Supplementary Information (SI) for Nanoscale.
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Supporting information

First-Principles Study of Anisotropic Planar 2D BC_2N for Sub-5 nm High-Performance P-Type Transistors

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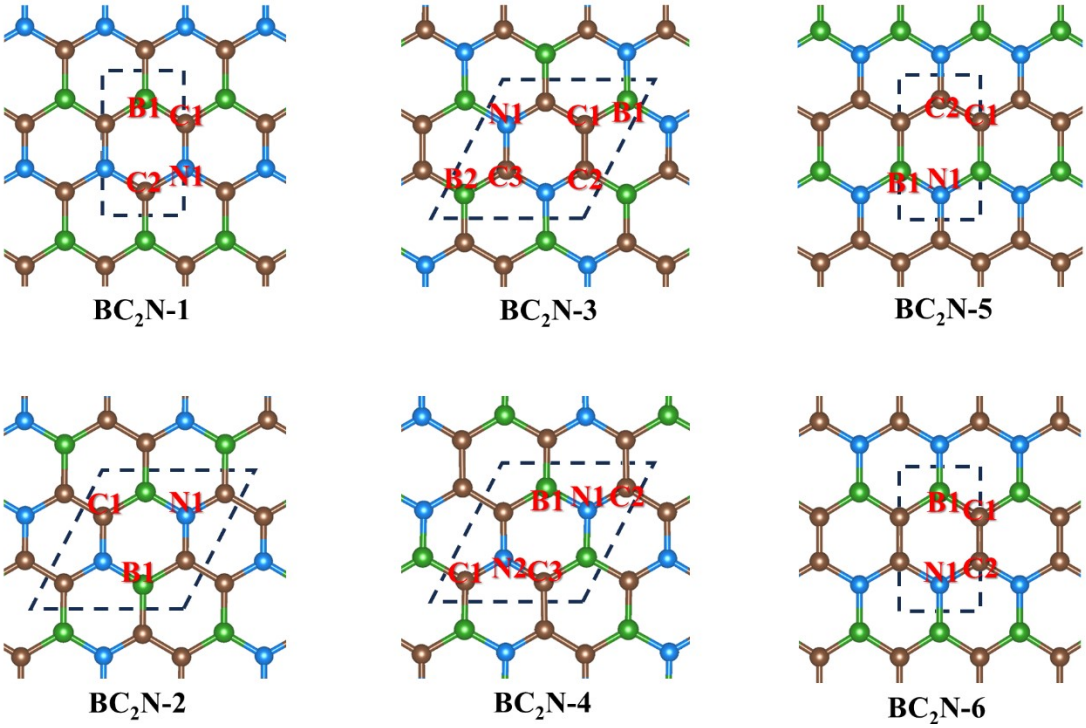

Fig. S1. Position of each atom in unit cell of six BC_2N structures.

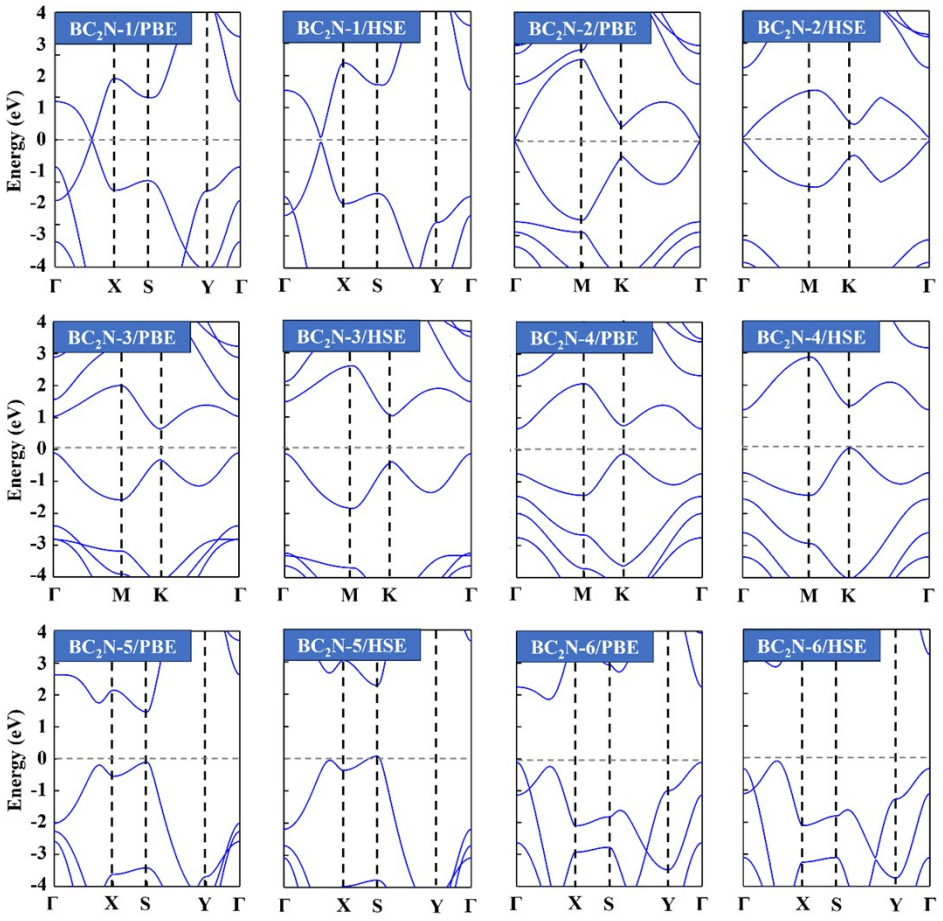

Fig. S2. Band structure of six BC_2N structures at the PBE and HSE level.

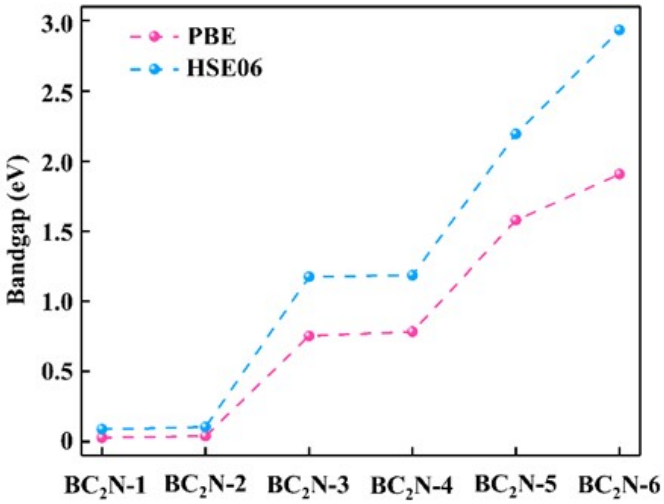

Fig. S3. Band gap variation of BC_2N based PBE and HSE06 calculation. The value of bandgap based HSE calculation is obvious higher than that of PBE calculation, but the trend of bandgap changes obtained by these two methods is consistent.

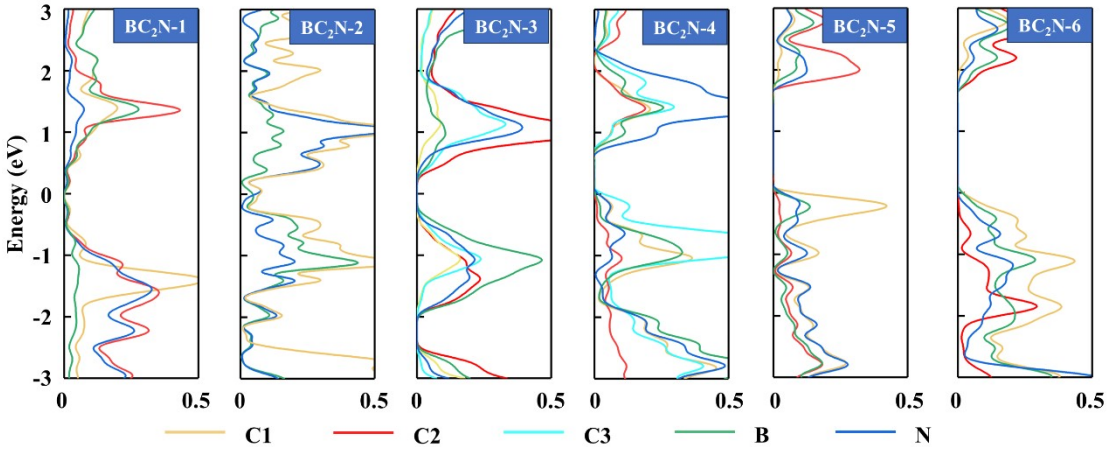

Fig. S4. PDOS of six BC_2N structures. The valance band maximum (VBM) of six structures is consisted with B and C atoms. The conduction band minimum (CBM) of BC_2N-1, 2, 3, 4, and 5 is consisted with N and C atoms, while that of BC_2N-6 is contributed by B and C atoms.

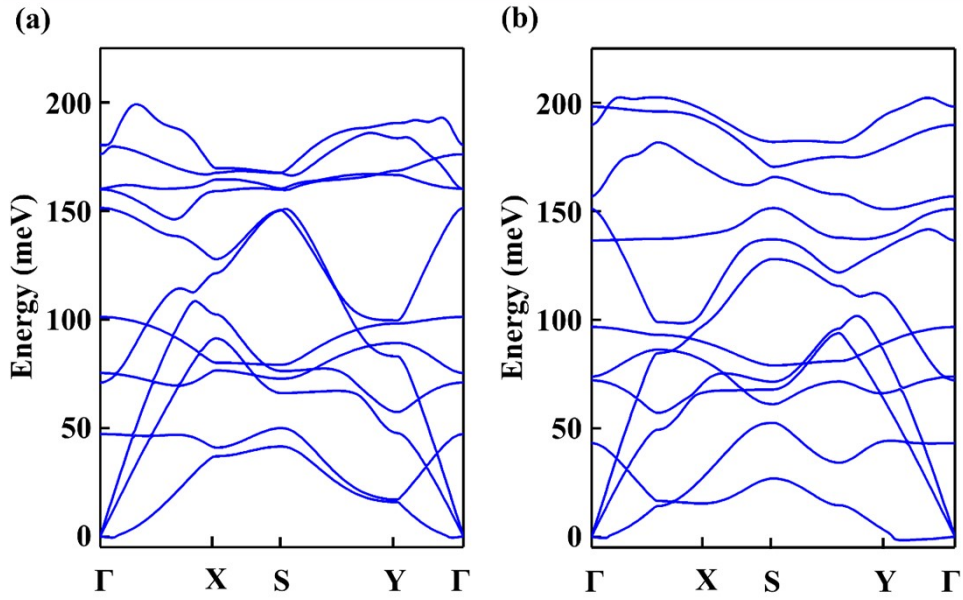

Fig. S5. Phonon band structure of (a) BC_2N-5 and (b) BC_2N-6. The phonon band structures of BC_2N-5 and BC_2N-6 do not have obvious phonon imaginary modes in the whole Brillouin zone, which indicates that the monolayer BC_2N-5 and BC_2N-6 are kinetically stable.

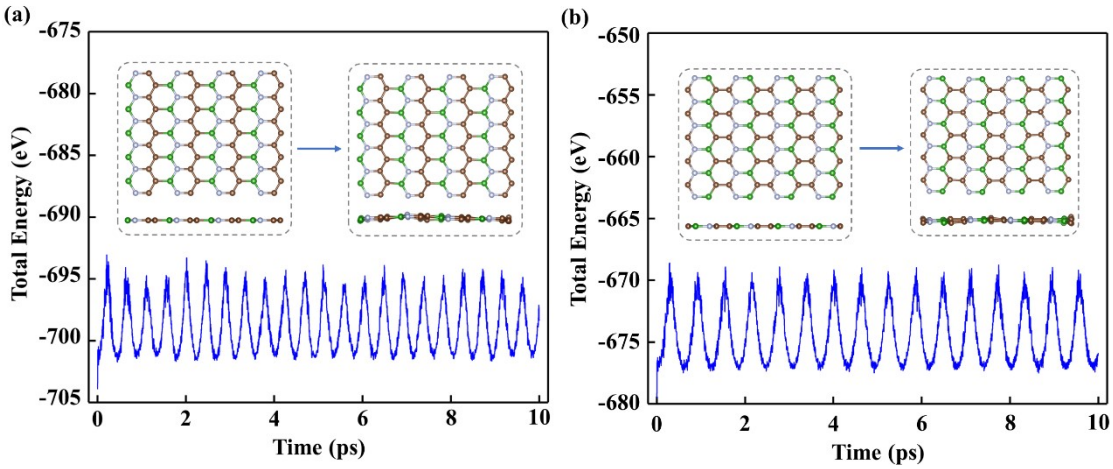

Fig. S6. Evolution of the total energies during the AIMD simulation for the pristine (a) BC_2N-5 and (b) BC_2N-6 nanosheet at 500 K. The snapshots for the final geometrical configurations at the end of the AIMD simulation are also depicted in the inset. The snapshots of the final geometry in **Fig. S6** clearly show that the structural integrity is well maintained. There was no bond breaking in the final geometry with only small atomic displacements. Thus, this confirms that the BC_2N-5 and BC_2N-6 systems have good thermal stability at 500 K.

Table S1. Bandgap, cohesive energy, space group, and lattice parameters of monolayer BC_2N.

Structure	E_g (eV) PBE	E_g (eV) HSE06	E_{coh} (eV)	Space group	a (Å)	b (Å)
BC_2N-1	0.028	0.088	-7.026	*pmmn*	4.391	2.489
BC_2N-2	0.039	0.105	-7.314	*pm*	5.073	5.073
BC_2N-3	0.753	1.175	-7.304	*pm*	5.030	5.030
BC_2N-4	0.783	1.186	-7.284	*pm*	5.033	5.033
BC_2N-5	1.578	2.193	-7.578	*pmmn*	4.358	2.484
BC_2N-6	1.906	2.933	-7.273	*pmmn*	4.351	2.497

Table S2. Bader charge of each atom of six BC_2N structures in unite cell.

structure	B1	B2	C1	C2	C3	N1	N2
BC_2N-1	-1.8735	/	0.9352	-0.1590	/	1.0973	/
BC_2N-2	-1.9016	/	0.2042	/	/	1.4932	/
BC_2N-3	-1.9927	-1.8278	0.4634	0.3411	-0.2807	1.4778	/

BC_2N-4	-1.955	/	0.9145	-0.4507	0.2656	1.7568	1.1612
BC_2N-5	-2.0331	/	0.5022	-0.3171	/	1.8479	/
BC_2N-6	-1.9875	/	1.2820	-0.5777	/	1.2832	/

Table S3. Comparison of the performance of the p-type monolayer BC_2N-6 FETs in this work along armchair and zigzag directions with the requirements of the ITRS 2013 requirements for HP transistors.

L_g (nm)	V_{dd} (V)	direction	I_{on} (μA/μm)	SS (mV/dec)	PDP (fJ/μm)	τ (ps)
10	0.74	zigzag	2415	63	0.281	0.116
		armchair	1660	63	0.155	0.093
9.7 (ITRS)			1450		0.510	0.477
7	0.69	zigzag	2310	70	0.184	0.080
		armchair	1793	92	0.114	0.063
7.3 (ITRS)			1170		0.360	0.451
5	0.64	zigzag	1653	103	0.055	0.033
		armchair	1554	93	0.059	0.038
5 (ITRS)			900		0.243	0.423
3		zigzag	74.9	227	0.024	0.324
		armchair	/	/	/	/
3^{+1UL}		zigzag	1072	124	0.034	0.032
		armchair	919	130	0.038	0.041
3^{+2UL}		zigzag	659	104	0.024	0.036
		armchair	576	108	0.022	0.039
1^{+2UL}		zigzag	148	205	0.015	0.102
		armchair	74	245	0.010	0.135
1^{+3UL}		zigzag	135	145	0.013	0.095
		armchair	101	215	0.013	0.126

< 5.1 (ITRS)	900	0.243	0.423