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

Supporting Information

Non-phase-separated 2D B-C-N alloys via molecule-like carbon doping in 2D BN: Atomic structures and optoelectronic properties

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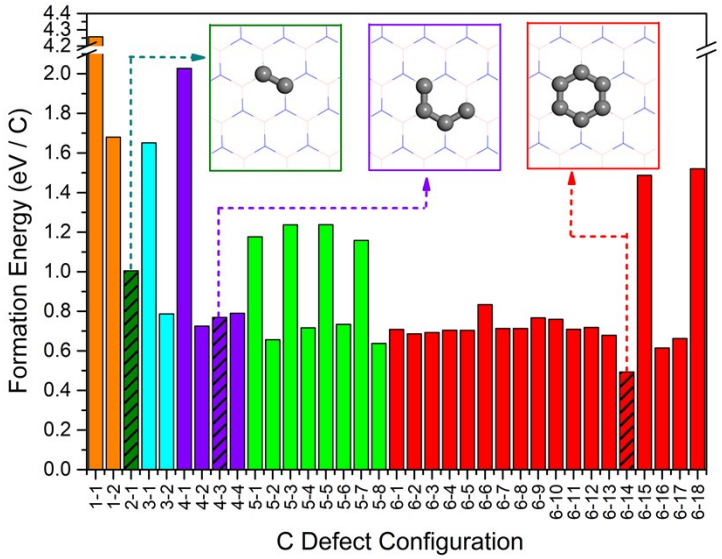

Fig. S1. Formation energy of carbon defect motifs in B-rich condition. Color coding of atom: pink for B, blue for N, and grey for C. The notification "*m*-*n*" is illustrated in the main text and is related to the defect motif shown in Fig. 1(a).

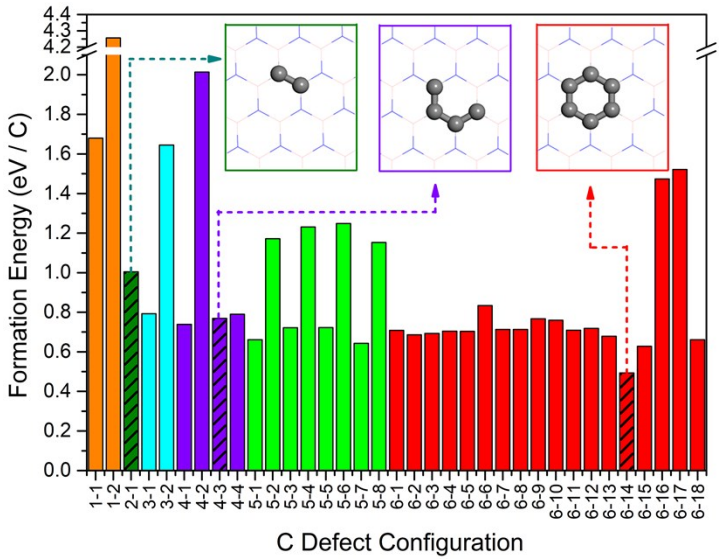

Fig. S2. Formation energy of carbon defect motifs in N-rich condition.

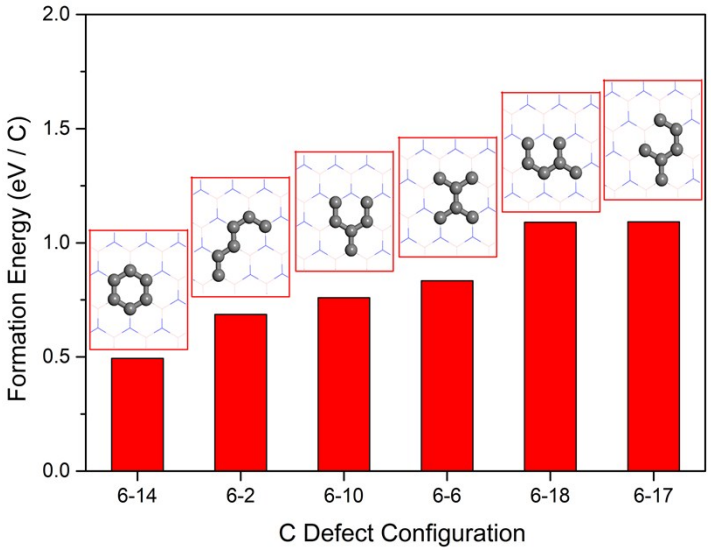

Fig. S3. Formation energies for the representative six-carbon defects. Their corresponding local pictures are shown in the insets. The notifications "*m*-*n*" are the same as Fig.1 in the main text.

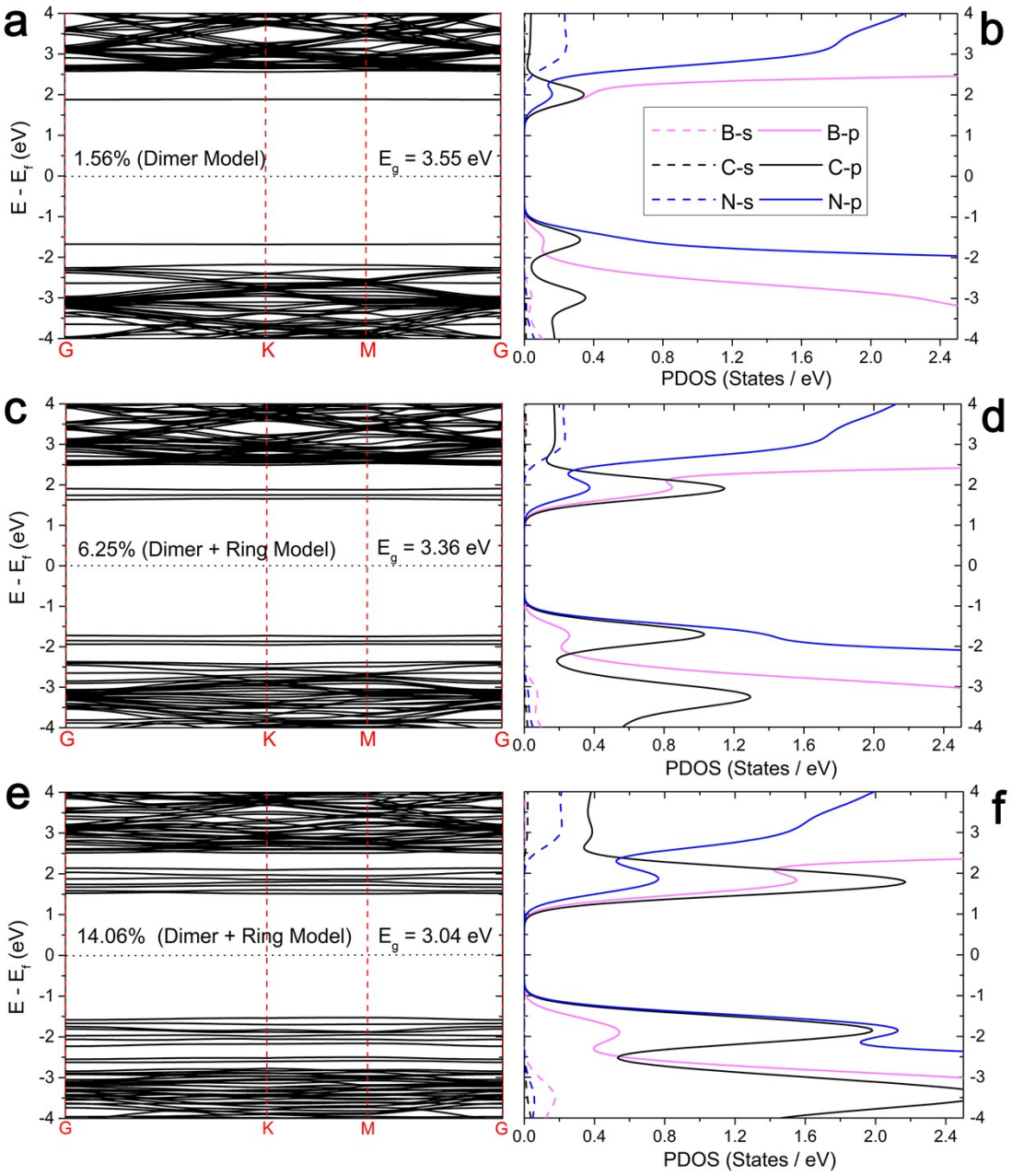

Fig. S4. Band structures and partial DOS (PDOS) of the typical B-C-N alloy models. (a), (c) and (e) are the band structures with carbon concentration of 1.56%, 6.25%, 14.06%, respectively. (b), (d), (f) are the PDOS of (a), (c), (e) respectively.