Supplemental Material: Interception of Layered LP-N and HLP-N at Ambient Conditions by Confined Template

Dong-xue Wang(王冬雪)[1], Jing Fu(付静)[2], Yi Li(李义)[3], Zhen Yao(姚震)[1,**], Shuang Liu(刘爽)[1,**], and Bing-bing Liu(刘冰冰)[1,**]

[1]State Key Laboratory of Superhard Materials, College of Physics, Jilin University, Changchun 130012, P.R. China

[2]Basic Science Department, Jilin Institute of Architecture and Technology, Changchun 130000, P.R. China

[3]College of Science, Liaoning University of Technology, Jinzhou 121000, P.R. China

*Supported by the National Key R&D Program of China (Grant No. 2018YFA0305900), the National Natural Science Foundation of China (Grant Nos. 12174143 and U2032215), and the Natural Science Foundation Project of Liaoning Province (Grant Nos. 2022- MS-377).

**Email: yaozhen@jlu.edu.cn; liu_shuang@jlu.edu.cn; liubb@jlu.edu.cn

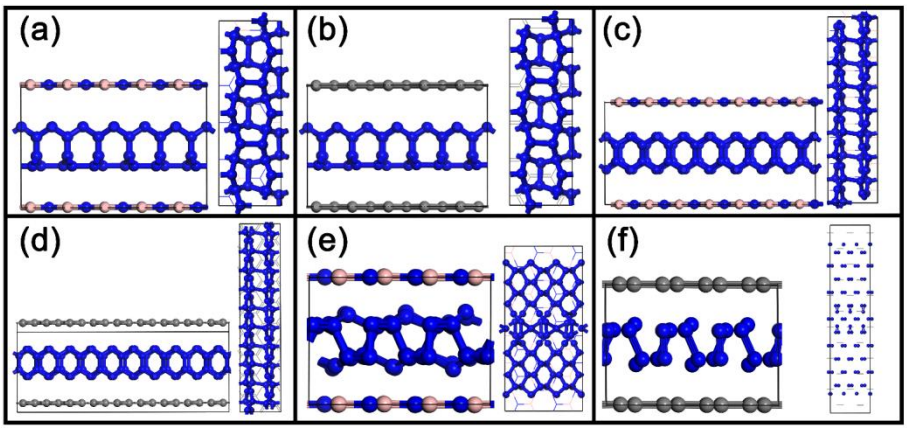

Figure S1: The images of relaxed structures of LP-N@h-BN (a), LP-N@graphene (b), HLP-N@h-BN (c), HLP-N@graphene (d), BP-N@h-BN (e), and BP-N@graphene (f) at 0 GPa.

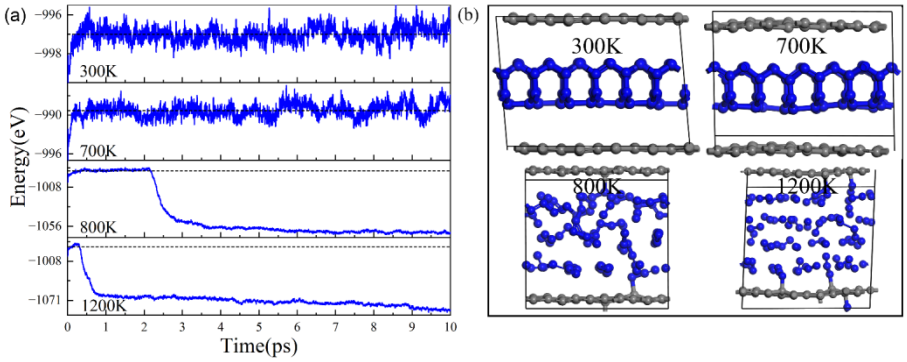

Figure S2: (a) Energy of LP-N@graphene as a function of time at 300 K, 700 K, 800 K, and 1200K in AIMDs. (b) Snapshots of LP-N@graphene after the AIMDs at 300 K, 700 K, 800 K, and 1200 K.

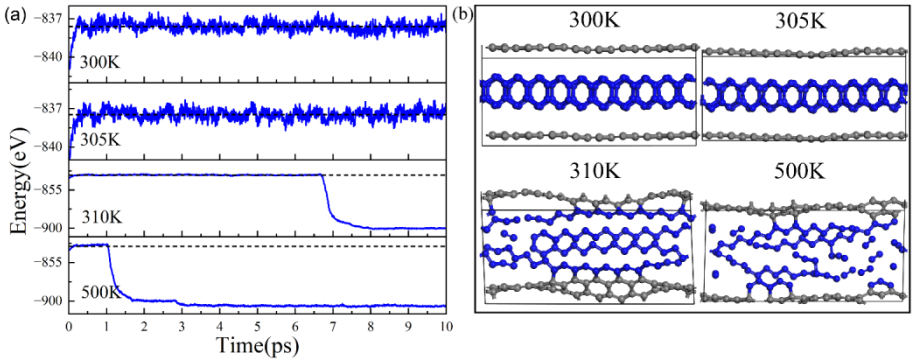

Figure S3: (a) Energy of HLP-N@graphene as a function of time at 300 K, 305 K, 310 K, and 500 K in AIMDs. (b) Snapshots of HLP-N@graphene after the AIMDs at 300 K, 305 K, 310 K, and 500 K.

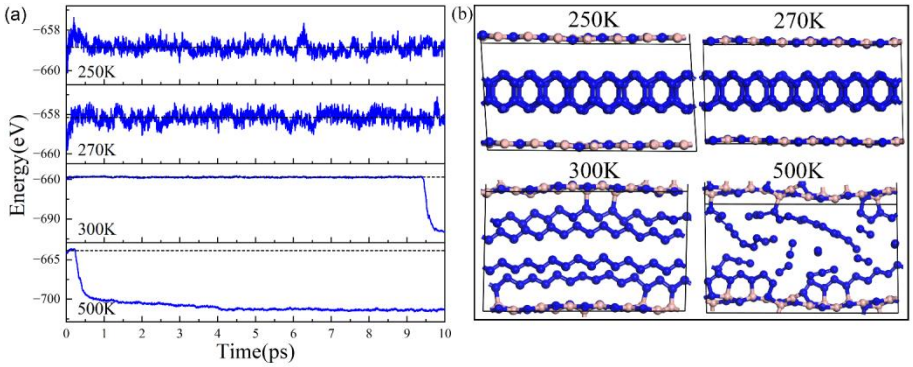

Figure S4: (a) Energy of HLP-N@h-BN as a function of time at 250 K, 270 K, 300 K, and 500K in AIMDs. (b) Snapshots of HLP-N@h-BN after the AIMDs at 250 K, 270 K, 300 K, and 500 K.

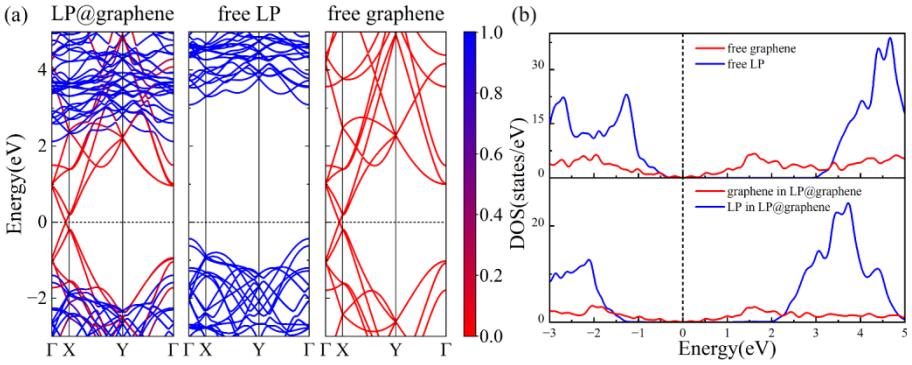

Figure S5: (a) Band structures of LP-N@graphene, free LP-N and free graphene. (b) DOSs of free LP-N, free graphene and their hybrid system.

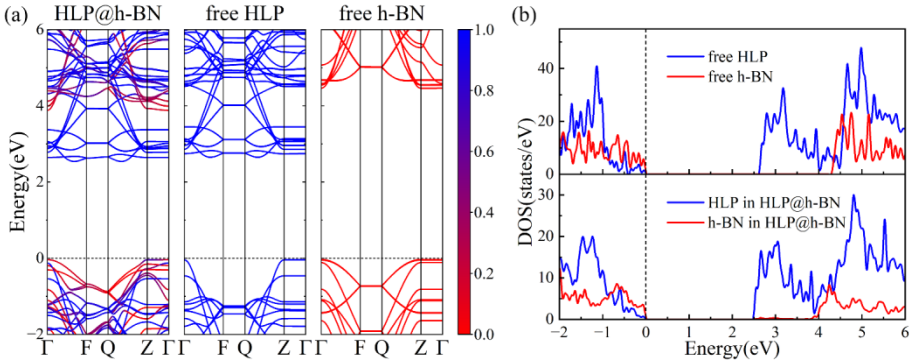

Figure S6: (a) Band structures of HLP-N@h-BN, free HLP-N and free h-BN. (b) DOSs of free HLP-N, free h-BN and their hybrid system.

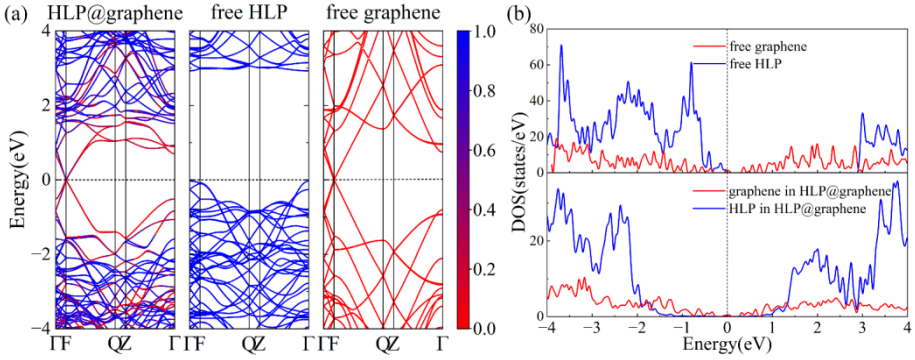

Figure S7: (a) Band structures of HLP-N@graphene, free HLP-N and free graphene. (b) DOSs of free HLP-N, free graphene and their hybrid system.

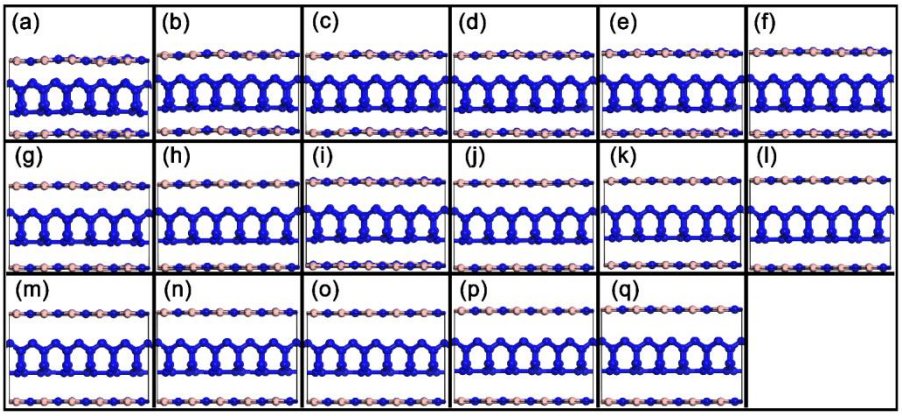

Figure S8: The images of relaxed LP-N@h-BN with interlayer spacing of 1.598 Å (a), 1.698 Å (b), 1.798Å (c), 1.898 Å (d), 1.998 Å (e), 2.098 Å (f), 2.198 Å (g), 2.298 Å (h), 2.398 Å (i), 2.498 Å (j), 2.598 Å (k), 2.698 Å (l), 2.798 Å (m), 2.898 Å (n), 2.998 Å (o), 3.098 Å (p), and 3.198 Å (q) at ambient pressure.

In this work, the values of |δ| for our constructed six confinement models are all smaller than 5%, indicating that the lattice matches well between the template and confined guest. The detailed calculations of |δ| see follows.

1). For LP-N@h-BN, the model is constructed by the 3×1 unit cell of LP-N (48 atoms) and 5×1 unit cell of h-BN (20 atoms). The details of the unit cell lattice constants are as follows.

For h-BN: oa=2.53, ob=4.35.

For LP-N: oa= 4.17, ob=4.15.

The lattice mismatch $\delta_{oa} = |(5*L_{h\text{-}BN}-3*L_{LP\text{-}N})/3*L_{LP\text{-}N}| = 0.92\%$; L refers to lattice constant oa. The lattice mismatch $\delta_{ob} = |(1*L_{h\text{-}BN}-1*L_{LP\text{-}N})/1*L_{LP\text{-}N}| = 4.77\%$; L refers to lattice constant ob.

2). For LP-N@graphene, the model is constructed by the 3×1 unit cell of LP-N (48 atoms) and 5×1 unit cell of graphene (20 atoms). The details of the unit cell lattice constants are as follows.

For graphene: oa=2.46, ob=4.26.

For LP-N: oa=4.17, ob=4.15.

The lattice mismatch $\delta_{oa} = |(5*L_{graphene}-3*L_{LP\text{-}N})/3*L_{LP\text{-}N}| = 1.68\%$; L refers to lattice constant oa. The lattice mismatch $\delta_{ob} = |(1*L_{graphene}-1*L_{LP\text{-}N})/1*L_{LP\text{-}N}| = 2.65\%$; L refers to lattice constant ob.

3). For HLP-N@h-BN, the model is constructed by the 4×1 unit cell of HLP-N (64 atoms) and 7×1 unit cell of h-BN (28 atoms). The details of the unit cell lattice constants are as follows.

For h-BN: oa=2.53, ob=4.35.

For HLP-N: oa=ob= 4.41.

The lattice mismatch $\delta_{oa} = |(7*L_{h\text{-}BN}-4*L_{HLP\text{-}N})/4*L_{HLP\text{-}N}| = 0.22\%$; L refers to lattice constant oa. The lattice mismatch $\delta_{ob} = |(1*L_{h\text{-}BN}-1*L_{HLP\text{-}N})/1*L_{HLP\text{-}N}| = 1.38\%$; L refers to lattice constant ob.

4). For HLP-N@graphene, the model is constructed by the 5×1 unit cell of HLP-N (80 atoms) and 9×1 unit cell of graphene (36 atoms). The details of the unit cell lattice constants are as follows.

For graphene: ob=2.46, oc=4.26.

For HLP-N: ob=oc= 4.41.

The lattice mismatch $\delta_{ob} = |(9*L_{graphene}-5*L_{HLP\text{-}N})/5*L_{HLP\text{-}N}| = 0.43\%$; L refers to lattice constant ob. The lattice mismatch $\delta_{oc} = |(1*L_{graphene}-1*L_{HLP\text{-}N})/1*L_{HLP\text{-}N}| = 3.38\%$; L refers to lattice constant oc.

5). For BP-N@h-BN, the model is constructed by the 7×3 unit cell of BP-N (84 atoms) and 6×2 unit cell of h-BN (48 atoms). The details of the unit cell lattice constants are as follows.

For h-BN: oa=2.53, ob=4.35.

For BP-N: oa= 2.13, ob= 2.86.

The lattice mismatch $\delta_{oa} = |(6*L_{h\text{-}BN}-7*L_{BP\text{-}N})/7*L_{BP\text{-}N}| = 1.40\%$; L refers to lattice constant oa. The lattice mismatch $\delta_{ob} = |(2*L_{h\text{-}BN}-3*L_{BP\text{-}N})/3*L_{BP\text{-}N}| = 1.35\%$; L refers to lattice constant ob.

6). For BP-N@graphene, the model is constructed by the 7×3 unit cell of BP-N (84 atoms) and 6×2 unit cell of graphene (48 atoms). The details of the unit cell lattice constants are as follows.

For graphene: oa=2.46, ob=4.26.

For BP-N: oa=2.13,ob= 2.86.

The lattice mismatch $\delta_{oa} = |(6*L_{graphene}-7*L_{BP\text{-}N})/7*L_{BP\text{-}N}| = 1.21\%$; L refers to lattice constant oa. The lattice mismatch $\delta_{ob} = |(2*L_{graphene}-3*L_{BP\text{-}N})/3*L_{BP\text{-}N}| = 0.68\%$; L refers to lattice constant ob.

Table S1. The lattice constants of initial models of LP-N@h-BN, LP-N@graphene, HLP-N@h-BN, HLP-N@graphene, BP-N@h-BN and BP-N@graphene.

Compounds	Lattice Parameters
LP-N@h-BN	a=12.568, b=4.249, c=7.347
	α=90.0°, β=90.0°, γ=90.0°

LP-N@graphene	a=13.220, b=4.459, c=7.941 α=87.5°, β=90.0°, γ=90.0°
HLP-N@h-BN	a=17.655, b=4.378, c=7.000 α=90°, β=90.0°, γ=90.0°
HLP-N@graphene	a=7.000, b=22.091, c=4.335 α=90°, β=90.0°, γ=90.0°
BP-N@h-BN	a=15.150, b=8.696, c=6.000 α=90°, β=90.0°, γ=90.0°
BP-N@graphene	a=15.150, b=8.696, c=6.000 α=90°, β=90.0°, γ=90.0°