Supplementry information

Unveiling the potential of BCN-Biphenylene monolayer as a high-performance anode material for alkali metal ion batteries: A first-principles study

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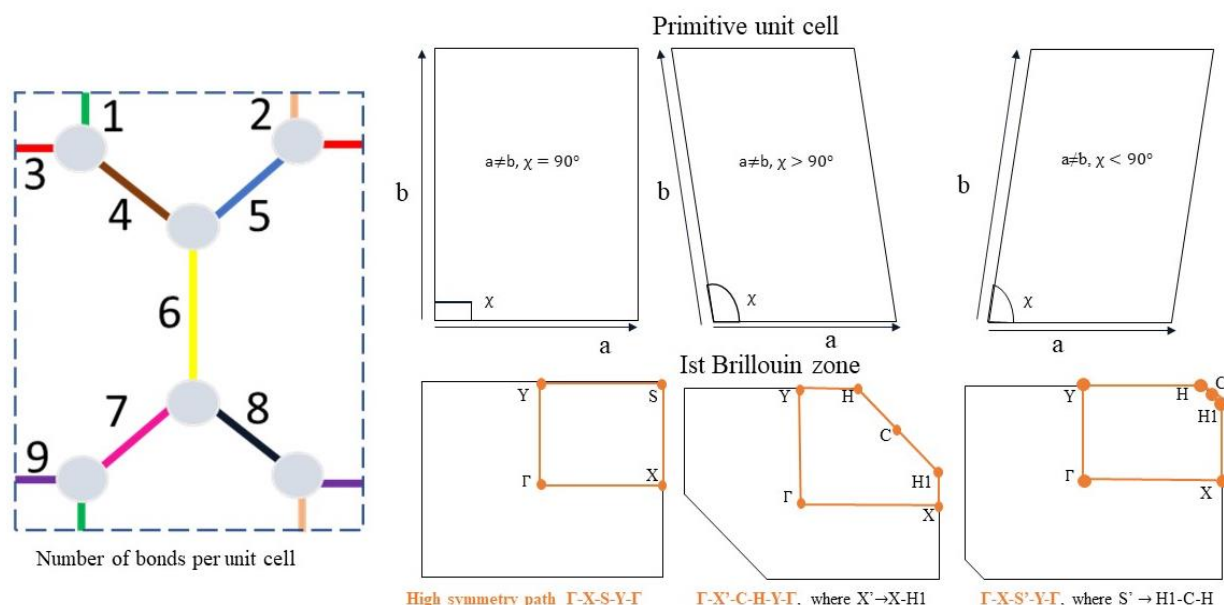
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Fig. S1 *numbers of bonds per unit cell, primitive unit cell and their corresponding Ist Brillouin zone along with high symmetry path*

Table S1 *lattice parameters, bond types, bond length and their count in different phases of CBN.*

Phases	Lattice constant (Å)		angle	Types of Bonds and their counts per unit cell											
x-CBN	a	b	a�b	B-B (Å)		C-C (Å)		N-N (Å)		C-N (Å)		B-N (Å)		B-C (Å)	
α-BCN	3.82	4.85	90.0°	1	1.68	1	1.38	1	1.42	2	1.43	2	1.43	2	1.52
β-BCN	3.87	4.57	90.0°	1	1.58	1	1.42	1	1.50	2	1.38	2	1.48	2	1.50
γ-BCN	3.92	4.46	90.0°	1	1.60	1	1.45	1	1.42	2	1.38	2	1.43	2	1.53
δ-BCN	3.78	4.86	91.4°	1	1.66	0	-	0	-	4	1.40*	2	1.46	2	1.50
η-BCN	3.86	4.55	92.5°	0	-	1	1.40	0	-	2	1.38	4	1.48*	2	1.53
θ-BCN	3.90	4.47	88.0°	0	-	0	-	1	1.40	2	1.35	2	1.47	4	1.52*
Few bonds with different bond length are marks as *, mention here, C-N(1.42 Å); B-N(1.47 Å); B-C(1.53 Å)															

Table S2 *Min. and max. value of Young moduli and Poisson ratio of different phases of CBN.*

bpn-BCN	Y(θ) (N/m)		ν(θ)	
X-BCN	Min.	Max.	Min.	Max.
α- BCN	143.93	194.84	0.28	0.42
β- BCN	170.80	225.62	0.30	0.39
γ- BCN	191.44	253.76	0.23	0.34

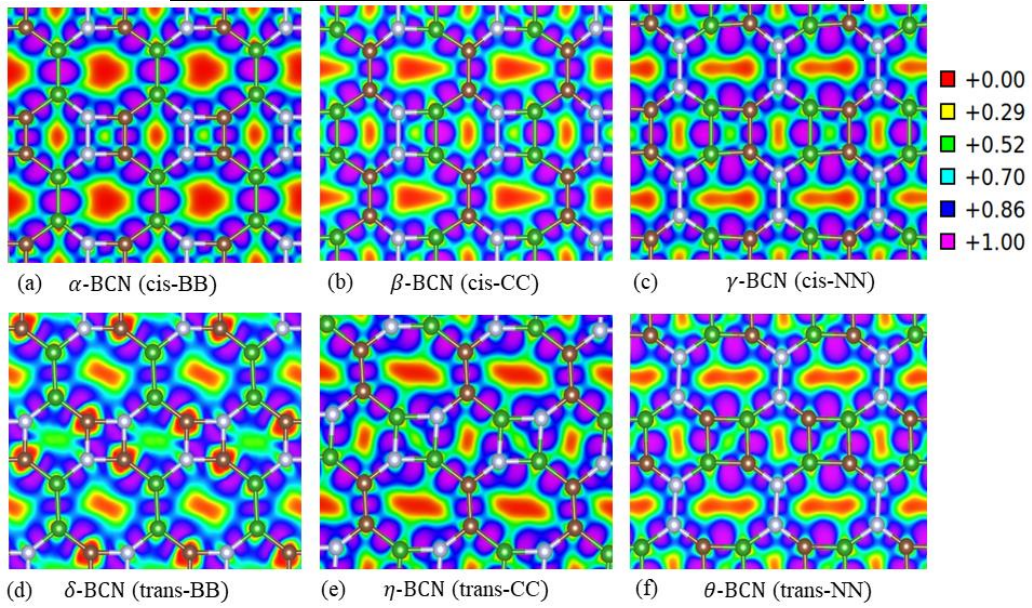|				
δ-BCN	143.94	203.64	0.29	0.45
θ-BCN	175.68	219.57	0.32	0.44
η- BCN	178.62	250.75	0.26	0.39

Fig. S2 displays the electron localized function (ELF) of multiple phases of bpn-BCN monolayers with an iso-surface value of 0.4 atomic units.
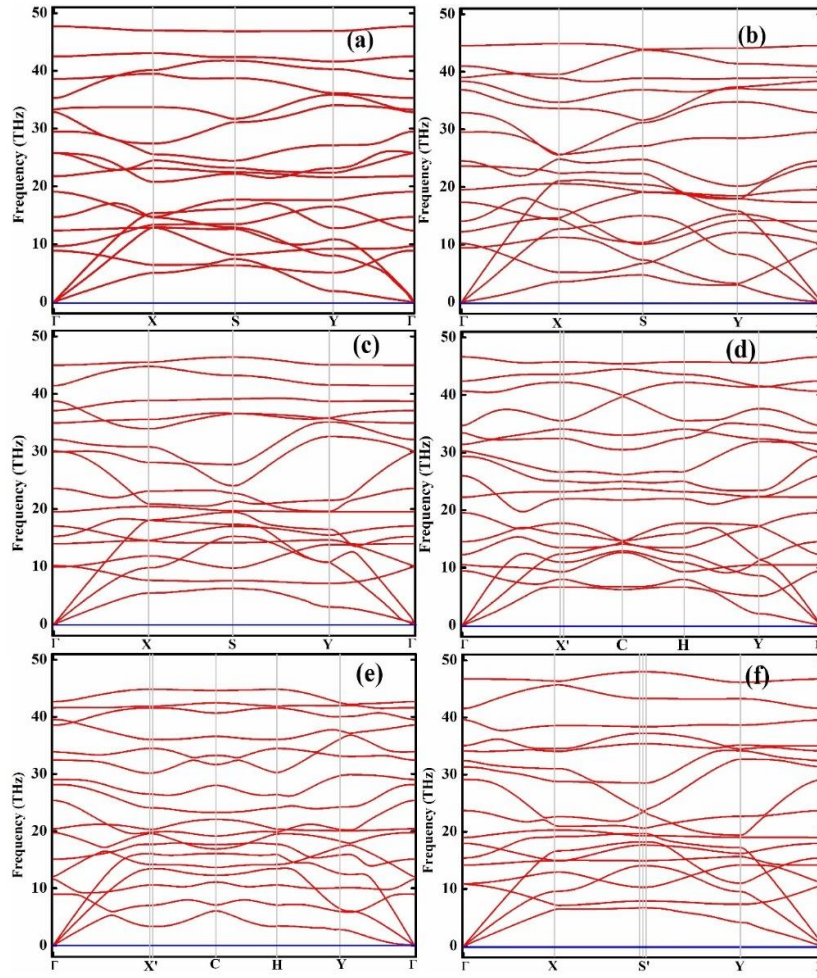
Fig. S3 *shows the phonon spectra of different phases of bpn-BCN monolayers; α- BCN, β-BCN, γ- BCN, δ-BCN, η- BCN and θ-BCN are marked in the figure as 'a' to 'f' respectively.*
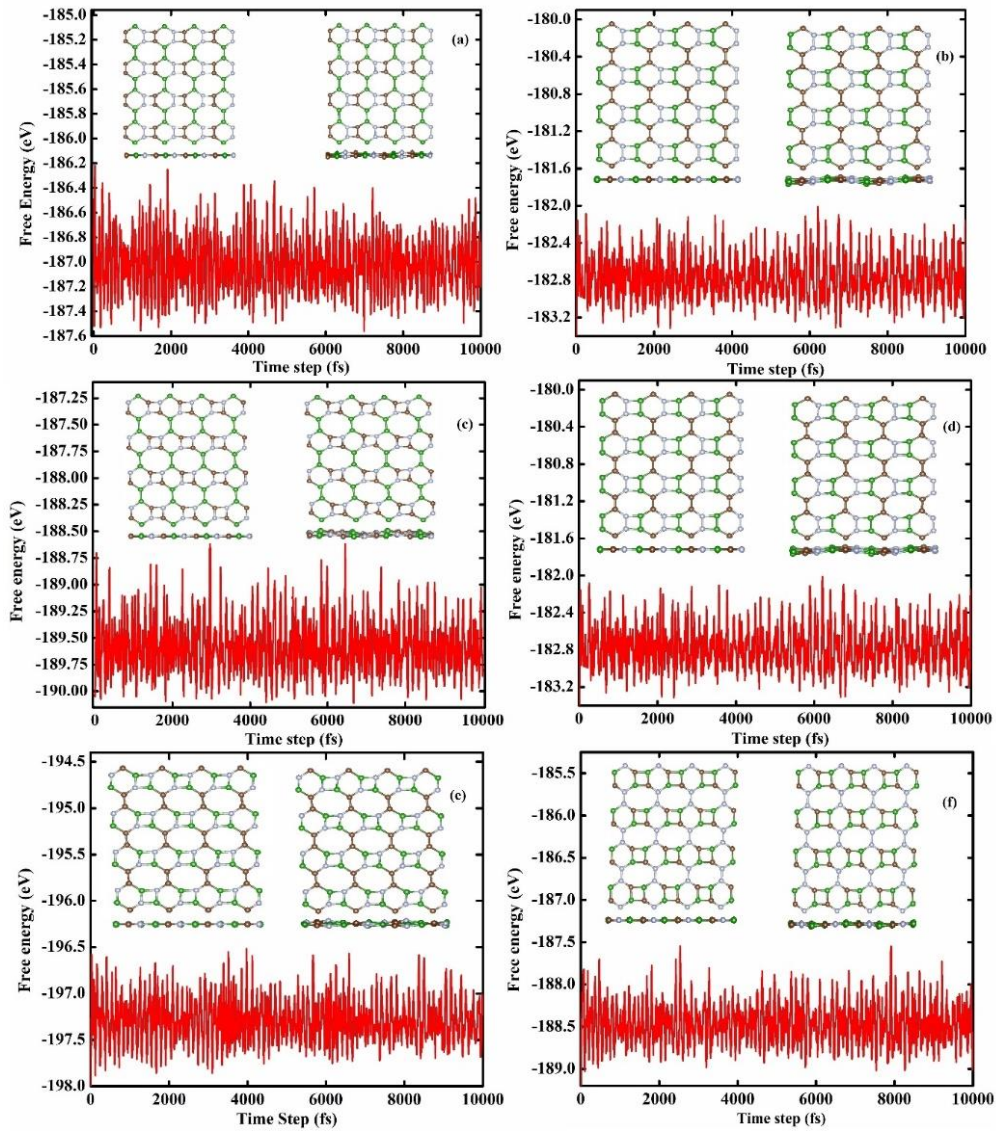
Fig. S4 *depicts ab initio molecular dynamics at 300K of different phases of bpn-BCN monolayers; α-BCN, β- BCN, γ- BCN, δ-BCN, η- BCN and θ-BCN are marked in the figure as 'a' to 'f' respectively.*

Note:- The energies of isolated single B, C, and N atoms, calculated by placing each atom in a cubic box with a box length of 20 Å, are follows: $E_B = -69.59$ eV, , $E_C = -144.70$ eV, and & $E_N = -261.07$ eV. On the other hand, the $\mu_C = -154.86$ eV is the energy of per carbon atom calculated from graphite, a stable carbon allotrope. In the N-rich environment, the energy per atom of the alpha-N_2 phase of solid nitrogen is $\mu_N = -270.22$ eV, whereas for the B-rich environment, the energy per atom of a metallic alpha-B phase is $\mu_B = -77.23$ eV.
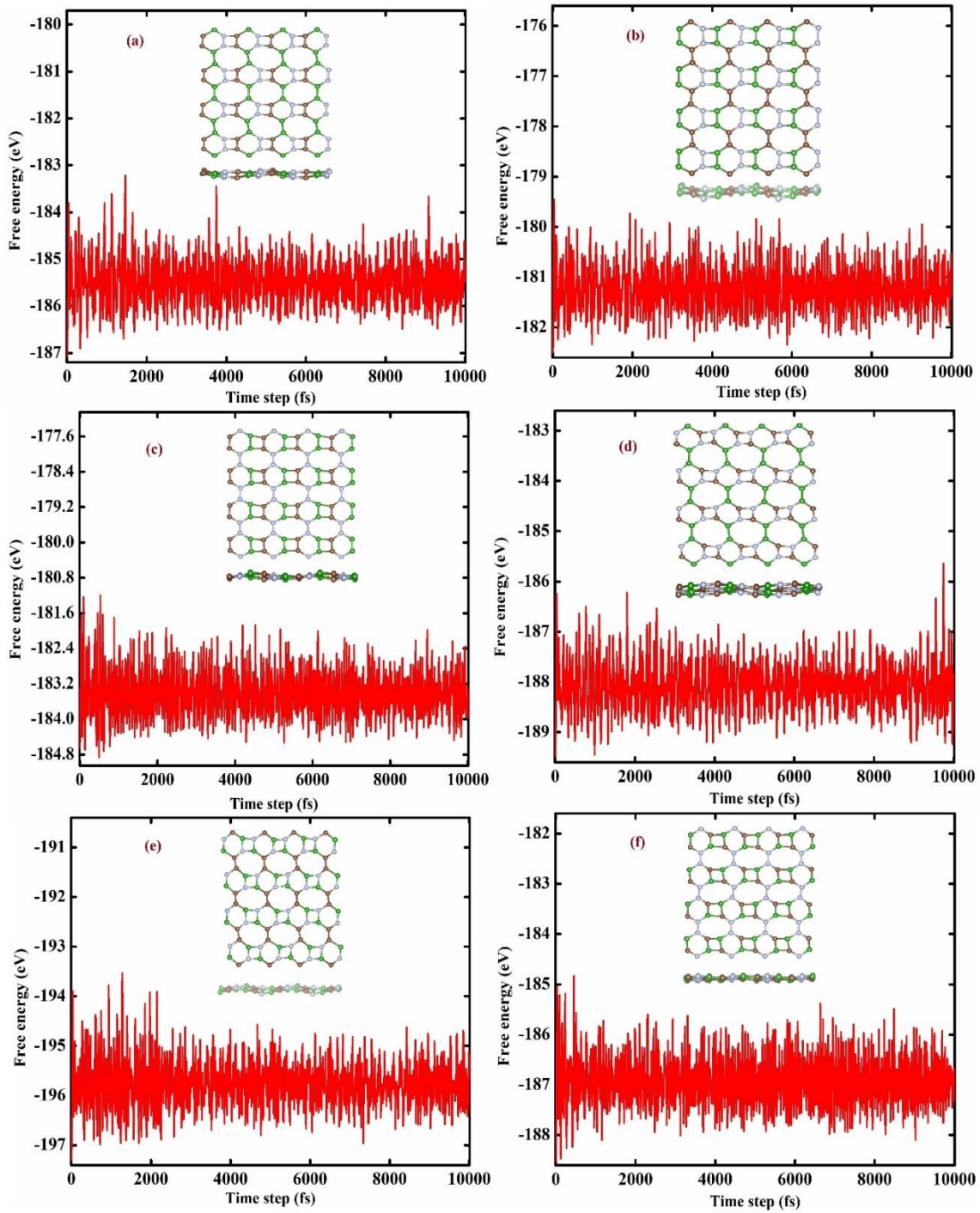
Fig. S5 *ab initio molecular dynamics at 800K, of different phases of bpn-BCN monolayer; α-BCN, β- BCN, γ- BCN, δ-BCN, η- BCN and θ-BCN are marked in the figure as 'a' to 'f' respectively.*
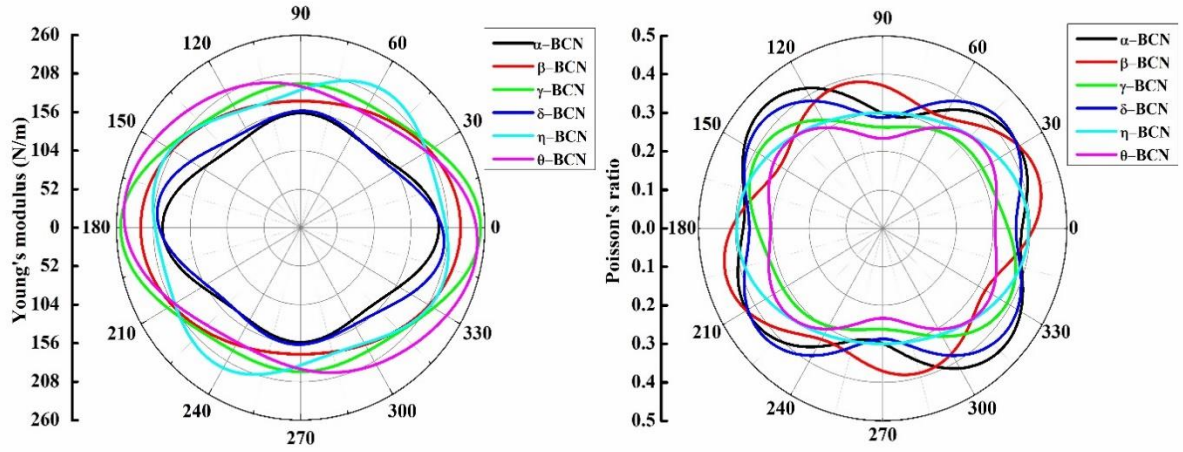
Fig. S6 *displays the angular dependence of Young's moduli (left panel) Y(Φ) and Poisson's ratio (right panel) υ(Φ) of different phases of the bpn-BCN monolayers, where the angle Φ is defined relative to the x-direction.*
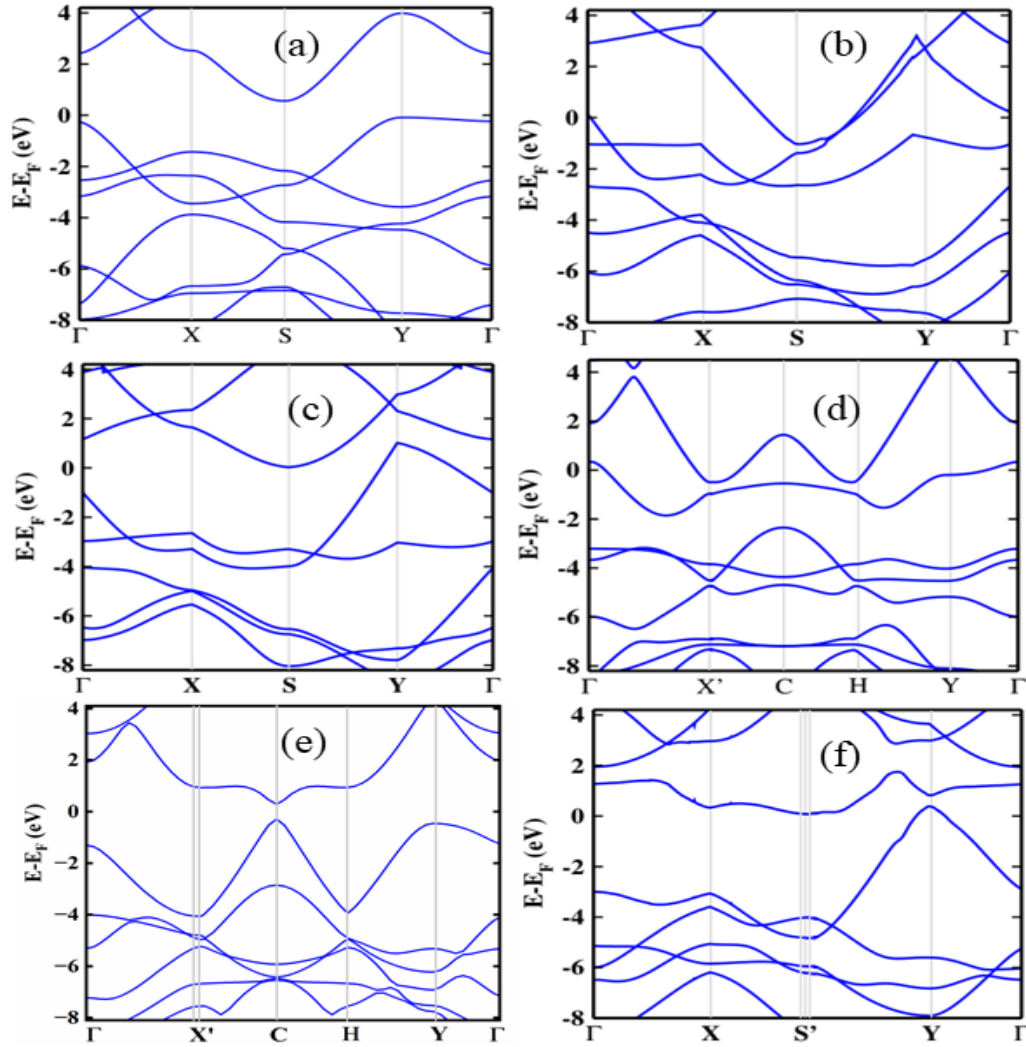

Fig. S7 *The electronic bands structures using HS06 hybrid exchange-correlation functional for different phases of bpn-BCN monolayer; α- BCN, β- BCN, γ- BCN, δ-BCN, η- BCN and θ-BCN are marked in the figure as a, b, c, d, e and f respectively.*
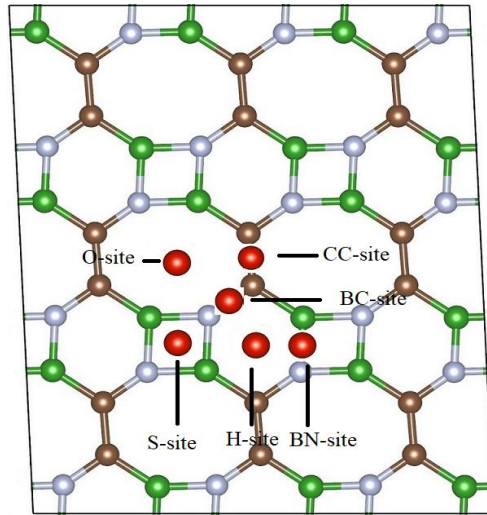
Fig. S8 *All possible adsorption sites for alkali metal atoms in bpn-BCN monolayer..*
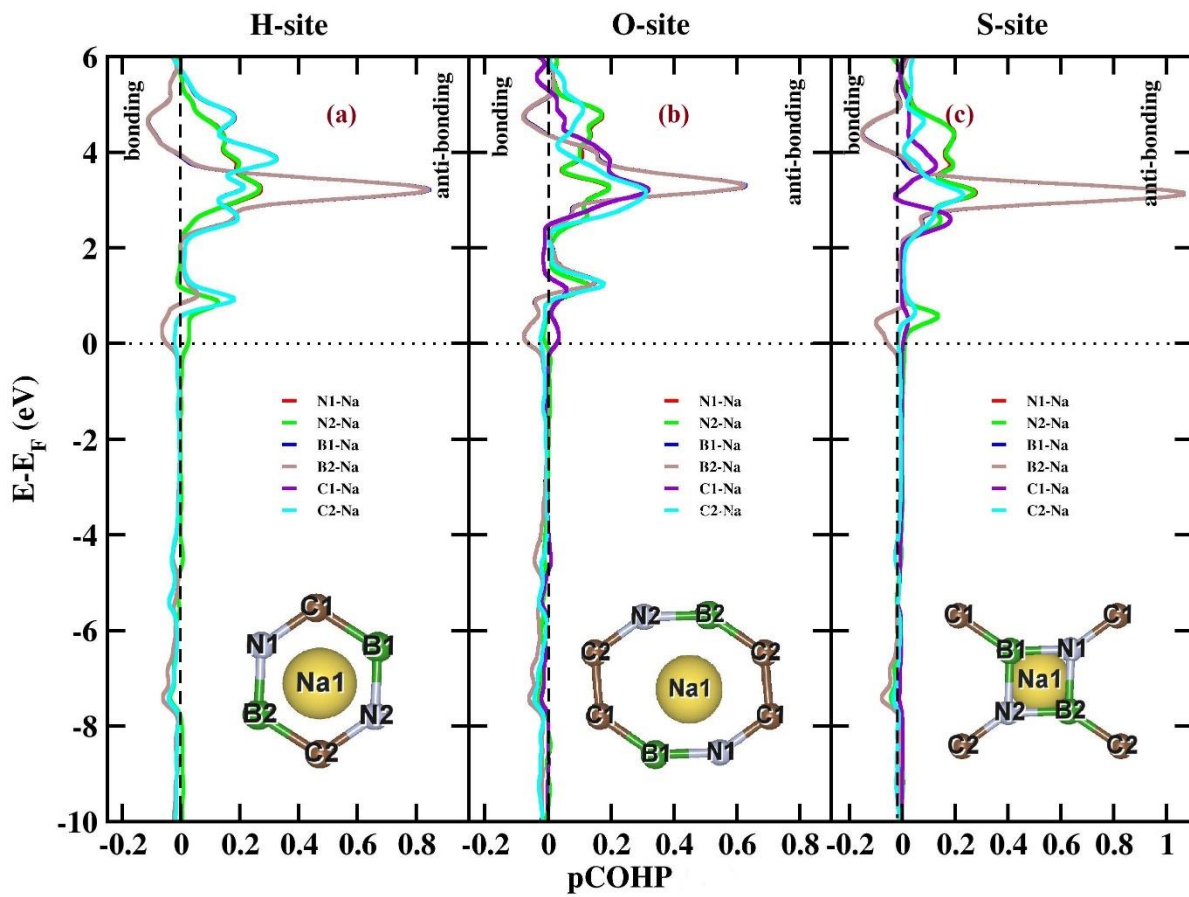

Fig. S9 *pCOHP analyses of the chemical bonding between the adsorbed Na atom and constituent atoms of the bpn-BCN monolayer for (a) H-site, (b) O-site, and (c) S-site, respectively.*
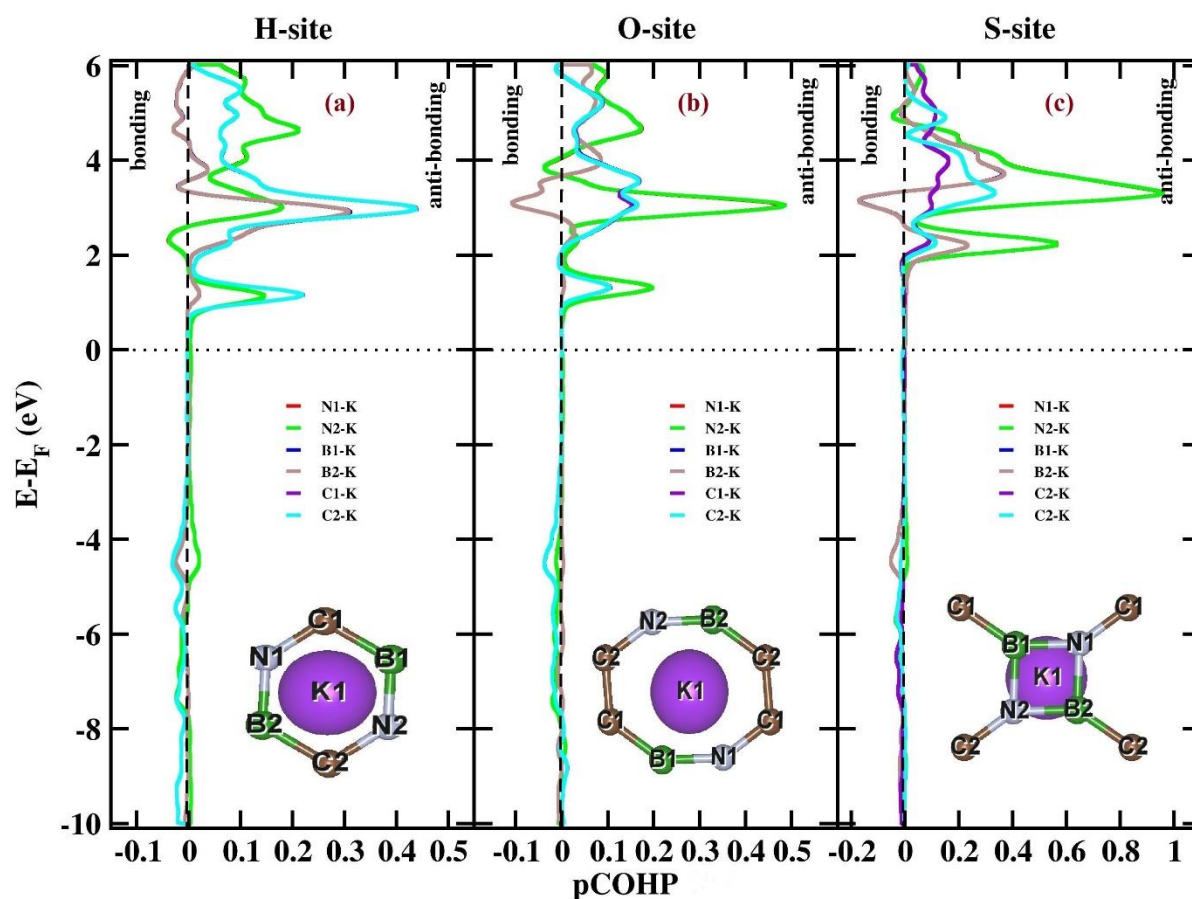
Fig. S10 *pCOHP analyses of the chemical bonding between the adsorbed K atom and constituent atoms of the bpn-BCN monolayer for (a) H-site, (b) O-site, and (c) S-site, respectively.*

Table S3 *ICOHP (eV) values for BCN atoms with all alkali metals at different H-, O-, and S-sites. Please refer to Fig. 5, Fig. S9 and Fig. S10 for labels of B, C, and N atoms.*

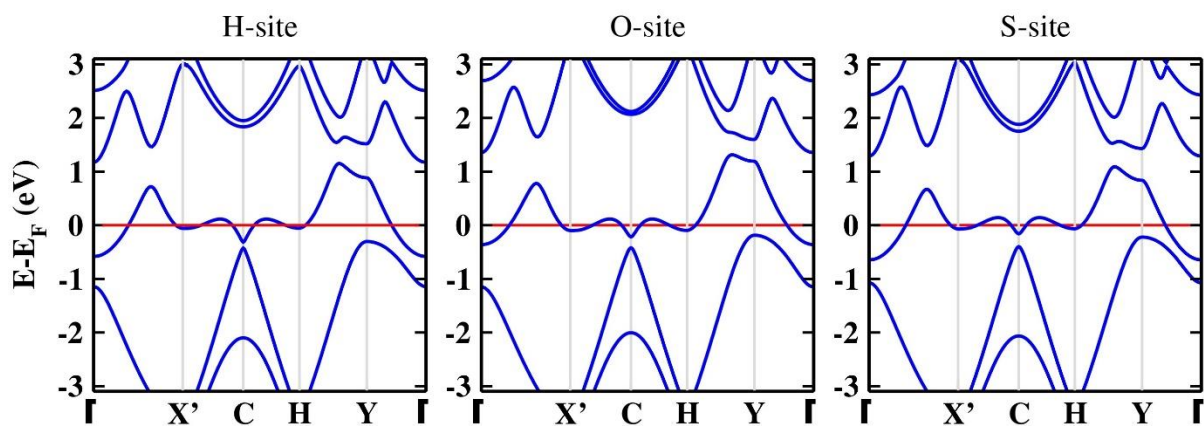| X=Li,	Li			Na			K		
Na, K	H-site	O-site	S-site	H-site	O-site	S-site	H-site	O-site	S-site
B1-X	-0.175	-0.171	-0.179	-0.431	0.313	-0.452	-0.284	-0.161	-0.442
B2-X	-0.187	-0.171	-0.179	-0.434	0.311	-0.431	-0.281	-0.157	-0.446
C1-X	-0.225	-0.218	-0.089	-0.531	-0.391	-0.220	-0.646	-0.346	-0.383
C2-X	-0.223	-0.217	-0.097	-0.533	-0.388	-0.224	-0.649	-0.345	-0.372
N1-X	-0.211	-0.179	-0.200	-0.428	-0.410	-0.436	-0.463	-0.508	-1.053
N2-X	-0.208	-0.178	-0.200	-0.431	-0.408	-0.431	-0.461	-0.513	-1.055

Fig. S11 *The electronic band spectra of Na metal absorbed bpn-BCN monolayer at H- O- and S-sites.*
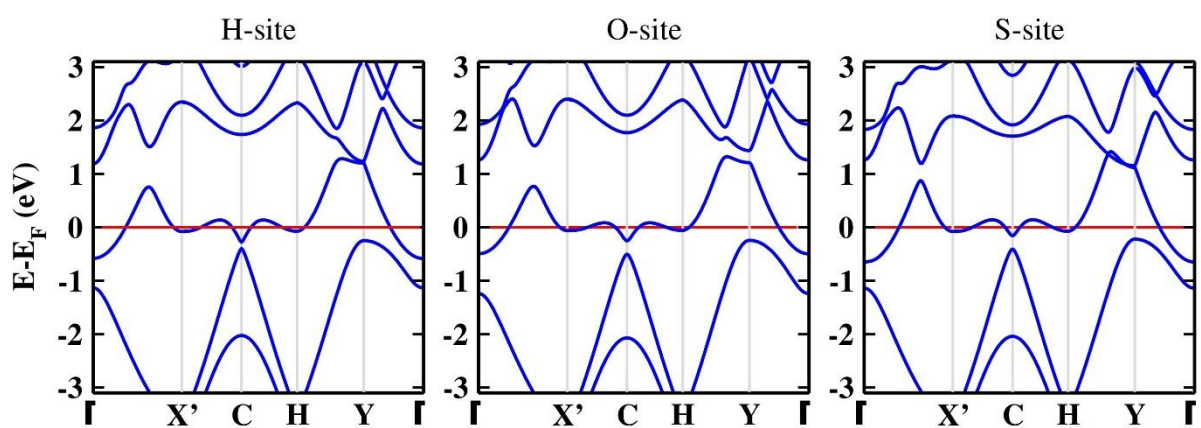

Fig. S12 *The electronic band spectra of K metal absorbed bpn-BCN monolayer at H- O- and S-sites.*
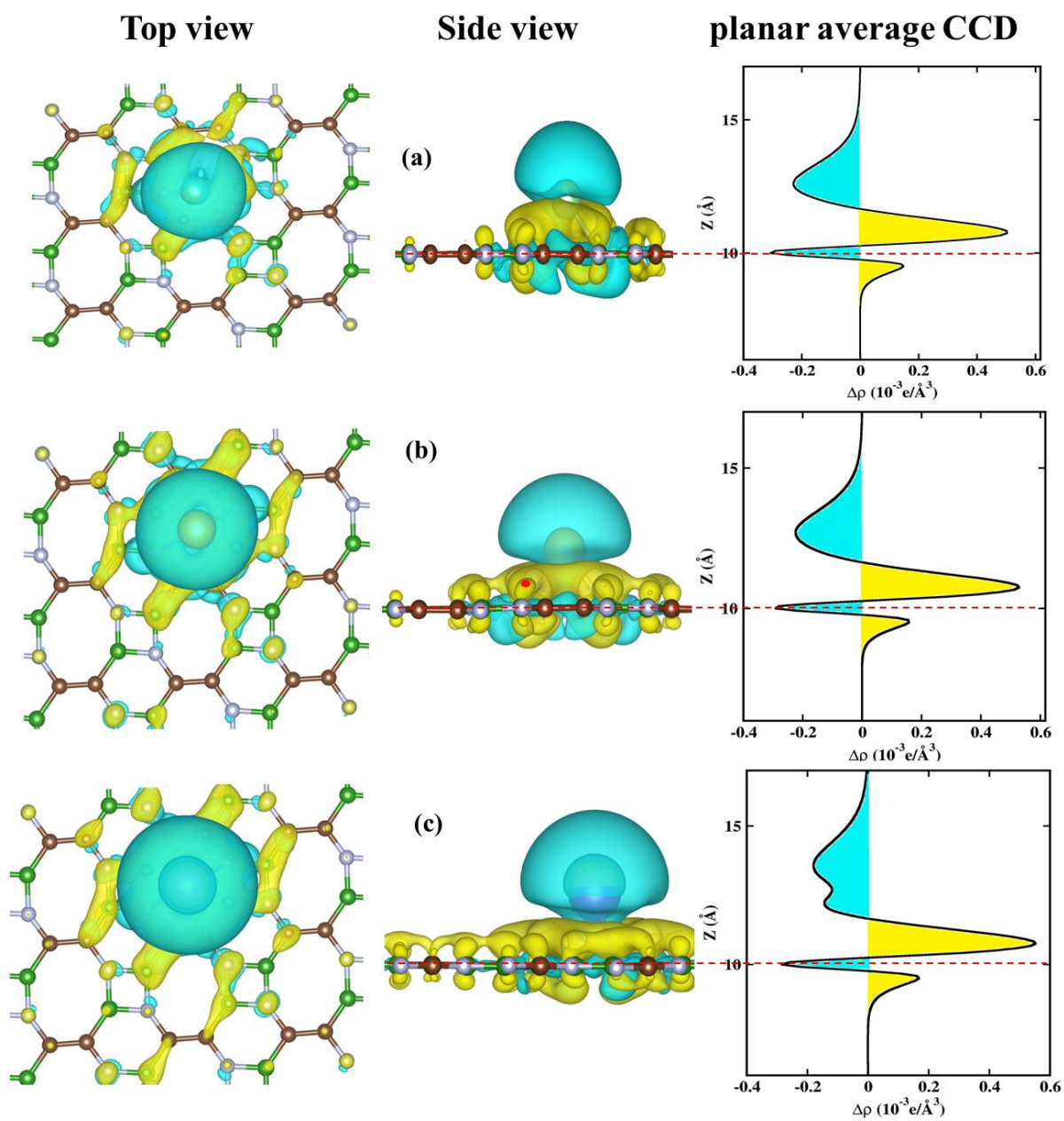
Fig. S13 *The top and side view along with average planar electron density difference for (a) Li- (b) Na- and K-metal adsorbed at (a) O-site on the bpn-BCN monolayer with iso-surface value of 0.001 eÅ⁻³.*
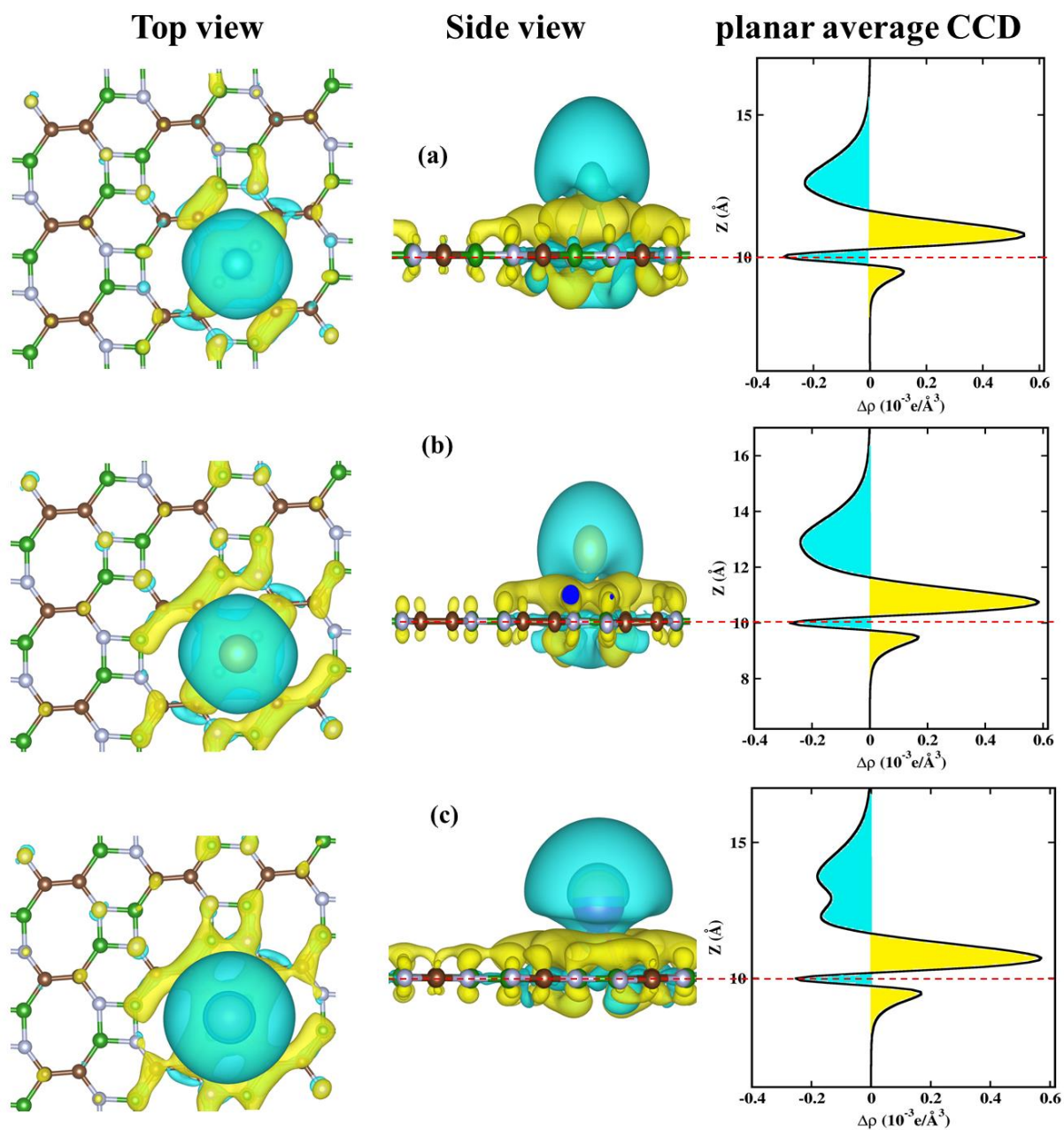
Fig. S14 *The top and side view along with average planar electron density difference for (a) Li- (b) Na- and K-metal adsorbed at (a) S-site on the bpn-BCN monolayer with iso-surface value of 0.001 eÅ⁻³.*