Supplementary Information:

A Novel Borophene Featuring Heptagonal Holes: Common Precursor of Borospherenes

Yuewen Mu [*,†], Qiang Chen[†], Na Chen[†], Haigang Lu[†] and Si-Dian Li[*,†]

[†]*Key Laboratory of Materials for Energy Conversion and Storage of Shanxi Province, Institute of Molecular Science, Shanxi University, Taiyuan 030006, China*

E-mail: ywmu@sxu.edu.cn; lisidian@sxu.edu.cn

Table S1: Optimized coordinates of the unit cell for H-borophene (POSCAR file for VASP).

paw_pbe
1.00000000000000
9.2706830000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 4.5048550000000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 15.8516080000000006
B
14
Direct
0.0366597140000025 0.8245489509999970 0.4988118249999971
0.3453187479999968 0.0989043789999968 0.5071740369999986
0.9147672539999974 0.5403838789999966 0.4940983569999986
0.5366597140000025 0.1754510490000030 0.5011881750000029
0.8453187479999968 0.9010956210000032 0.4928259630000014
0.4147672539999974 0.4596161210000034 0.5059016430000014
0.9633402870000012 0.1754510490000030 0.5011881750000029
0.6546812520000032 0.9010956210000032 0.4928259630000014
0.0852327460000026 0.4596161210000034 0.5059016430000014
0.4633402870000012 0.8245489509999970 0.4988118249999971
0.1546812520000032 0.0989043789999968 0.5071740369999986
0.5852327460000026 0.5403838789999966 0.4940983569999986
0.7500000000000000 0.6074652100000009 0.5171749149999982
0.2500000000000000 0.3925347899999991 0.4828250859999983

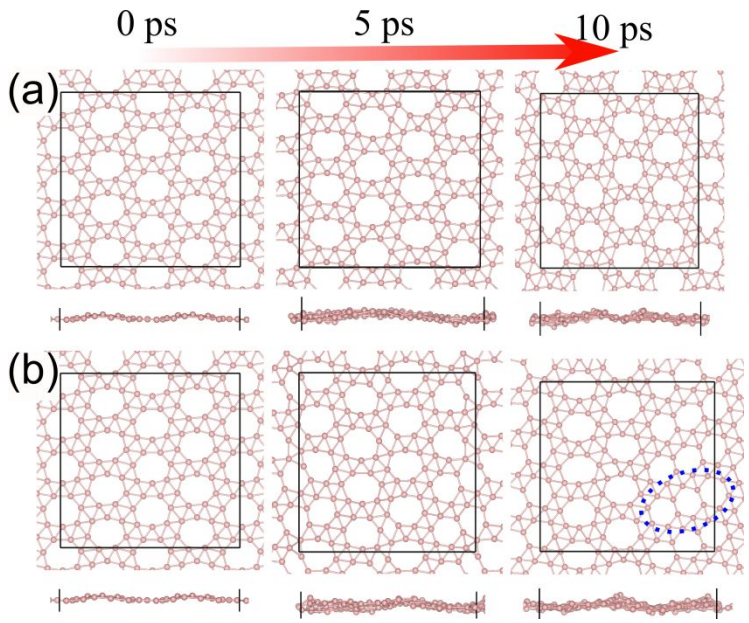

Figure S1. Snapshots (top and side views) of Born-Oppenheimer molecular dynamics (BOMD) simulations for (2×4) H-borophene over 10 ps with a time step of 1 fs at (a) 500 K and (b) 800 K. Adjacent hexagonal holes were labeled by a blue dotted ellipse.

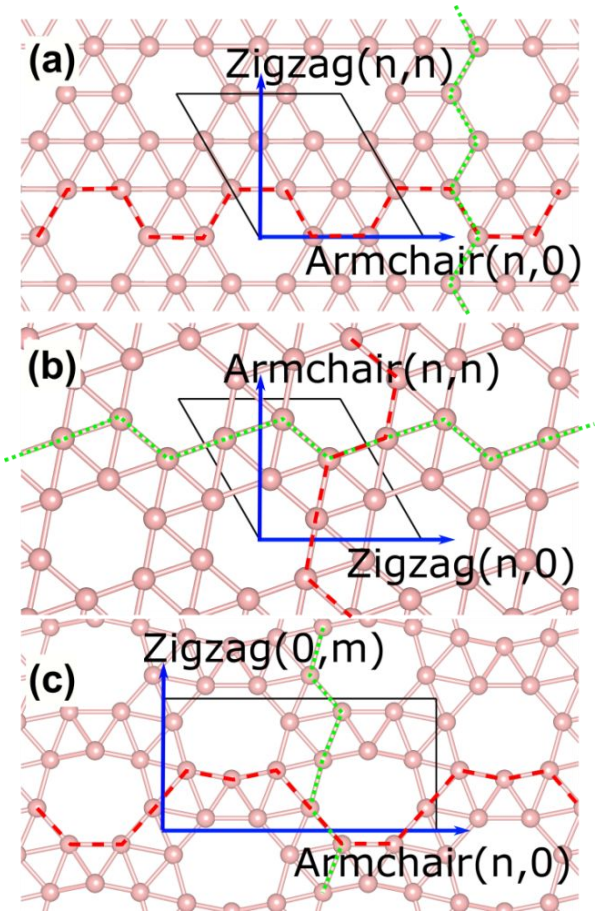

Figure S2. Illustrations of armchair and zigzag directions with indices for (a) α sheet, (b) snub sheet and (c) H-borophene. Green dotted and red dashed lines represent typical zigzag and armchair edges for these three sheets, respectively. Black solid rectangles stand for their unit cells.