Supplementary Materials for

DFT characterization of a new possible two-dimensional BN allotrope with a biphenylene network structure

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1. Layered configuration design

The 6 considered different possible construction patterns were obtained by displacing the second layer of *pbn*-BN in *a* and *b* lattice directions with the relative rotational angle α as another adjustable variable. All the representative *a, b* and α quantities selected based on geometric structure symmetry were listed in Tab. 1 with all obtained configurations given in Fig. S1. The initial layer distance was set at a layer thickness of single layer *h*-BN (~3.4 Å). Then the total energy of the 6 independent bilayer structures with different layer distances were calculated as shown in Fig. S2.

Table S1 The 6 different representative *a, b* and α quantities selected used in design of the double layer structure of *pbn*-BN and the corresponding lowest total energy after optimizing the distance between the two layers.

No. / Quanti	Displacement *a*	Displacement *b*	Angle α (π)	Energy (eV)
1	0	0	0	-204.362
2	0.5	0	0	**-204.374**
3	0	0.5	0	-204.371
4	0.5	0.5	0	-204.364
5	0.25	0.5	0	-204.367
6	0.25	0.5	1.0	-204.366

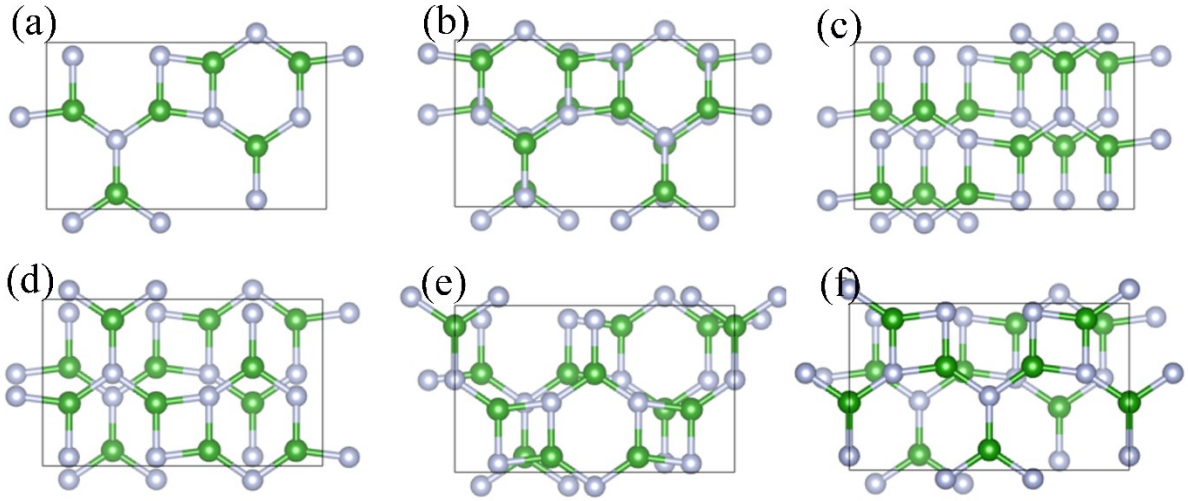

Figure S1 The 6 configurations corresponding to the representative considered *a, b* and α quantities selected based on geometric structure symmetry listed in Tab. 1.

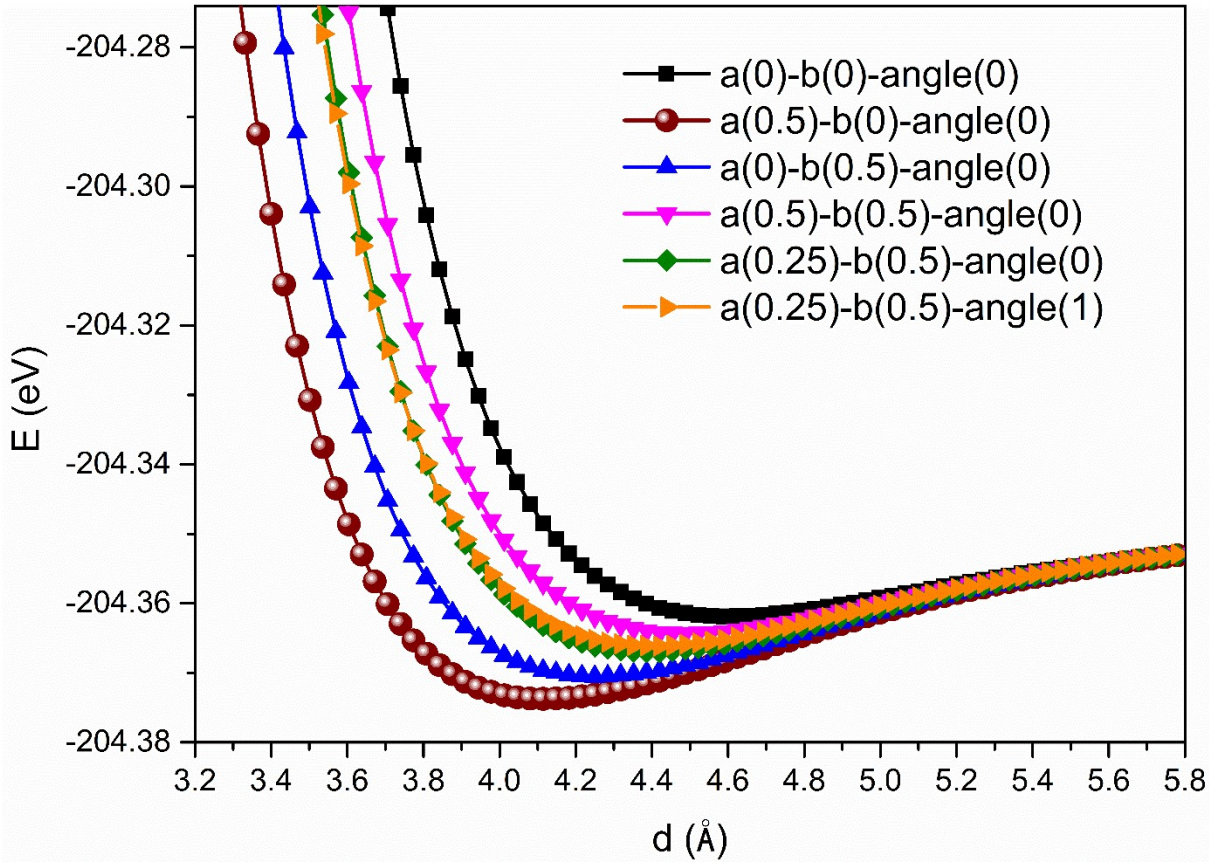

Figure S2 The total energy *E* change versus the layer distance *d* between the two layers in a bilayer *bpn-BN* structure. The 6 independent *a, b* and α quantities are given in the legends.