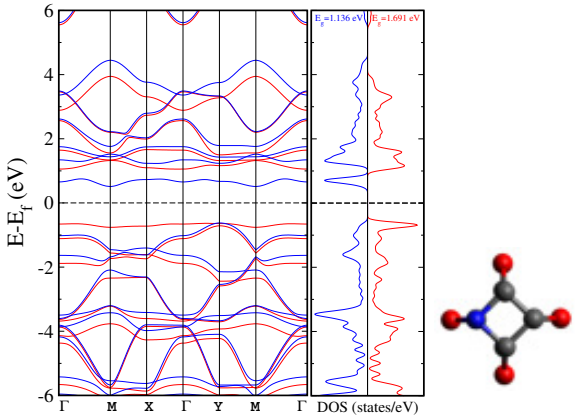

Figure S.7: The electronic band structure of twin T-graphene with nitrogen doping at another C_A site.

Table S.1: SIESTA output. outcoor: Relaxed atomic coordinates (scaled by 1 Ang):

0.01598005	1.13140202	-1.05918179	1	1	C
1.05580617	2.17158466	-1.04465189	1	2	C
0.01581531	3.21165784	-1.05977538	1	3	C
-1.02406901	2.17142077	-1.07417659	1	4	C
-0.01404037	1.13221182	1.05869533	1	5	C
1.02584514	2.17232723	1.07333284	1	6	C
-0.01424269	3.21231634	1.05805908	1	7	C
-1.05413603	2.17210997	1.04359808	1	8	C
0.00079362	4.24844409	-0.00114266	1	9	C
-2.07548627	2.17166997	-0.02996814	1	10	C
0.00105937	0.09535573	0.00019445	1	11	C
2.07717658	2.17183302	0.02898819	1	12	C

Table S.2: SIESTA output. outcell: Unit cell vectors (Ang):

5.493257	-0.000149	0.077997
-0.000149	5.493819	-0.001857
0.311986	-0.007427	19.091743

Table S.3: SIESTA output.

outcell: Cell vector modules (Ang) :	5.493811	5.493820	19.094293
outcell: Cell angles (23,13,12) (deg):	90.0417	88.2503	90.0034
outcell: Cell volume (Ang**3) :	576.0353		