

Electronic Supplemental Information for

“Coro-graphene and Circumcoro-graphyne: Novel Two-Dimensional Materials with Exciting Electronic Properties”

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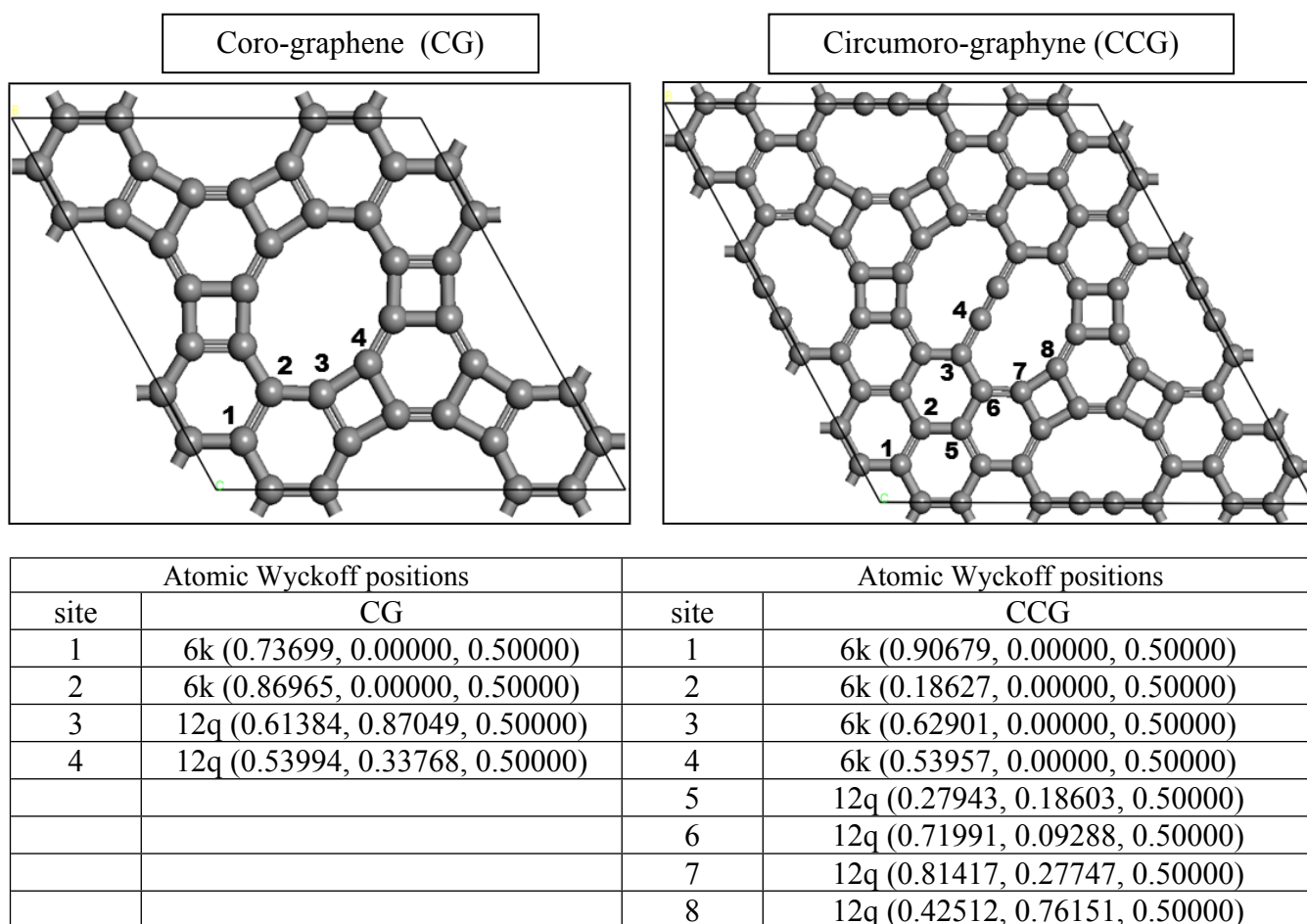


Fig. S1. The different atomic Wyckoff positions of CG and CCG.

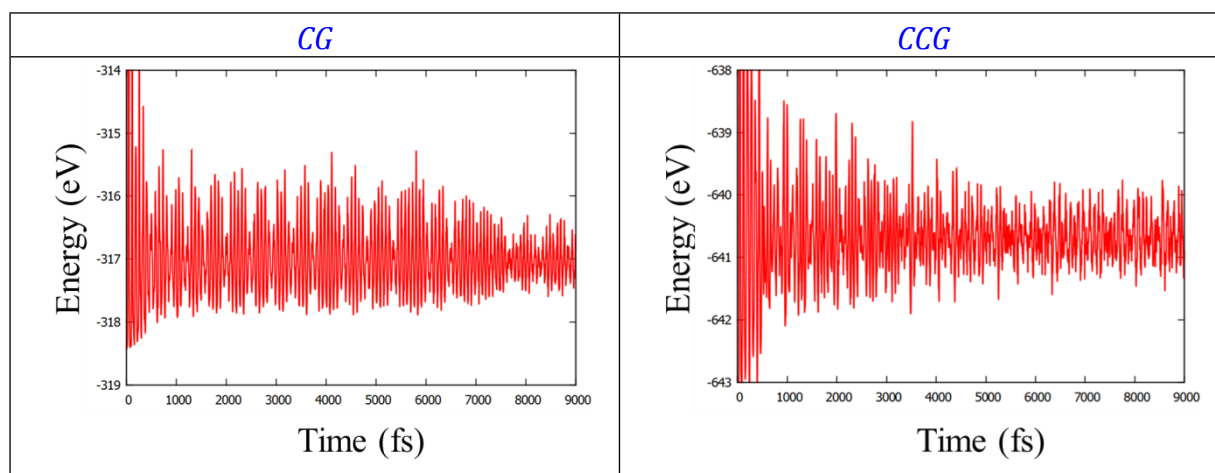


Fig. S2. Total energy fluctuation of CG and CCG at 300 K for 9ps.

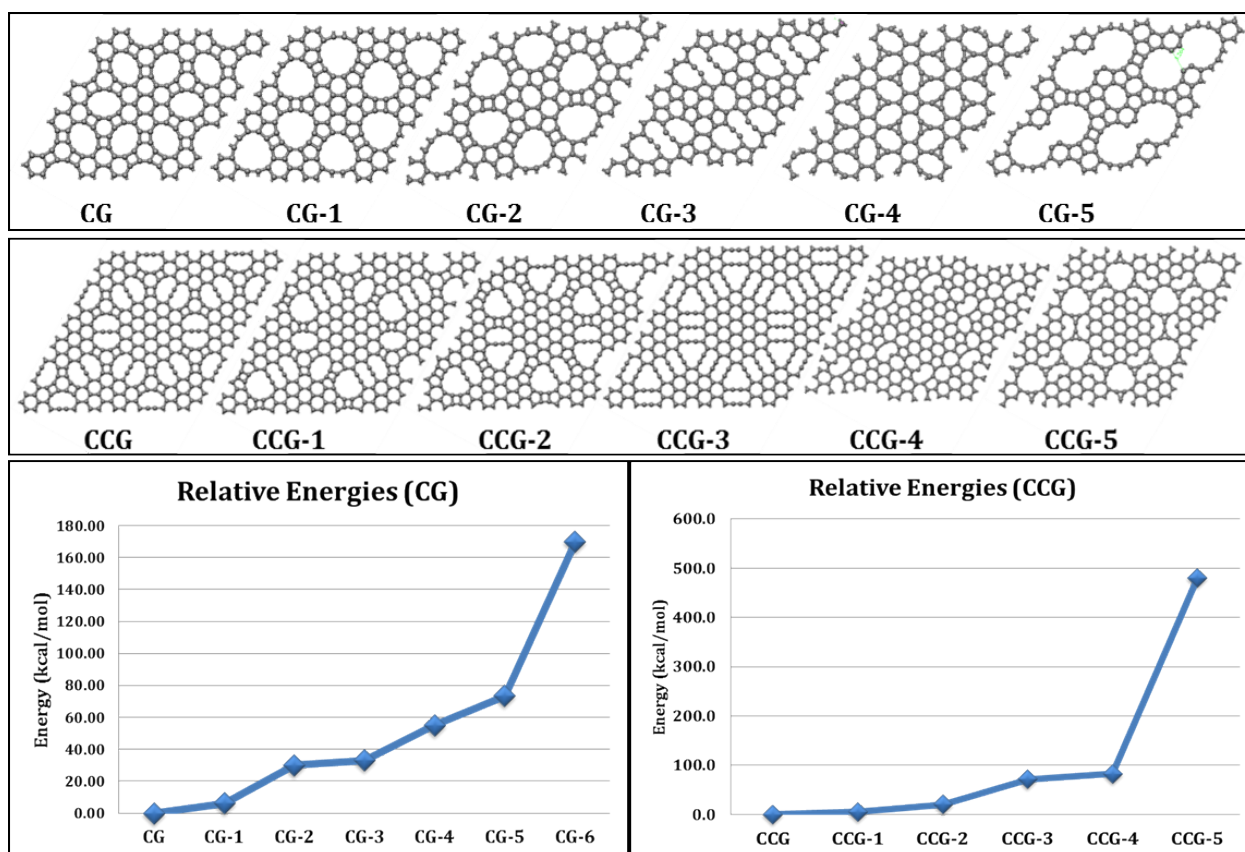


Fig. S3. The relative energies of various carbon based 2D materials with the same number of atoms as that of CG and CCG.

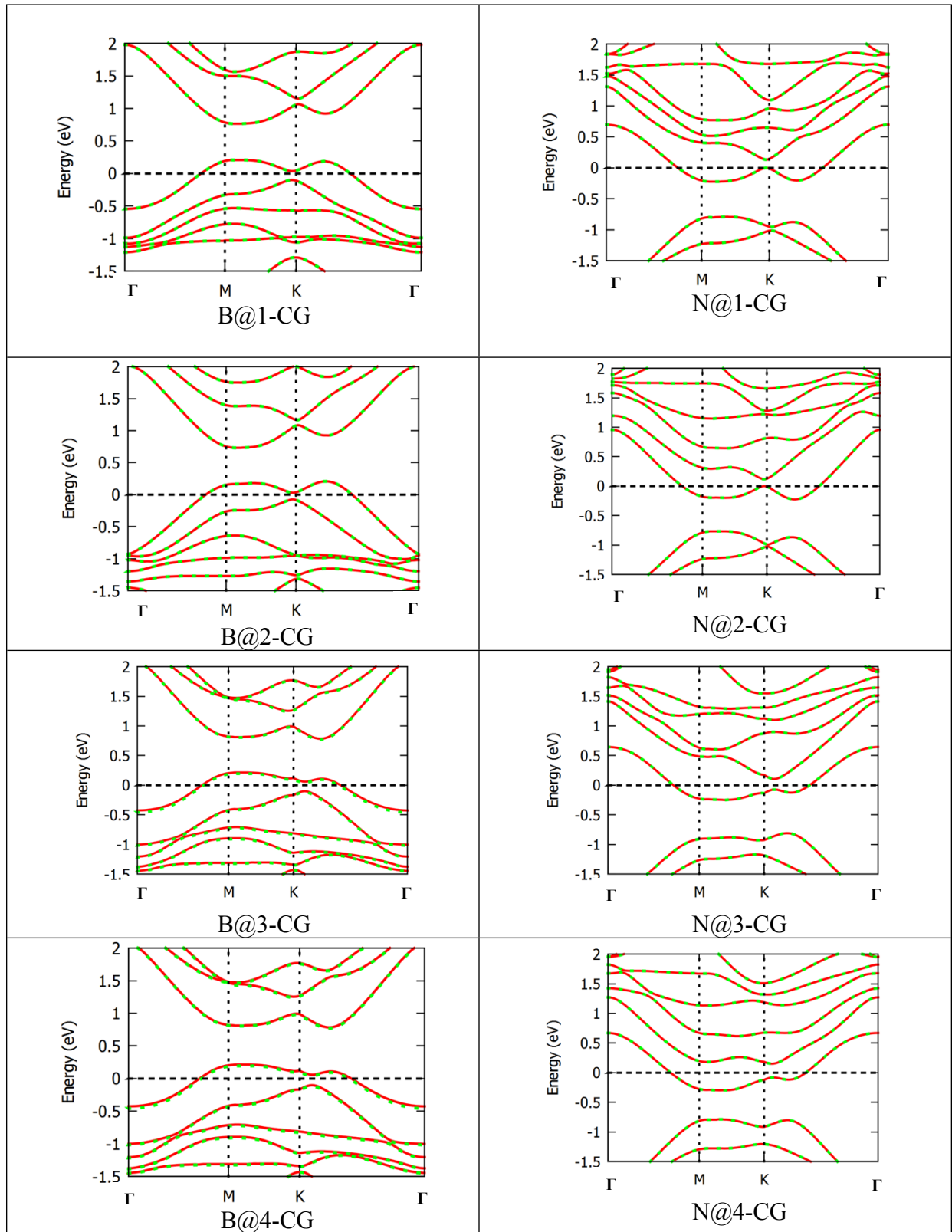
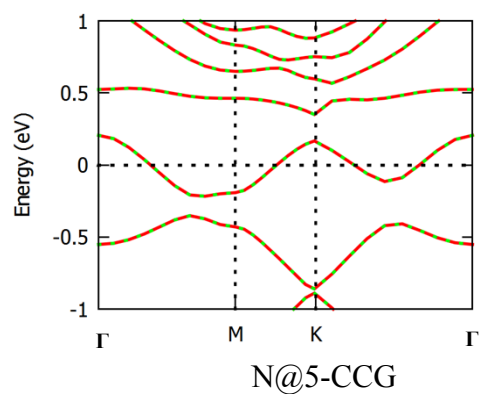
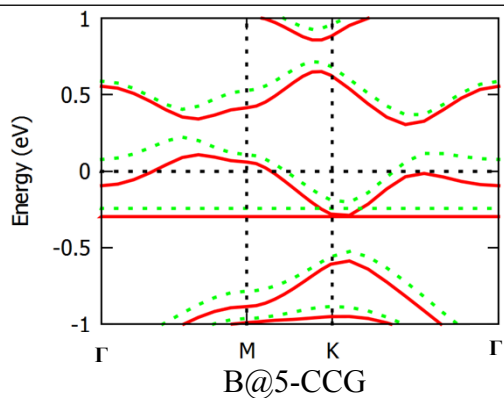
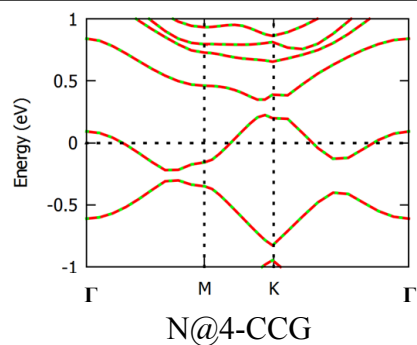
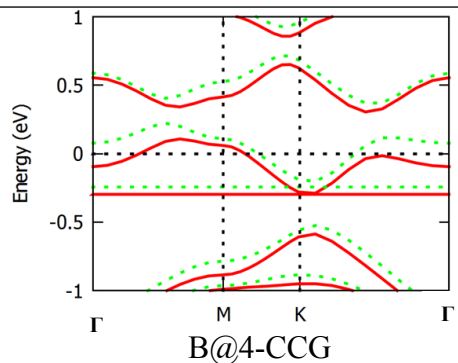
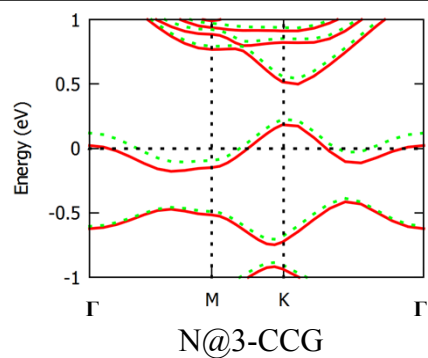
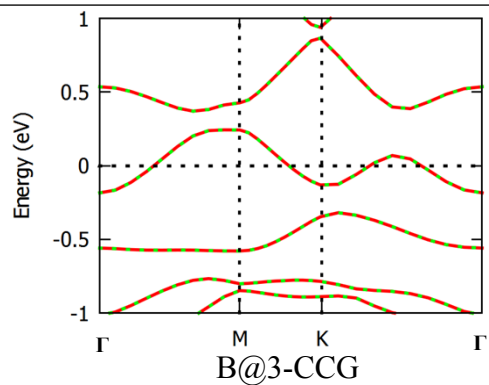
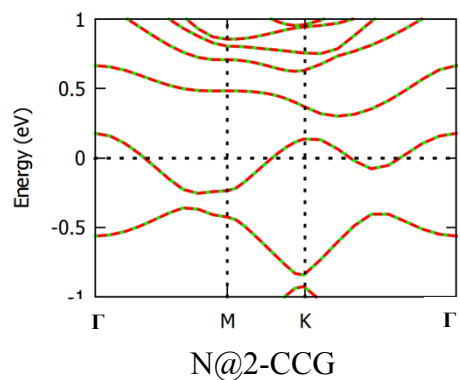
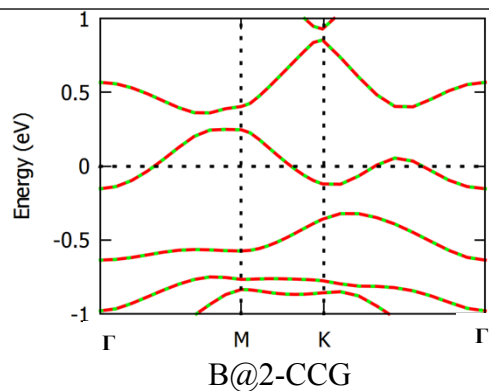


Fig. S4. The spin polarised band structure of B and N doped CG at various doping sites. The fermi level is set to be zero in all cases. The red colour line is corresponding to the up spin and green colour dotted line is for down spin. B@1-CG represents the CG sheet is doped with B atom at carbon atomic site 1.



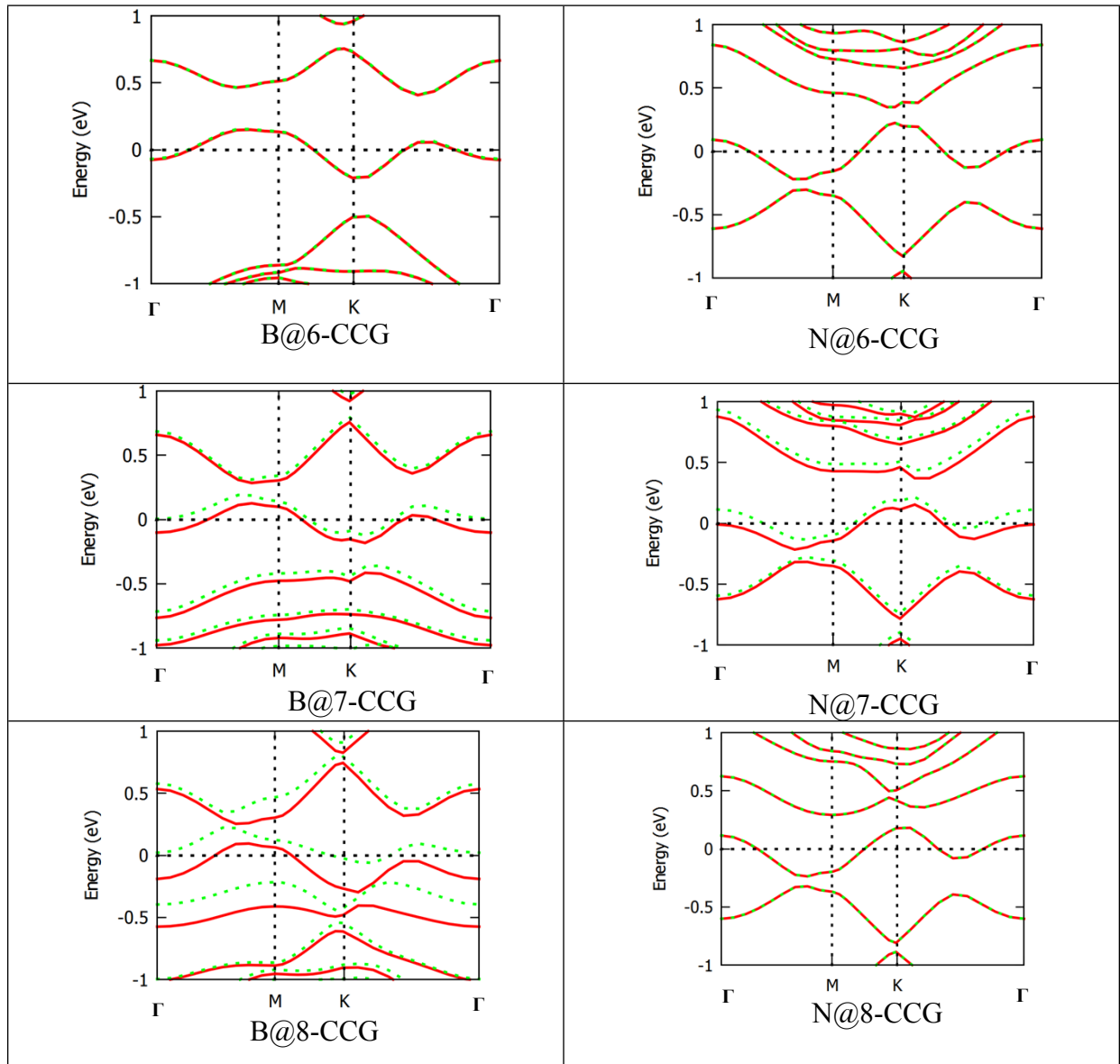


Fig. S5. The spin polarised band structure of B and N doped CCG at various doping sites. The fermi level is set to be zero in all cases. The red colour line is corresponding to the up spin and green colour dotted line represents the down spin. B@1-CCG represents the CCG sheet is doped with B at carbon atomic site 1.