Supplementary Information (SI) for Journal of Materials Chemistry C.
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Supporting information for:

Stability and electro-optical properties of hydrogen functionalized-monolayer BC_3H_3: A theoretical study

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Calculated details of carrier mobility

The carrier mobility of the BC_3H_3 monolayer can be calculated by the effective mass approximation[1] and deformation potential theory proposed by Bardeen and Shockley.[2] It can be obtained by the following equation:[3]

$$\mu_{x/y} = \frac{e\hbar^3 C_{x/y}}{k_B T (m^*_{x/y}) m_d (E_d^{x/y})^2}, \quad (1)$$

where $m^*_{x/y}$ and m_d are the effective mass of the charge carrier (electron or hole) along the *x*/*y* transport direction (two lattice vector directions of orthogonal structure, as shown in Fig. S6) and average effective mass of the charge carrier ($m_d = \sqrt{m_x^* m_y^*}$), respectively. The effective mass m^* of the carrier is calculated by the $\frac{1}{m^*} = \frac{1}{\hbar^2}\frac{\partial^2 E(k)}{\partial k^2}$, $E(k)$ is the energy at the wave vector k of electronic band structure. $E_d^{x/y} = \frac{\partial E_{edge}}{\partial \delta_{x/y}}$ is called as the deformation potential constant, being fitted by the positions of the band edges (valence band maximum VBM for the hole or conduction band minimum CBM for the electron) under the small uniaxial strain ($\delta_{x/y}$).

$C_{x/y} = \frac{1}{S_0}\frac{\partial^2 E_{tot}}{\partial \delta_{x/y}^{\ 2}}$, k_B, and T are the elastic modulus, Boltzmann constant, and temperature, respectively.

Table S1 Lattice constant (a_0/b_0), bond length between the atoms ($L_{B\text{-}C}$, $L_{C\text{-}C}$, $L_{C\text{-}H}$), and formation energy (E_f). Units of length and energy are Å and eV, respectively.

Name	a_0/b_0	$L_{B\text{-}C}$	$L_{C\text{-}C}$	$L_{C\text{-}H}$	E_f
BC_3	5.165	1.563	1.419	———	———
BC_3H_3-1	5.278	1.573	1.546	1.115	-0.314
BC_3H_3-2	5.408	1.587	1.572	1.106	2.429
BC_3H_3-3	5.232	1.562	1.571	1.107/1.116	-0.869
BC_3H_3-4	5.150	1.569	1.527	1.109/1.140	-0.581

Table S2 Calculated in-plane elastic constant $C_{x/y}$ (N/m), effective mass $m^*_{x/y}$ (m_0), deformation-potential constant $E_d^{x/y}$(eV), and carrier mobility $\mu_{x/y}$ ($cm^2 \cdot V^{-1} \cdot s^{-1}$) of BC_3H_3 monolayer with type-3 configuration along the x and y directions at 300 K.

Name	Carriers	$C_{x/y}$	$m^*_{x/y}$	$E_d^{x/y}$	$\mu_{x/y}$
type-3	electron	245.602/186.032	0.820/1.484	-2.450/-3.275	943/221
	hole	245.602/186.032	0.339/0.729	-2.694/-3.455	2226/1183

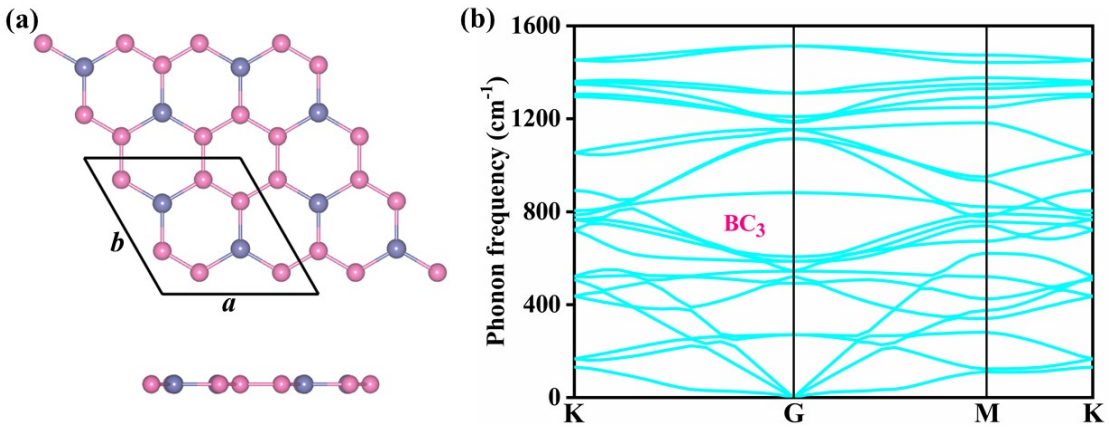

Fig. S1 Optimized configuration (a) and phonon spectrum (b) of BC_3 monolayer. C atom is marked by light pink.

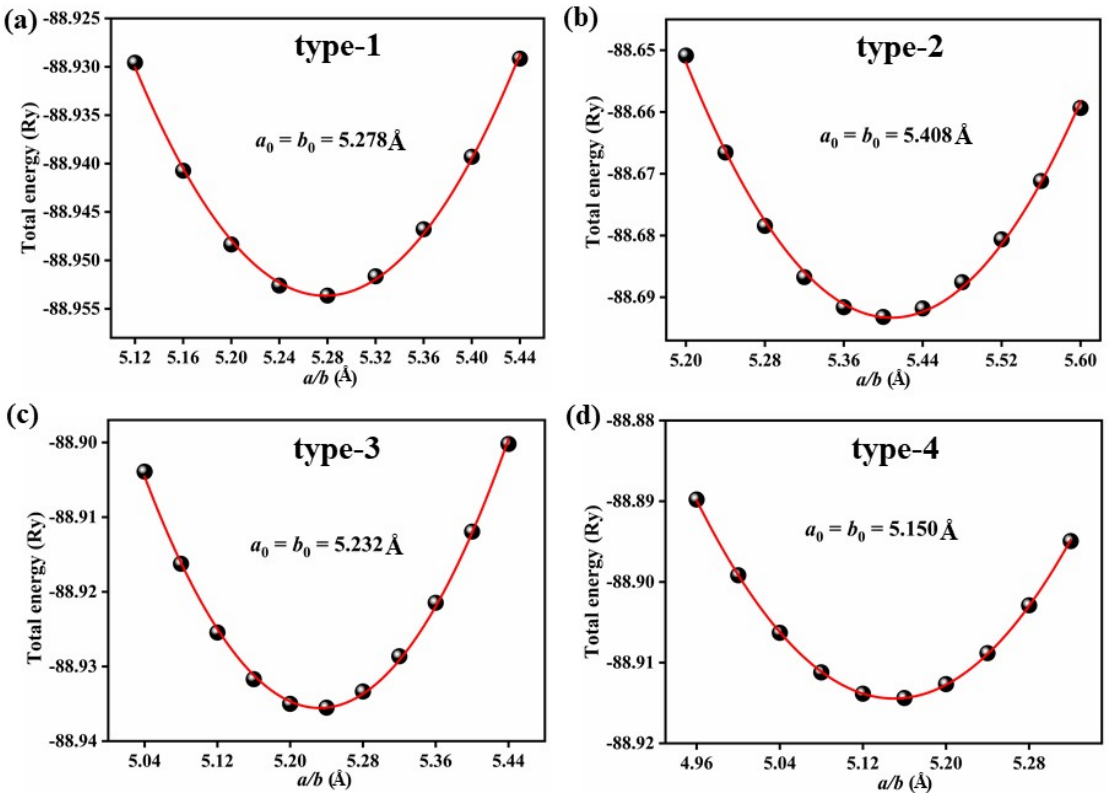

Fig. S2 Total energies of BC_3H_3 monolayer under different lattice constants: (a) type-1, (b) type-2, (c) type-3, and (d) type-4.

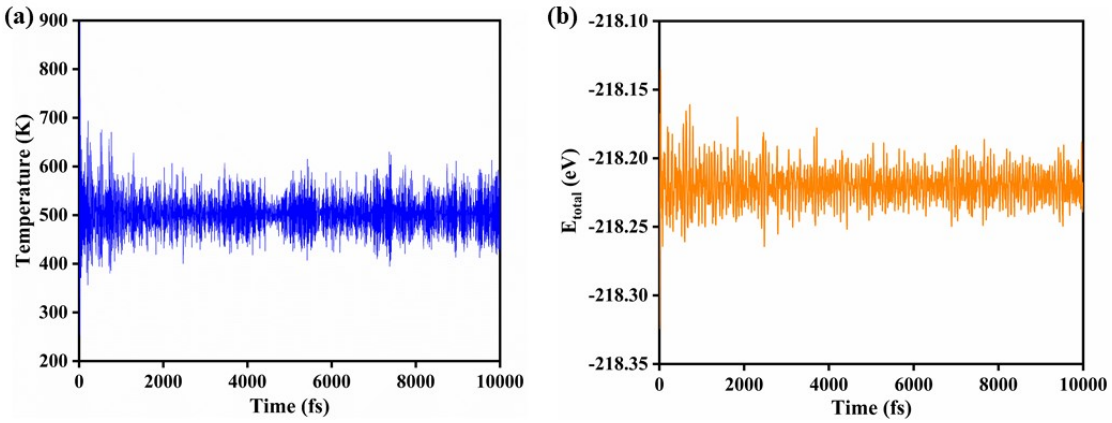

Fig. S3 Variable temperature (a) and total energy (b) of BC_3H_3 monolayer with type-4 configuration during heating 10 ps at the temperature of 500 K.

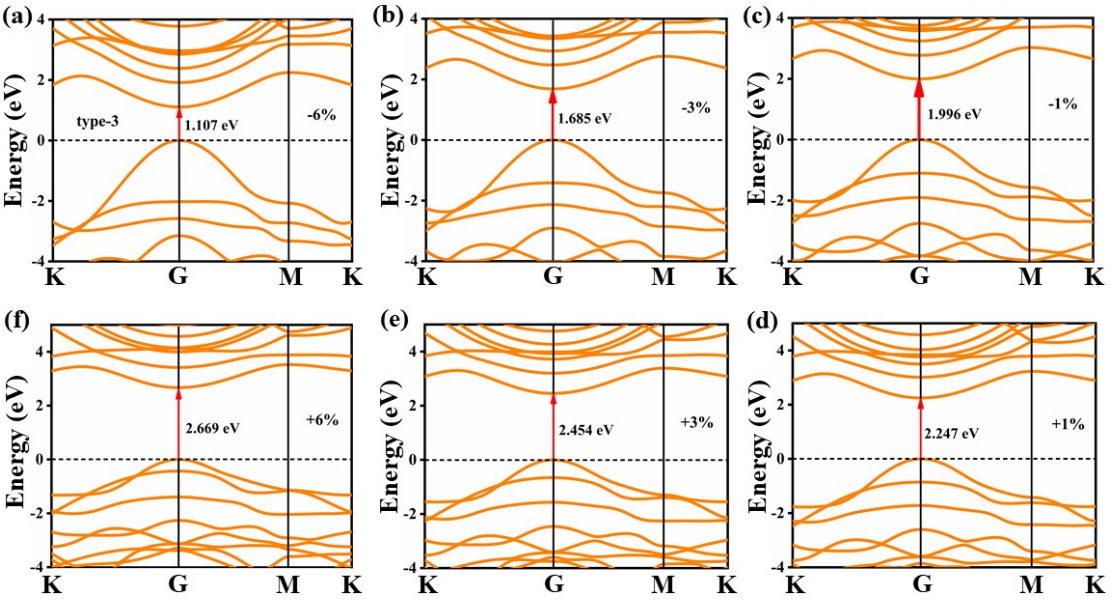

Fig. S4 Band structures of BC_3H_3 monolayer with type-3 configuration under different biaxial strains.

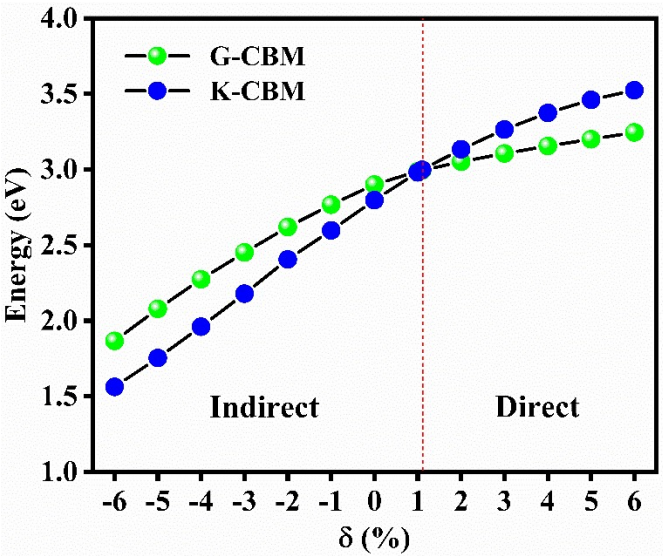

Fig. S5 Positions of CBMs at **G** and **K** points relative to the VBM for the type-4 BC_3H_3 monolayer under different biaxial strains.

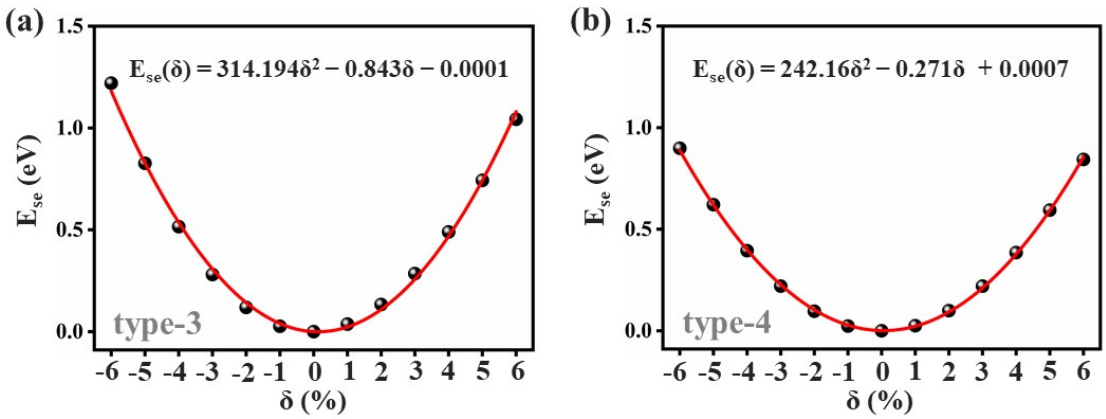

Fig. S6 Strain energies (E_{se}) of BC_3H_3 monolayers with type-3 and type-4 configurations under the biaxial strain (δ) ranging from -6% to +6%. "-" shows the compressive strain.

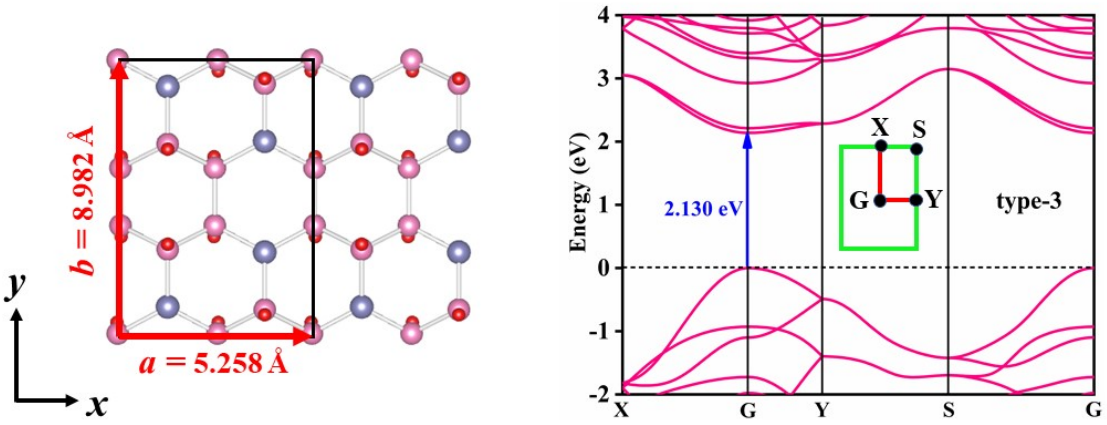

Fig. S7 Optimized orthogonal structure and PBE band structure of BC_3H_3 monolayer with the type-3 configuration. *x* and *y* show transport directions.

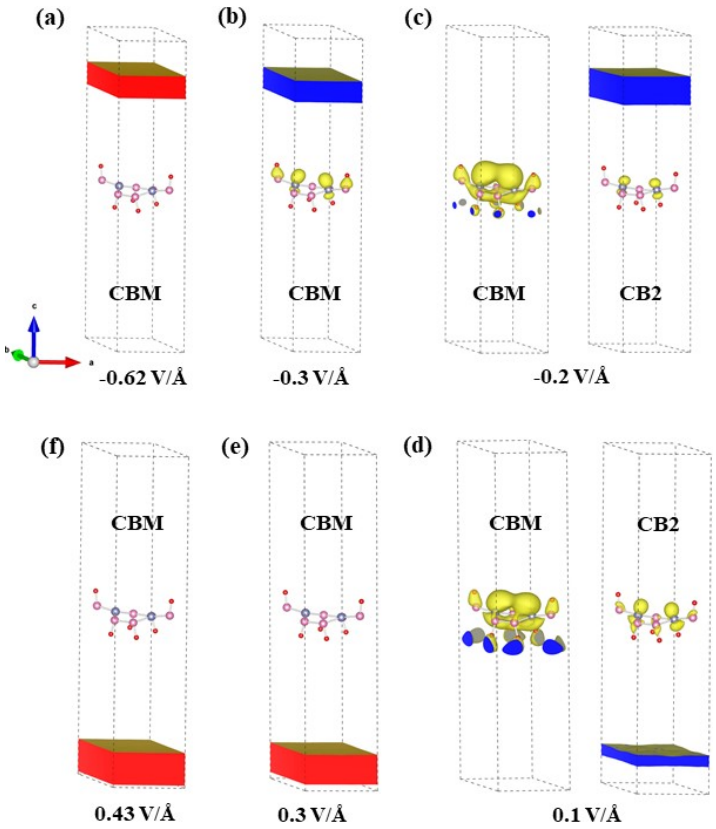

Fig. S8 Decomposed charge density of the CBM at **G** point for the type-3 configuration: (a) -0.62 V/Å, (b) -0.3 V/Å, (c) -0.2 V/Å, (d) 0.1 V/Å, (e) 0.3 V/Å, and (f) 0.43 V/Å. The CB2 shows the second conduction band at **G** point. The isovalue is set to be 1.5×10^{-3} e/Å^3.

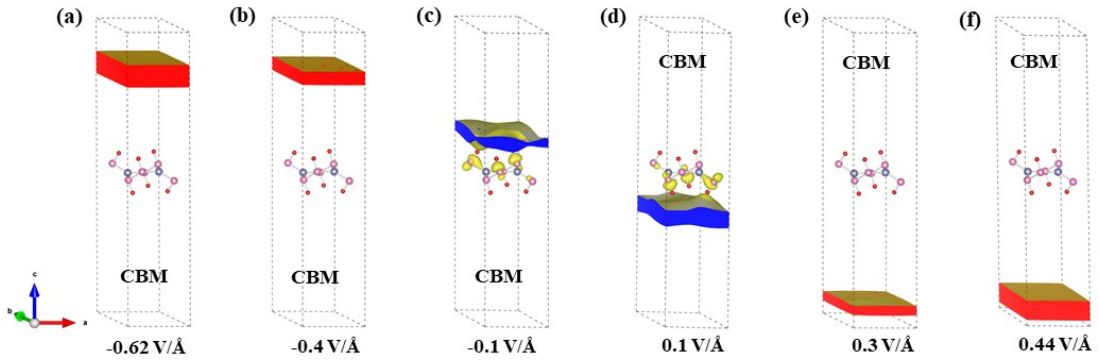

Fig. S9 Decomposed charge density of the CBM at **G** point for the type-4 configuration: (a) -0.62 V/Å, (b) -0.4 V/Å, (c) -0.1 V/Å, (d) 0.1 V/Å, (e) 0.3 V/Å, and (f) 0.44 V/Å. The CB2 shows the second conduction band at G point. The isovalue is set to be 1.5×10^{-3} e/Å^3.

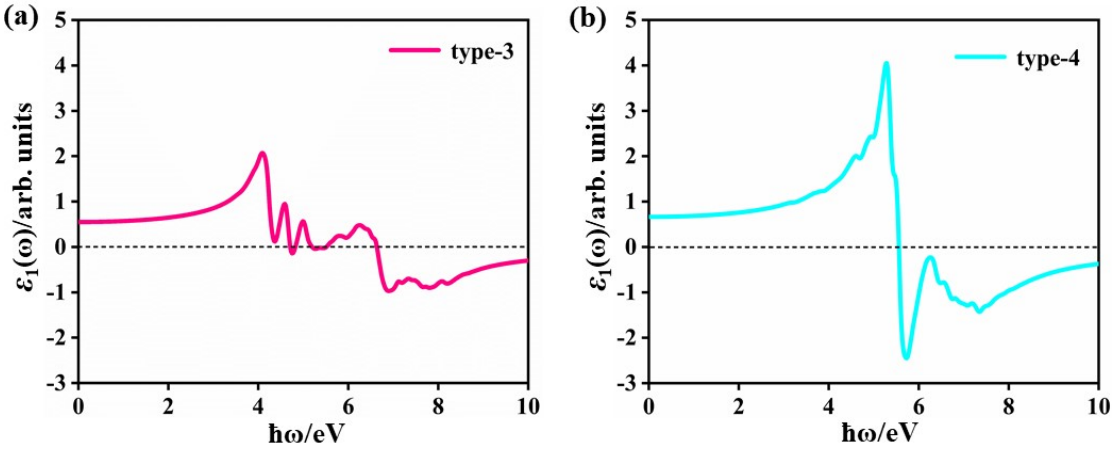

Fig. S10 Real part ε_1 (ω) of frequency-dependent dielectric function ε(ω) of BC_3H_3 monolayer with type-3 and type-4 configurations for including the electron-hole coupling (G_0W_0+BSE). Lorentzian broadening of 100 meV is considered in these curves.

References

1 J. Xi, M. Long, L. Tang, D. Wang and Z. Shuai, *Nanoscale*, 2012, **4**, 4348–4369.

2 J. Bardeen and W. Shockley, *Phys. Rev*, 1950, **80**, 72–80.

3 J. Qiao, X. Kong, Z.-X. Hu, F. Yang and W. Ji, *Nat. Commun.*, 2014, **5**, 4475.