Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information for

Tunable electron property induced by B-doping in g-C_3N_4

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	Energy(eV/atom)
With dispersion term	-8.249
Without dispersion term	-8.217
difference	0.032

Table. S1 The energy of g-C_6N_7B with and without dispersion term.

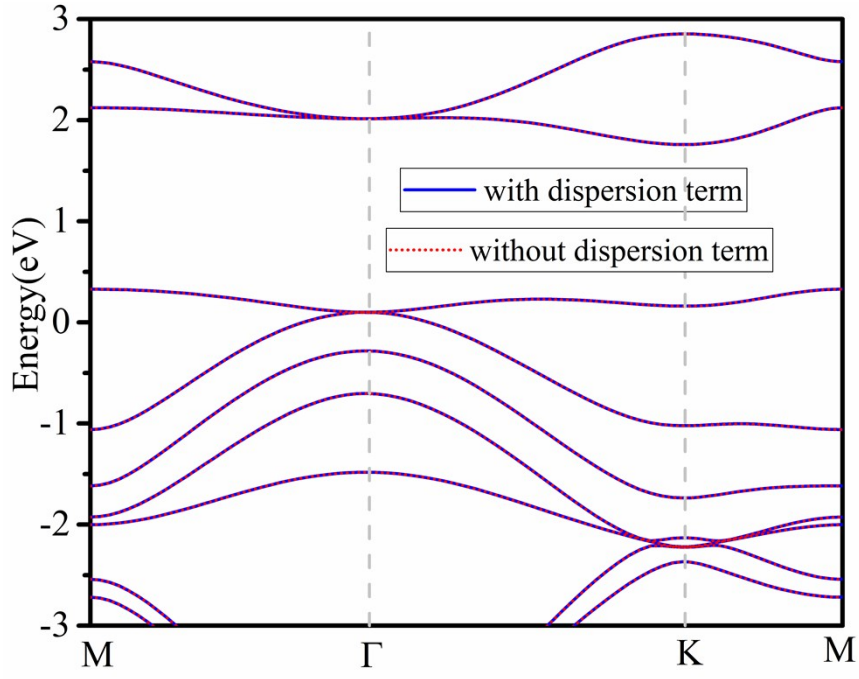

Fig. S1 The electronic band structure of g-C_6N_7B with and without dispersion term. The Fermi level was set as zero.

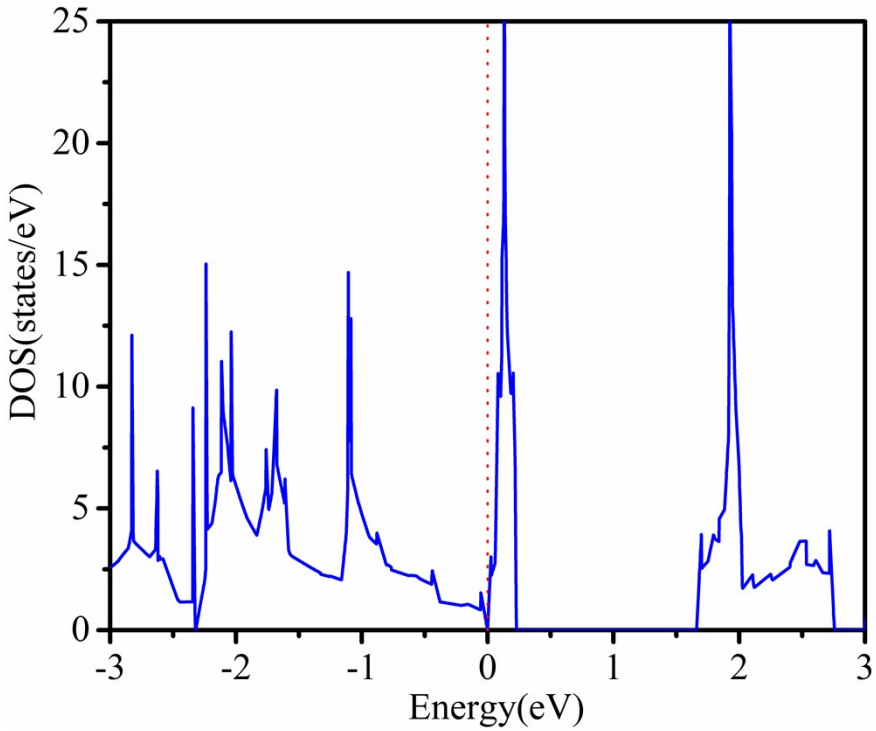

Fig S2. The total density of states of g-C_6N_7B, the Fermi level was set as zero

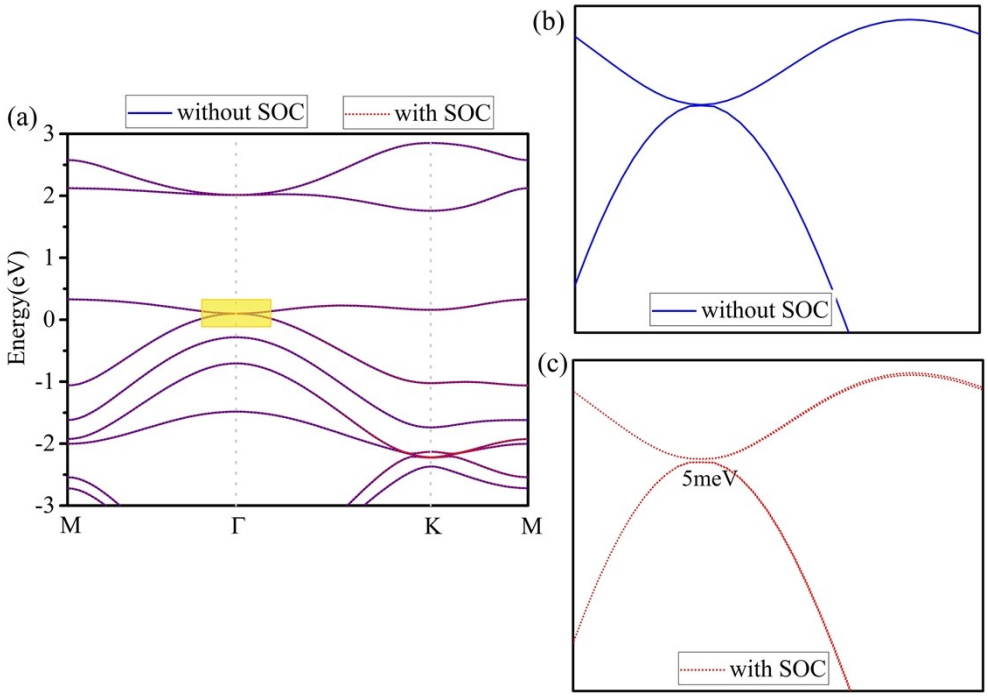

Fig S3. (a) The band structure of g-C_6N_7B without and with SOC, (b) and (c) is the enlarged view for the yellow part in Fig S3. (a) without and with SOC, respectively.

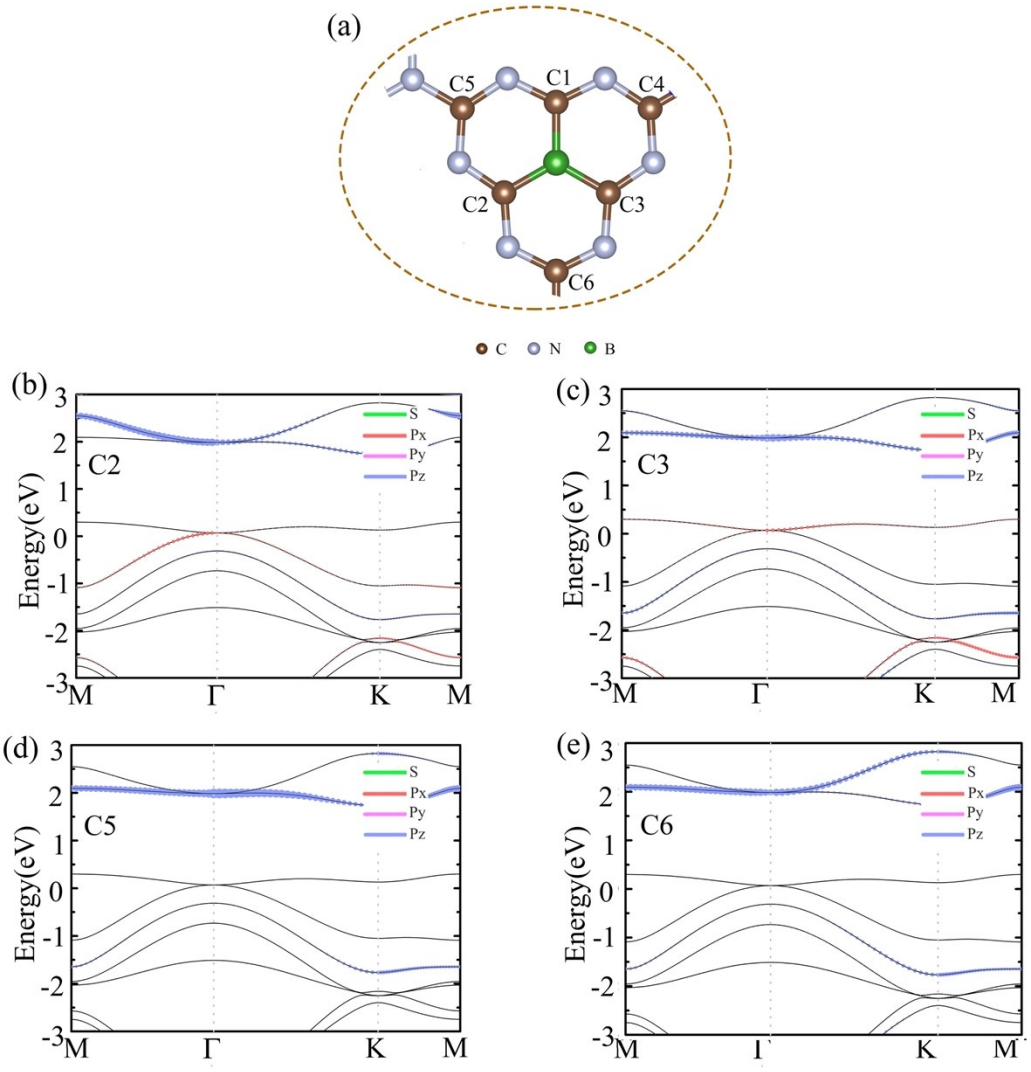

Fig. S4 (a) The geometry structure of g-C_6N_7B. (b)-(e) The orbital-resolved band structure of the g-C_6N_7B on different atoms, labelled in (a).