Supporting Information

BC_2N Monolayer as High-performance Anode Material for Potassium-Ion Batteries

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Table S1

Independent elastic constants (C_{ij}), Young's modulus (Y^{2D}) in N m^{-1} and Poisson's ratio (V^{2D}) of BC_2N.

	C_{11}	C_{22}	C_{12}	C_{66}	$Y^{2D}_{[01]}$	$Y^{2D}_{[10]}$	$V^{2D}_{[01]}$	$V^{2D}_{[10]}$
BC_2N	302.824	294.118	58.101	118.392	274.454	291.684	0.186	0.216

Table S2

Stable adsorption sites and adsorption energies of K on BC_2N surfaces.

K site	T_1	T_2	T_3	H_1	H_2	H_3	B_1	B_2	B_3	B_4
BC_2N	-0.481	-0.480	-0.506	-0.560	-0.606	-0.570	H2	H1	H3	H3

Table S3

Structural information of the BC_2N monolayer.

Phase	**Space Group**	**Lattice Parameters(Å, °)**	**Wyckoff Positions (fractional)**			
			Atoms	***x***	***y***	***z***
BC_2N	*Cmmm*	a = 5.06590	B (4j)	0.50000	-0.33085	-0.50000
		b = 8.63750	C (8q)	0.73817	-0.08125	-0.50000
		c = 30.00000	N (4j)	0.50000	-0.16268	-0.50000
		α = 90.00000				
		β = 90.00000				
		γ = 90.00000				

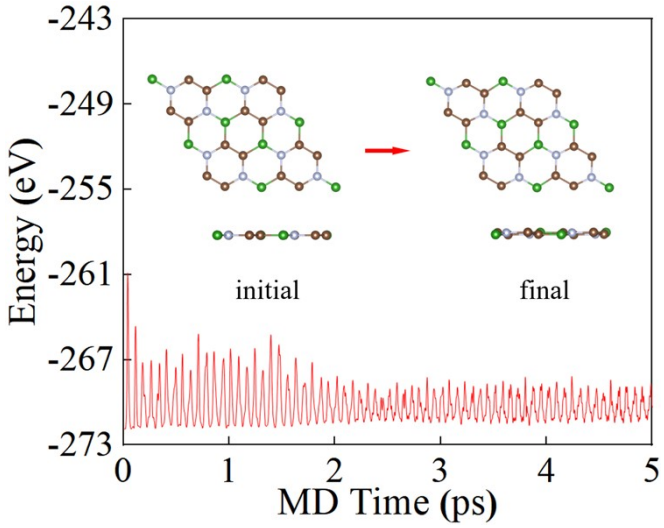

Fig. S1. The ab-initio molecular dynamics simulations at 350 K and 5 ps with the free-energy evolution and final structure of BC_2N.

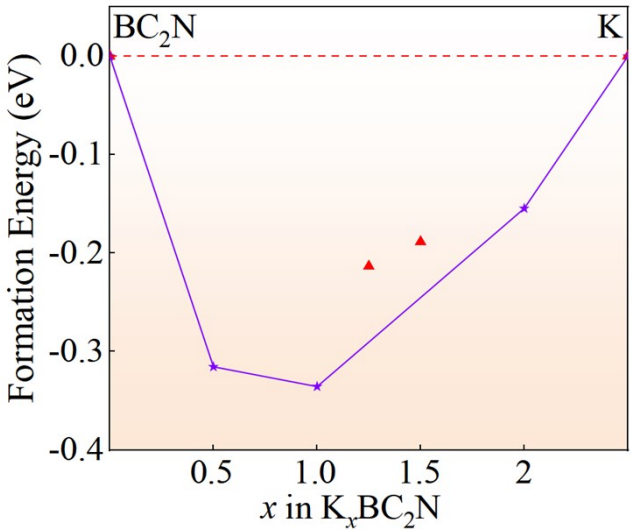

Fig. S2. The formation energies of K_xBC_2N systems with respect to the BC_2N monolayer and the K bulk metal.

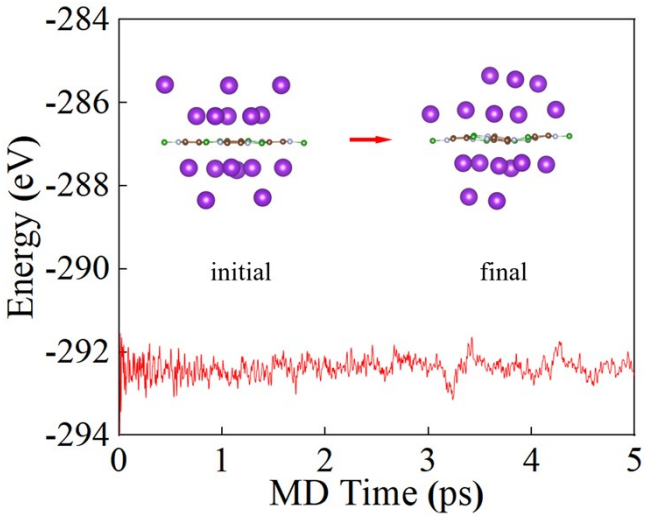

Fig. S3. Ab-initio molecular dynamics simulation showing the free energy evolution and final structure of BC_2N at 300 K and 5 ps in the saturated adsorption state.

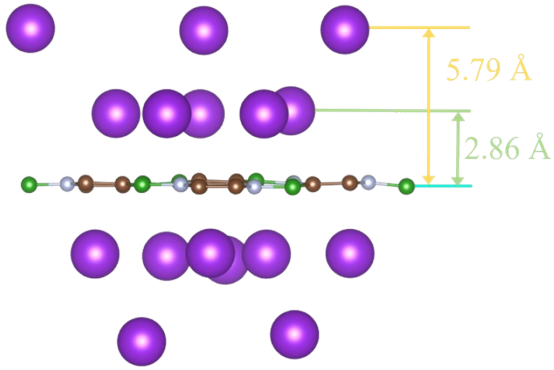

Fig. S4. Comparing the interlayer spacing between the adsorbed K-ions layers on the substrate K_2BC_2N.

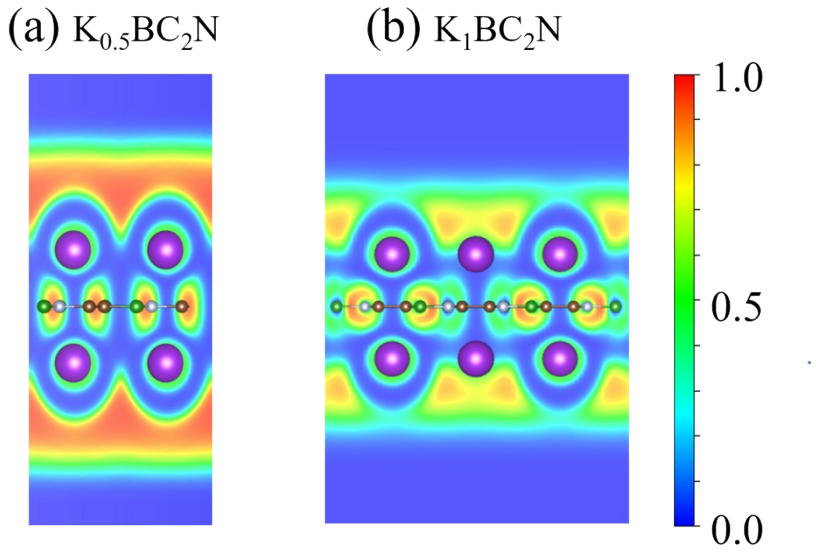

Fig. S5. Electron localization function (ELF) maps of (a) $K_{0.5}BC_2N$, (b) K_1BC_2N.

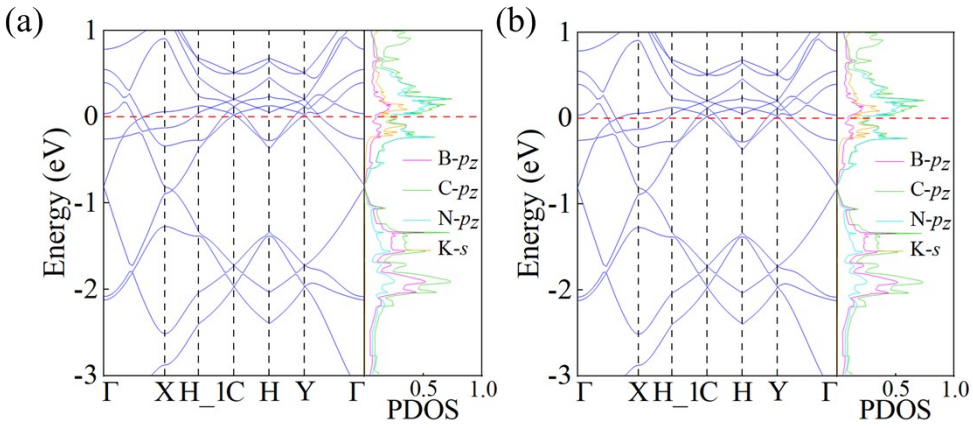

Fig. S6. The band structures and density of states for (a) $K_{0.5}BC_2N$, (b) K_1BC_2N. The Fermi level is set to 0 eV and labeled with a horizontal dashed line.