Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information for:

Novel hydrogenated boron-carbon monolayer with high stability and promising carrier mobility

Dong Fan, Shaohua Lu, Chengke Chen, Meiyan Jiang, Xiao Li, and Xiaojun Hu*

College of Materials Science and Engineering, Zhejiang University of Technology, Hangzhou 310014, China

Table S1 | Calculated lattice parameters, elastic constants, in-plane Young's modulus and Poisson's ratio of graphene at GGA-PBE level.

Phase	Lattice Parameters(Å)	C_{11}/ GPa	C_{22}/ GPa	C_{12}/ GPa	C_{66}/G Pa	In-plane stiffness /GPa·nm	Poisson's ratio
Graphene	**a**=**b** =2.47 α =β=90° γ = 120°	358	358	65	147	346.73	0.18
Borophone[*1]	**a** = 5.004 **b** = 2.889 α = β = γ = 90°	398	170	-7	94	398(**a**)[*3] 170(**b**)[*3]	-0.04(**a**) -0.02(**b**)
B_2C Graphene[*2]	**a** = 2.558 **b** = 3.453 α = β = γ = 90°	642.8	533.7	79.0	230.6	524.0	0.12
***h*-BCH**	**a**=**b** =2.624 α =β=90° γ = 120°	228.2	228.2	35.4	96.6	223	0.155
***t*-BCH**	**a** = **b** = 2.841 α = β = γ = 90°	233.9	233.9	17.8	35.5	233	0.076

*For *h*-BCH, we use its orthorhombic lattice to calculate the elastic constants.

*The in-plane Young's modulus and Poisson's ratio can be derived the elastic constants by:

$$E_a = \frac{C_{11}C_{22}\text{-}C_{12}C_{21}}{C_{22}} \quad E_b = \frac{C_{11}C_{22}\text{-}C_{12}C_{21}}{C_{11}}$$

$$\nu_a = \frac{C_{21}}{C_{22}} \quad \nu_b = \frac{C_{12}}{C_{11}}$$

***1**: Mannix, A. J., et al. *Science* 350.6267(**2015**):1513-1516.

***2**: Calculated by equations in Ref: Wu, X., Pei, Y., & Zeng, X. C. (**2009**). *Nano letters*, 9(4), 1577-1582

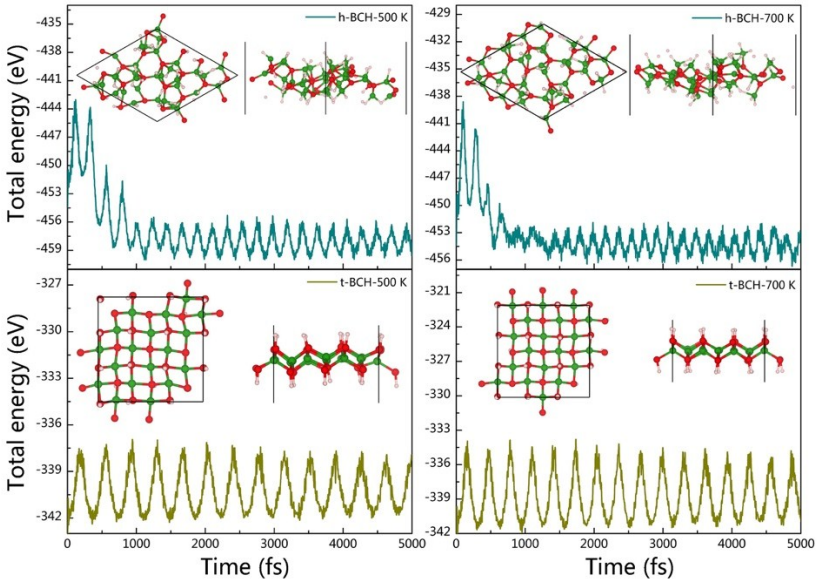

Fig. S1 | Evolution of total energy of *h*-BCH and *t*-BCH from AIMD simulations at 500 and 700 K. Snapshots at the corresponding temperatures at the end of 5 ps AIMD simulations are also inserted.

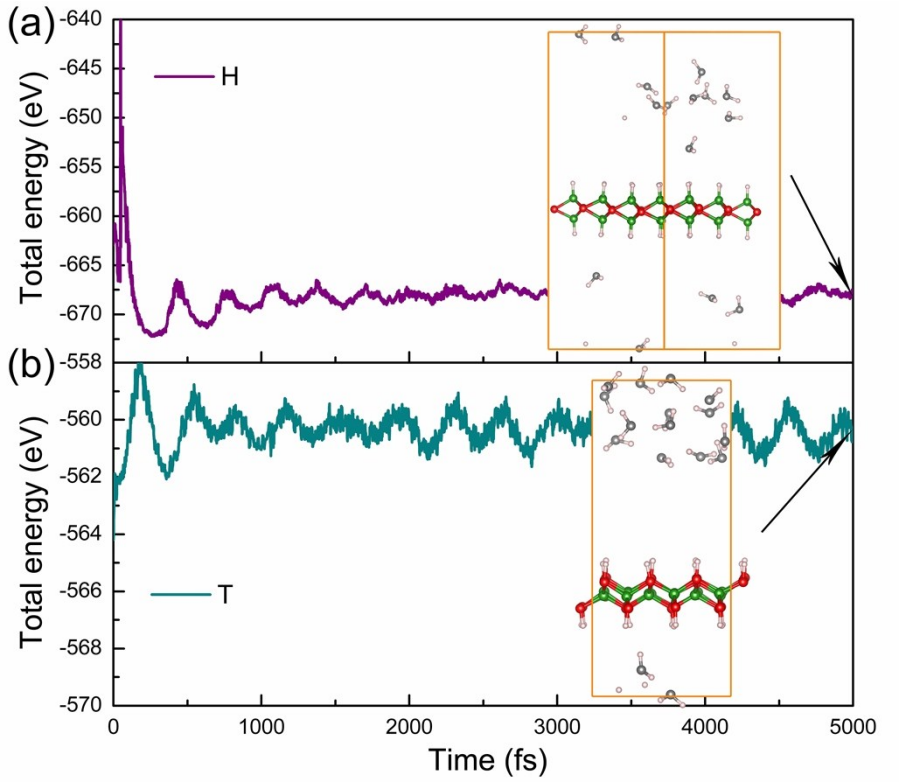

Fig. S2 | Evolution of total energy and snapshots of (a) *h*-BCH and (b) *t*-BCH with the interaction of low-density water molecule from AIMD simulations at 300 K.

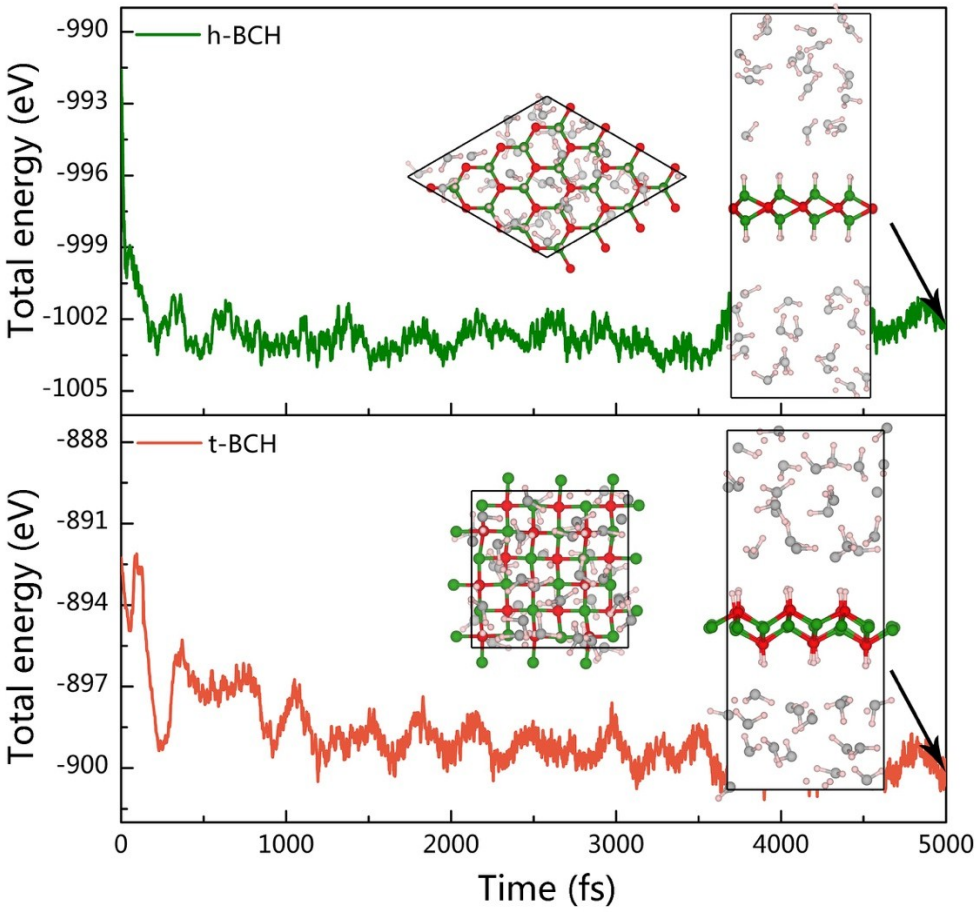

Fig. S3 | Evolution of total energy and snapshots of *h*(*t*)-BCH with the interaction of high-density water molecule from AIMD simulations at 300 K.

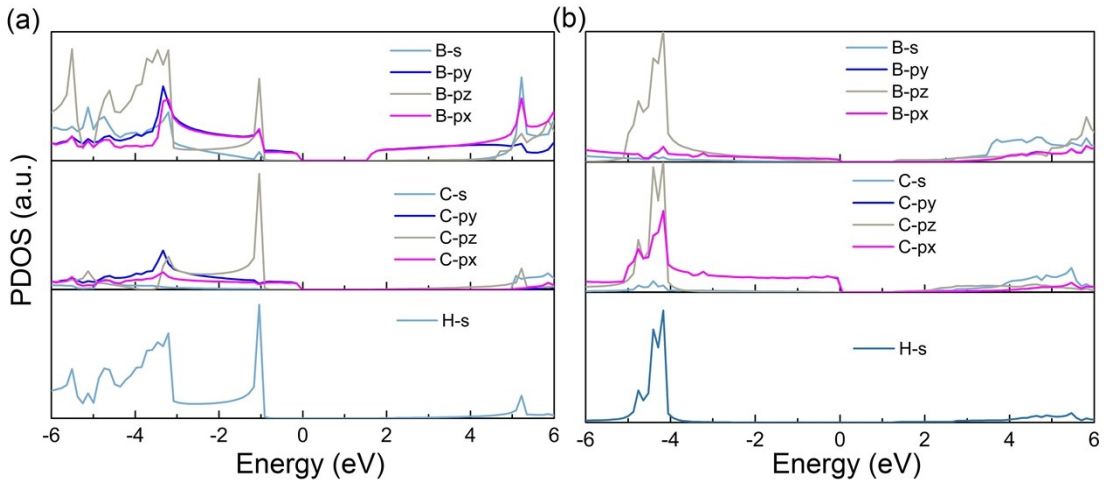

Fig. S4 | Electronic partial density of states (PDOS) of the *h*-BCH (left) and *t*-BCH (right) at the PBE level.

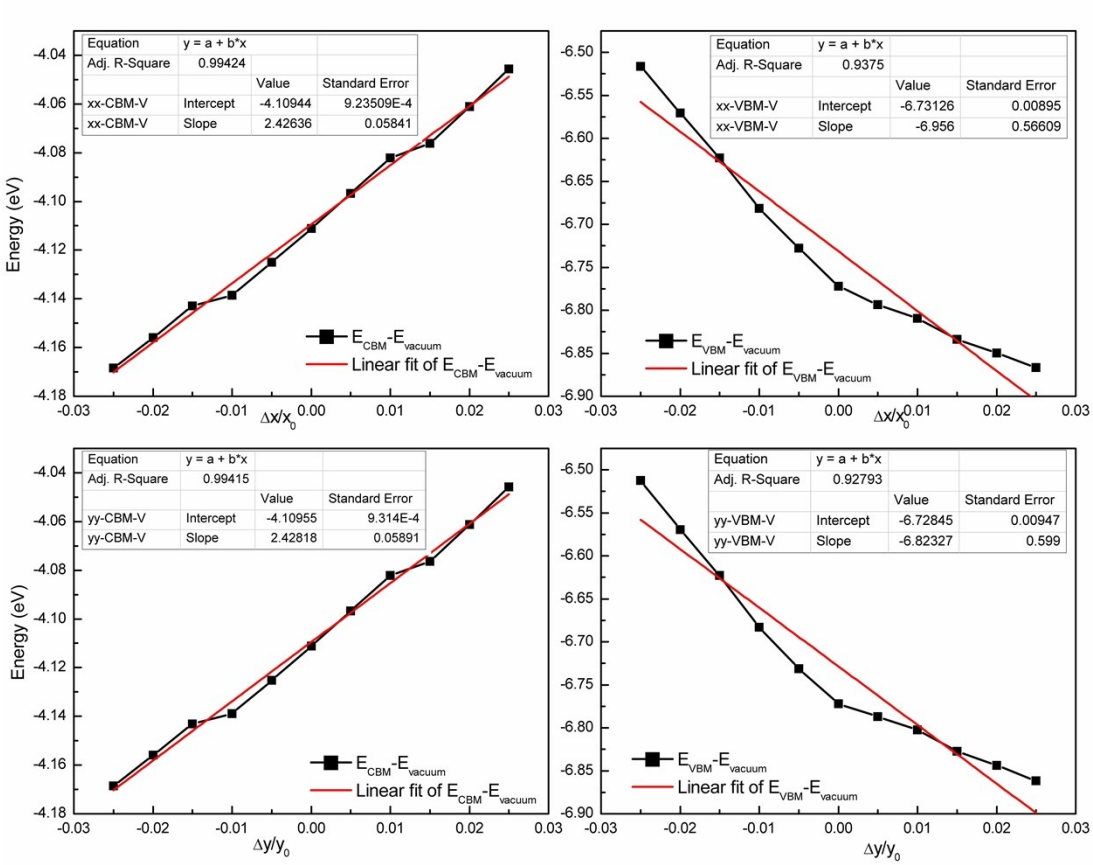

Fig. S5 | Band energy of the CBM and VBM of *h*-BCH. Band energies were calculated with the HSE06 functional. Red solid lines are the fitting curves. Insets show the standard errors of the fitted slope, which corresponds to the deformation potential.

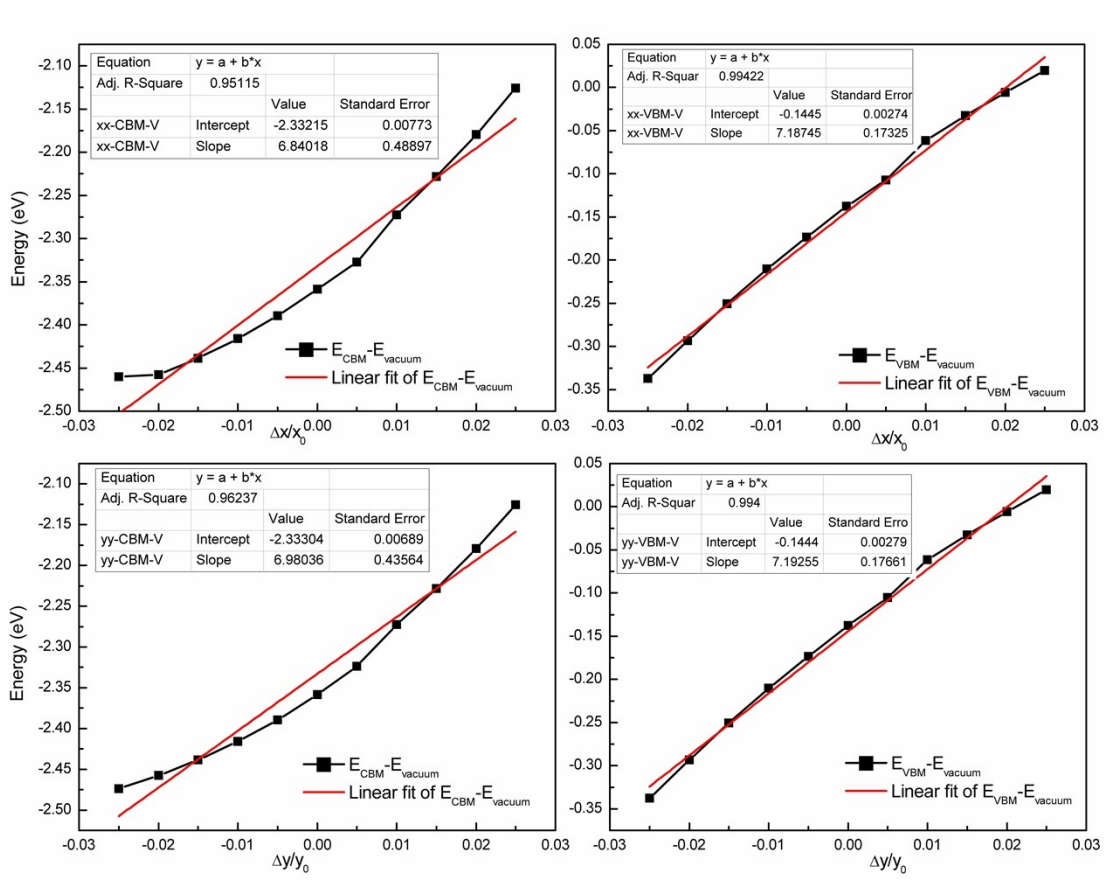

Fig. S6 | Band energy of the CBM and VBM of *t*-BCH. Band energies were calculated with the HSE06 functional. Red solid lines are the fitting curves. Insets show the standard errors of the fitted slope, which corresponds to the deformation potential.