

Supplementary Information
of
**Enhanced Stability and Epitaxial Growth Mechanism of
Honeycomb Borophene Monolayer on a Two-Dimensional
Ti₂C Substrate**

Kaiwen Pu^{a,b}, Xianying Dai^{a,b*}, Yuyu Bu^{a,b*}, Yiwei Guo^{a,b}, Qiu Jin^{a,b}, Jianjun Song^{a,b},

Tianlong Zhao^{a,b}, Tianmin Lei^c

a. School of Microelectronics, Xidian University, Xi'an 710071, China

*b. State Key Discipline Laboratory of Wide Bandgap Semiconductor Technologies,
Xidian University, Xi'an 710071, China*

*c. School of Advanced Materials and Nanotechnology,, Xidian University, Xi'an
710126, China*

* E-mail address: xydai@xidian.edu.cn (X. Dai)

* E-mail address: yybu@xidian.edu.cn (Y. Bu)

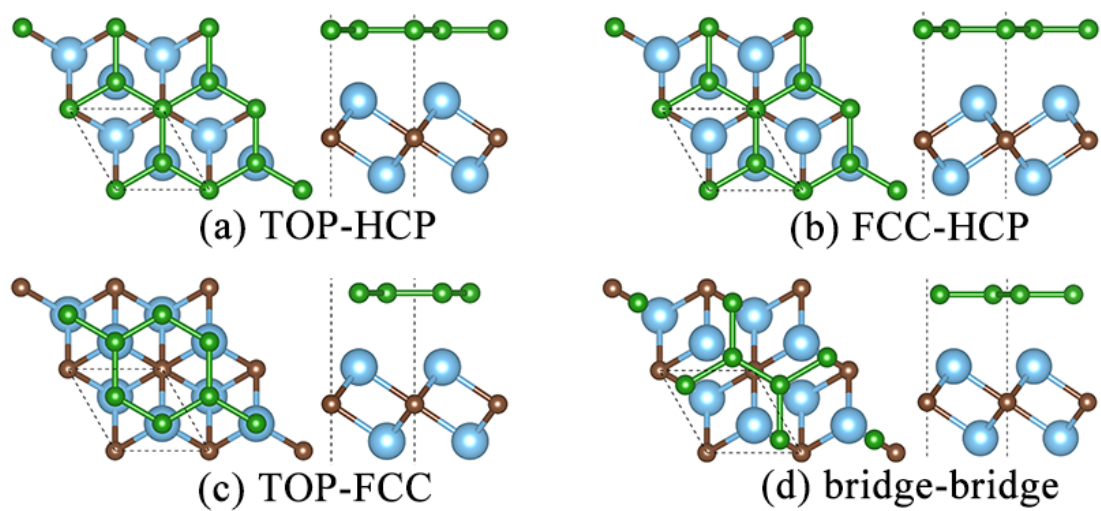


Figure S1. Initial structures of TOP-HCP (a), FCC-HCP (b), TOP-FCC (c) and bridge-bridge (d).

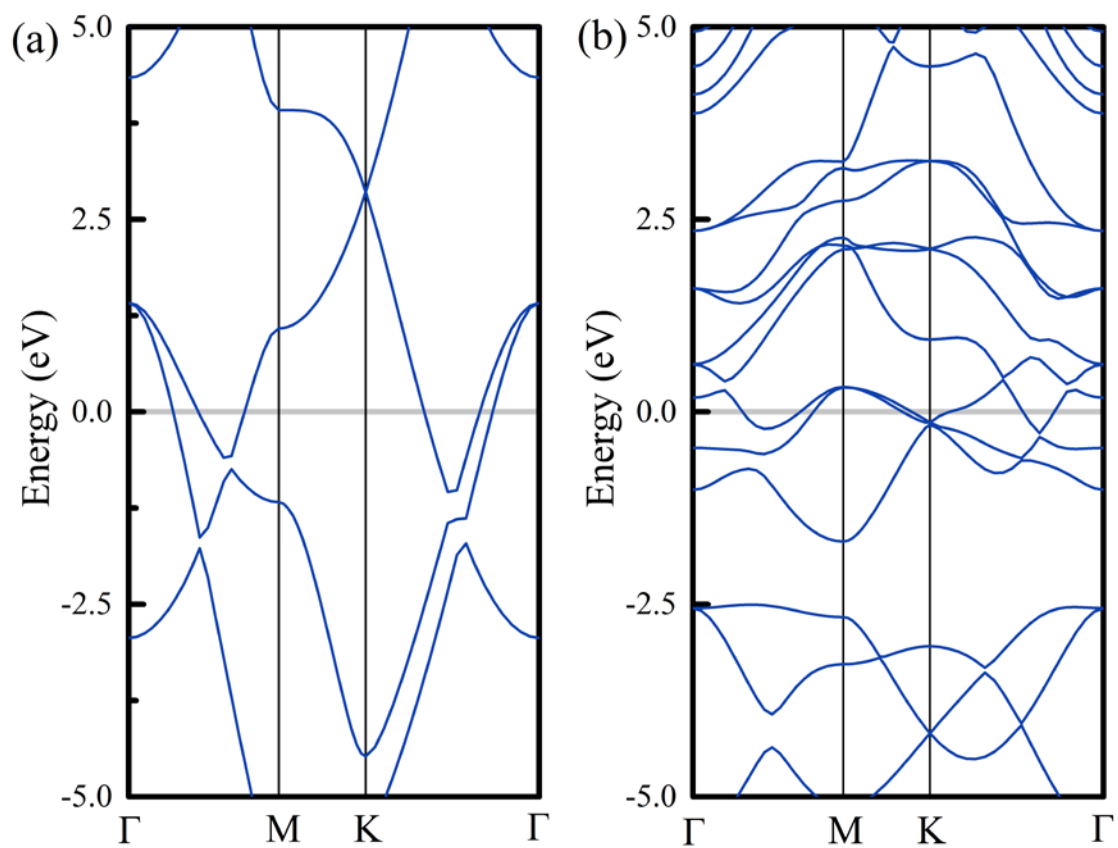


Figure S2. Band structures of free-standing honeycomb borophene (a) and Ti_2C (b), respectively.

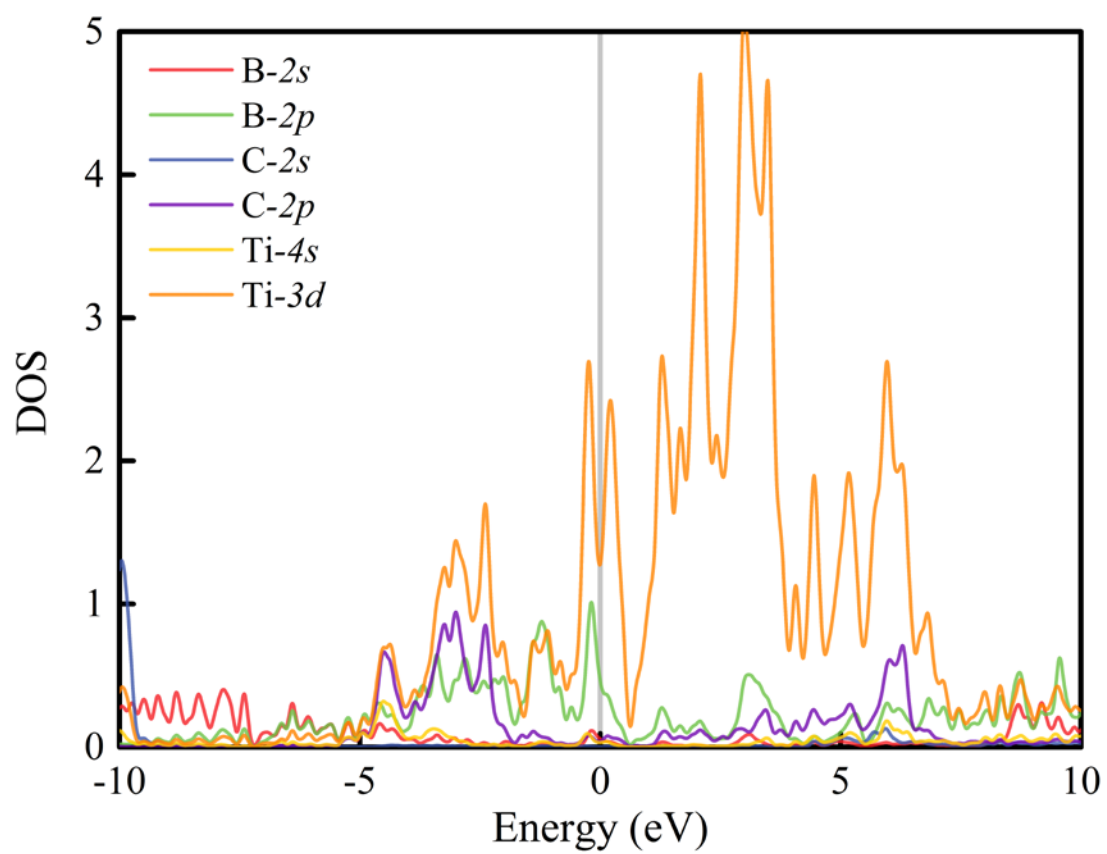


Figure S3. PDOS of borophene/Ti₂C system.