Supplementary Material

Size-Tunable Energy Gap of Hydrogen-Terminated Biphenylene Segments

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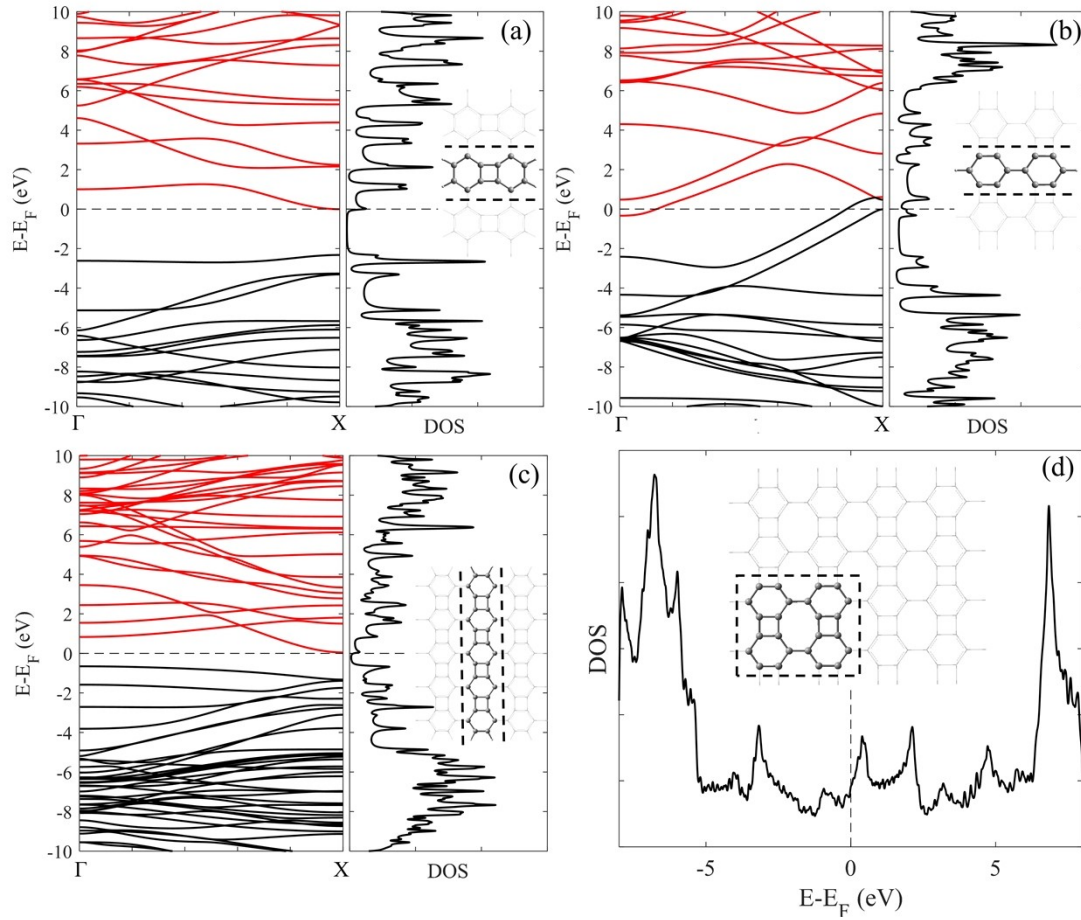
Fig. S1 Band structure and density of states (DOS) of one-dimensional (a) AC-BP and (b) ZZ-BP with the width of two benzene rings as well as (c) AC-BP with the width of five benzene rings. (d) DOS of two-dimensional BP sheet. The unit cells are inserted in each figure. The valence bands are plotted with black lines and the conduction bands are plotted in red. 500 k-points are used in the calculations.
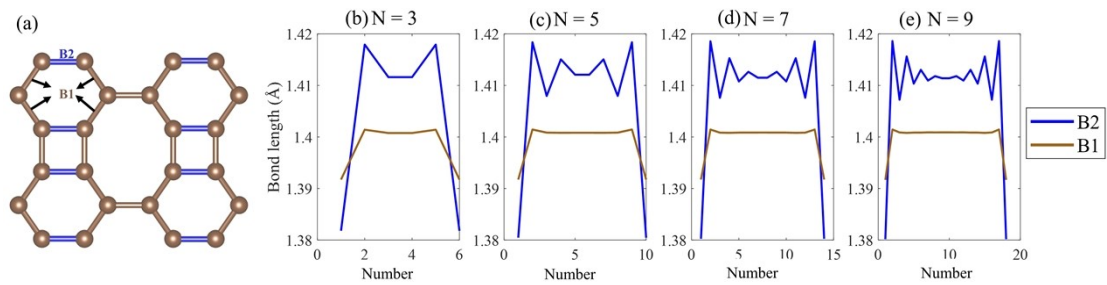

Fig. S2 (a) Structure of unit cell of two-dimensional BP network. (b)-(e) Bond length variation of B1 and B2 for AC-BP and ZZ-BP with N= 3, 5, 7, 9, respectively.
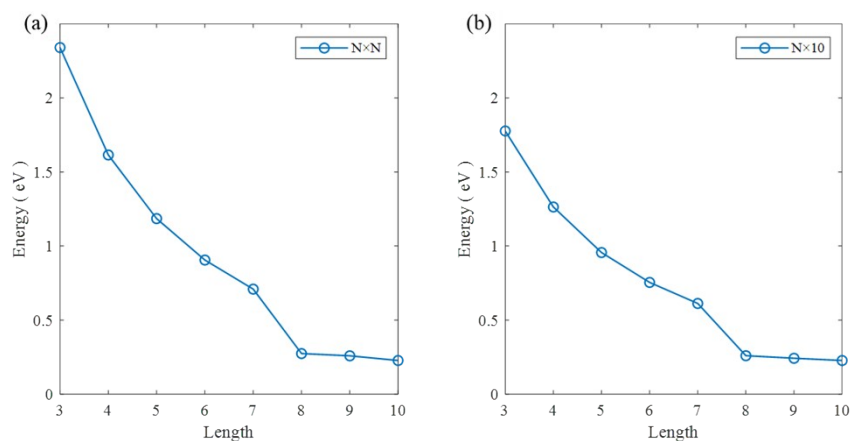
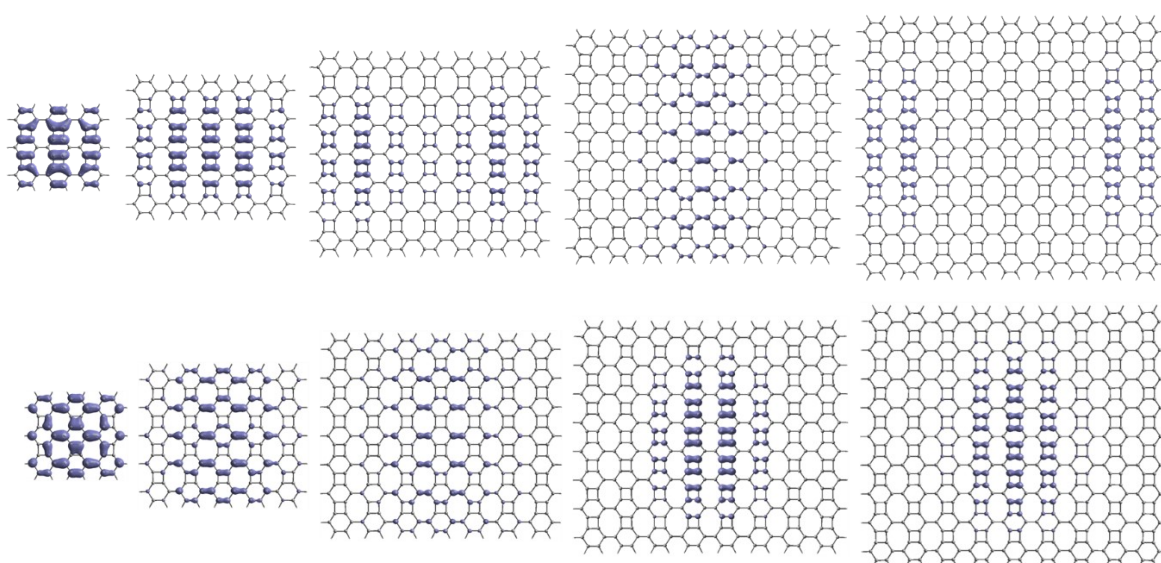**Fig. S3** Energy gap of (a) $N \times N$ and (b) $N \times 10$ BP structures (N=3~10).

Fig. S4 Electron density distribution at HOMO and LUMO state of $N \times N$ BP structures with N=3, 5, 7, 8 and 9. The isosurface value is 0.0005 e/Bohr³.
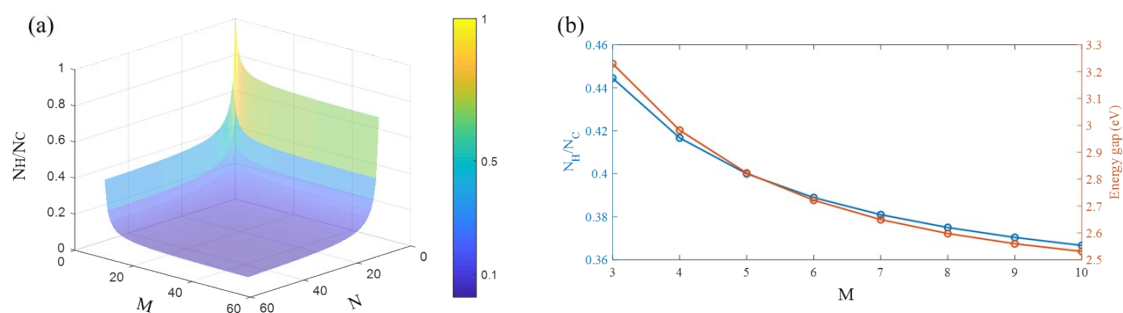

Fig. S5 (a) Relationship between the length and N_H/N_C and the energy gap for Armchair 2*N. (b) Relationship between the length and width and N_H/N_C for BP nano-segments.