Supplementary Information

Theoretical investigations of a new two-dimensional semiconducting boron-carbon-nitrogen structure

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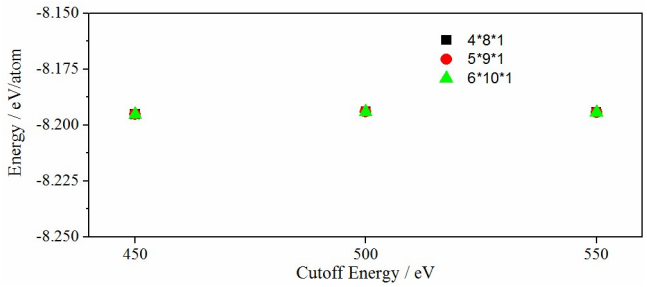

Fig. S1 Convergence test based on different cutoff energies (450, 500 and 550 eV) and k-point grids (4×8×1, 5×9×1 and 6×10×1).

Compared with two experimental synthesized BCN structures (denoted as BCN_v1 and BCN_v3) [*ACS Nano*, 2017, **11**, 2486-2493.], oC-$B_{12}C_{12}N_{12}$ has a higher energy, as shown in Fig. S2. The energy difference between BCN_v3 and oC-$B_{12}C_{12}N_{12}$ is 0.4 eV/atom.

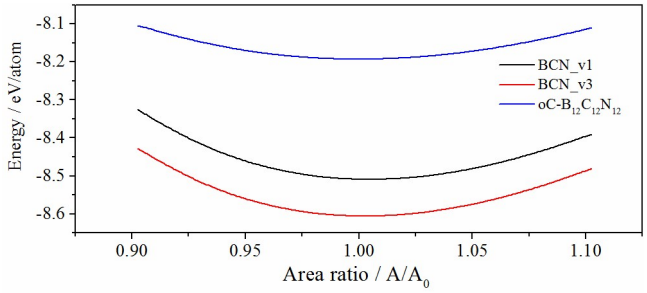

Fig. S2 Total energies of different BCN structures as a function of area ratio.