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 (\( N = 3 \sim 10 \)).

**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/Bohr\(^3\).

**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.