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SUPPLEMENTARY INFORMATION

BCN Monolayer for High Capacity Al based Dual-Ion Batteries

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Contents

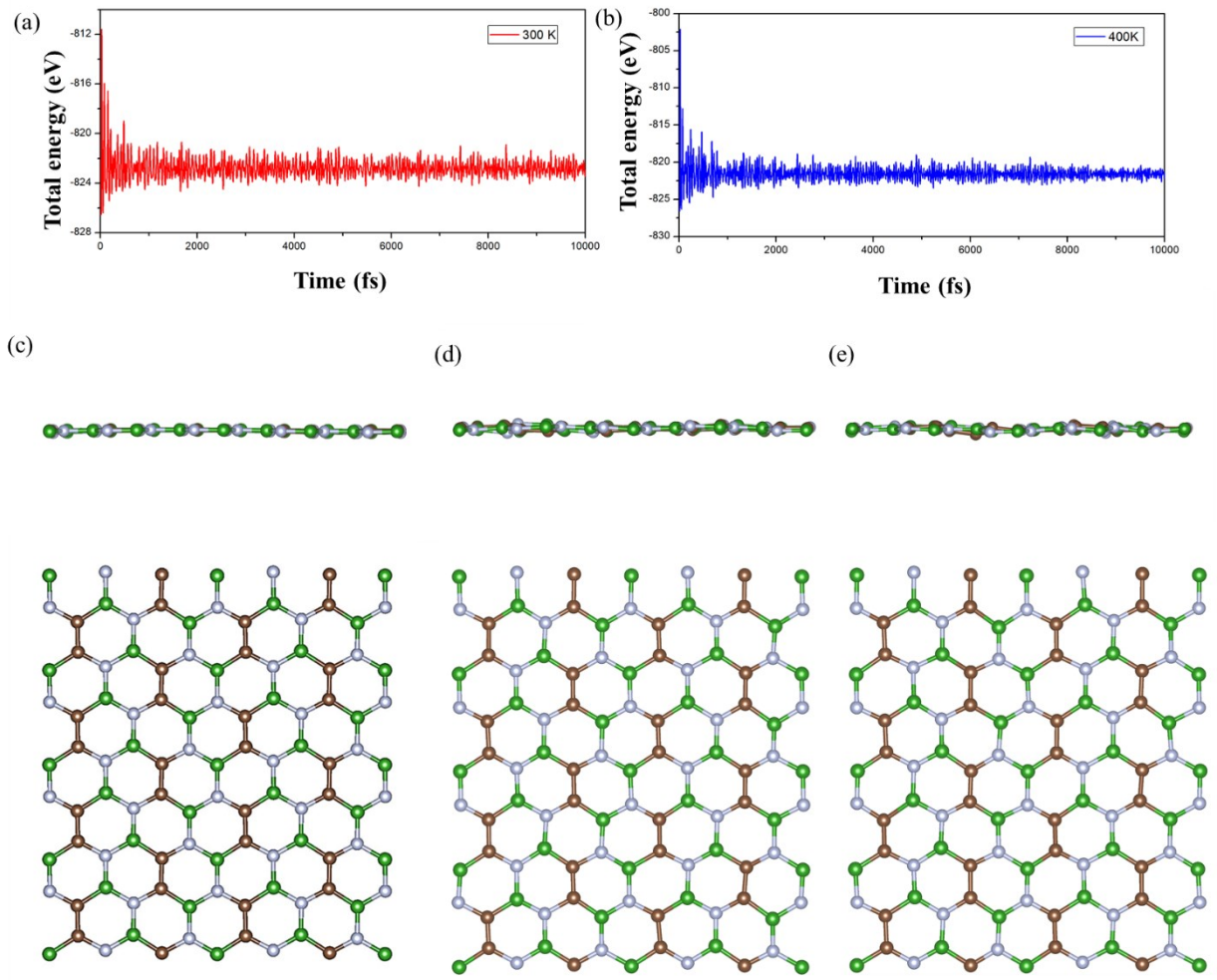

Fig. S1 Total energy vs time plot for AIMD simulations of the BCN monolayer at (a) 300 K and (b) 400 K. The side and top views of (c) initial structure (d) structure after 20 ps simulation at 300 K and (e) at 400 K.

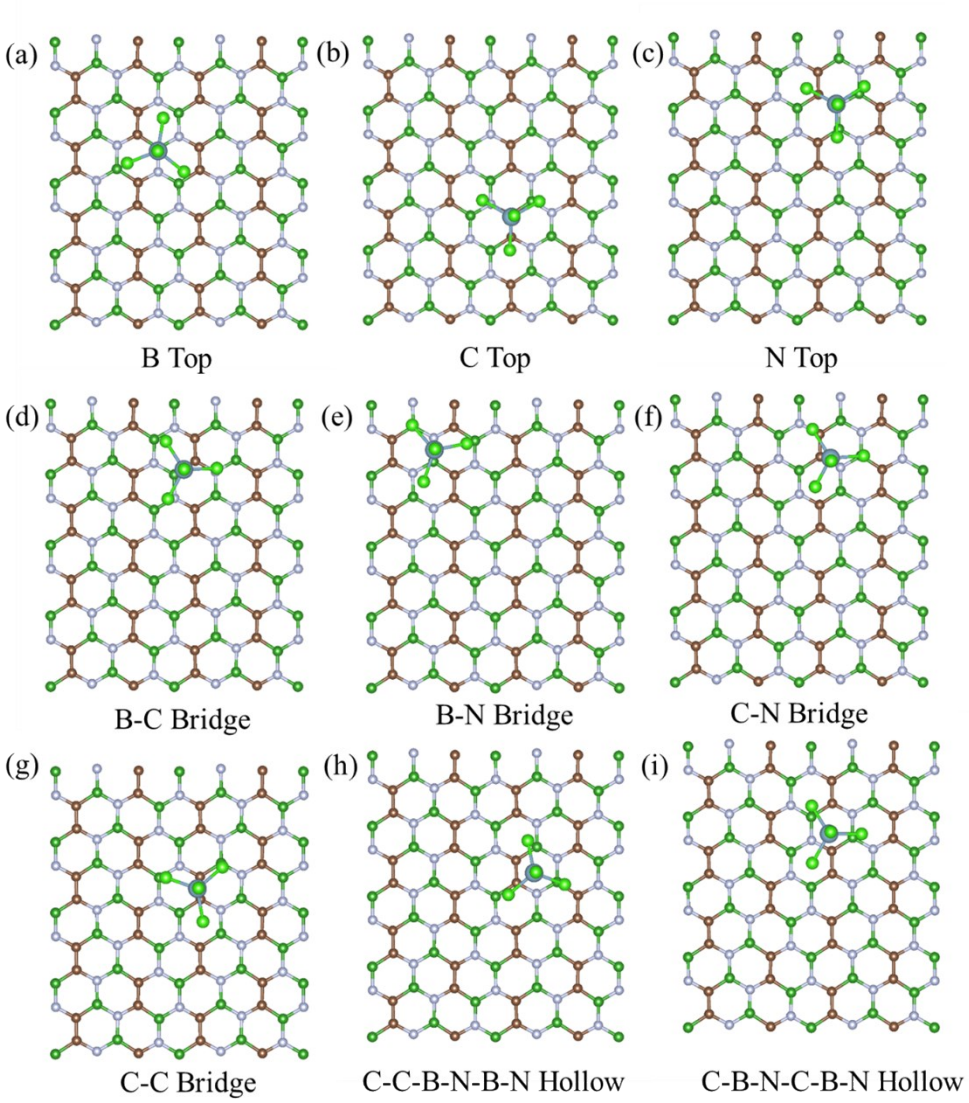

Fig. S2 Top view of the $AlCl_4$ adsorbed BCN monolayer at (a) B Top, (b) C Top, (c) N Top, (d) B-C Bridge, (e) B-N Bridge, (f) C-N Bridge, (g) C-C Bridge, (h) C-C-B-N-B-N Hollow and (i) C-B-N-C-B-N Hollow sites.

Table S1 The relative adsorption energy of $AlCl_4$ for all possible adsorption sites available and the average distance of Al of the adsorbed $AlCl_4$ from BCN monolayer at each site.

Sites		Relative Adsorption energy (eV)	Average Distance (Å)
1	B Top	0.03	3.91
2	C Top	0.02	3.88
3	N Top	0.04	3.97
4	B-C Bridge	0.06	3.88
5	B-N Bridge	0.02	3.93
6	C-N Bridge	0.03	3.89
7	C-C Bridge	0.01	3.87
8	C-C-B-N-B-N Hollow	0.00	3.85
9	C-B-N-C-B-N Hollow	0.03	3.90

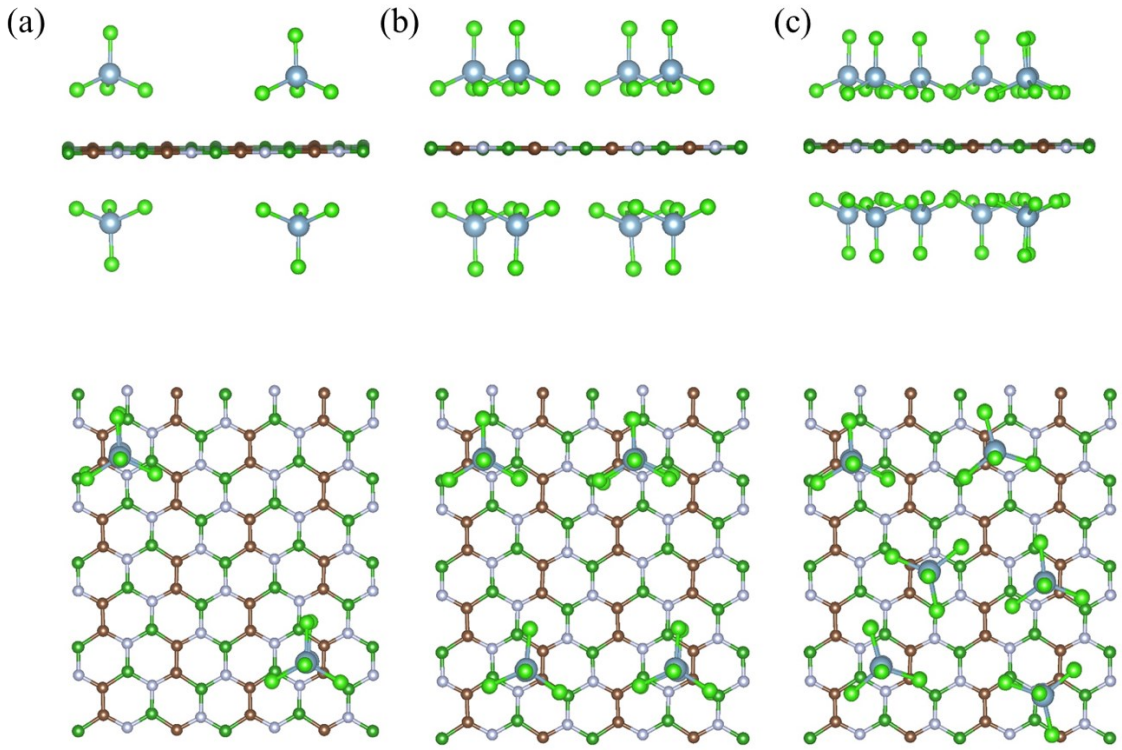

Fig. S3 Side and top views of the most stable configuration of $AlCl_4$ adsorbed BCN monolayer at different $AlCl_4$ concentrations (a) $(AlCl_4)_4$BCN (b) $(AlCl_4)_8$BCN (c) $(AlCl_4)_{12}$BCN.

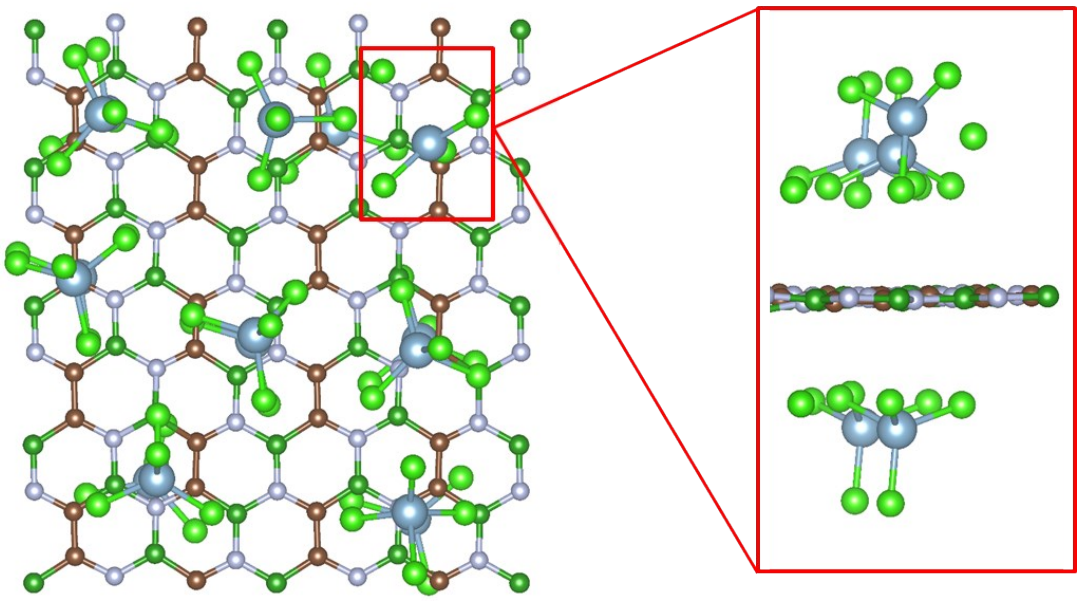

Fig. S4 Top view of the optimized configuration of 15 $AlCl_4$ absorbed BCN monolayer. Inset figure showing side view of $AlCl_4$ dissociation.

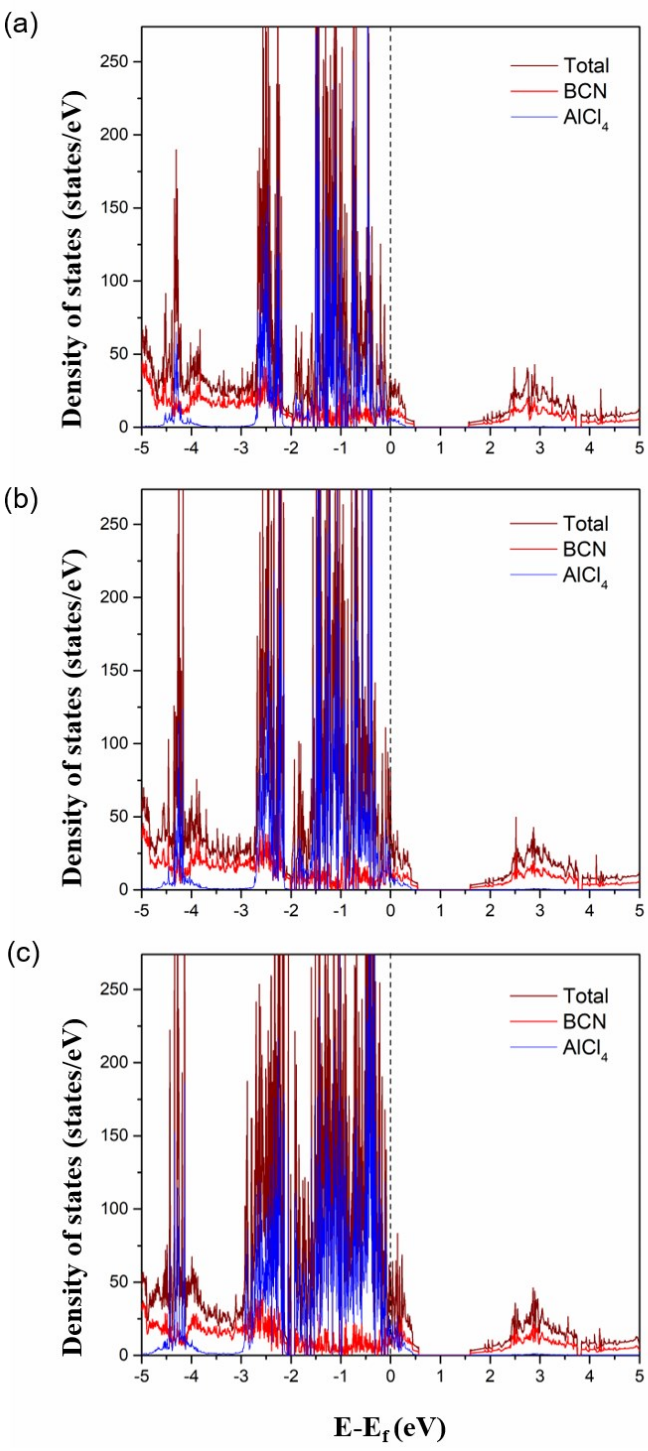

Fig. S5 Total and partial density of states of (a) 7 $AlCl_4$ adsorbed BCN monolayer, (b) 10 $AlCl_4$ adsorbed BCN monolayer, (c) 14 $AlCl_4$ adsorbed BCN monolayer. The Fermi level is set at zero.

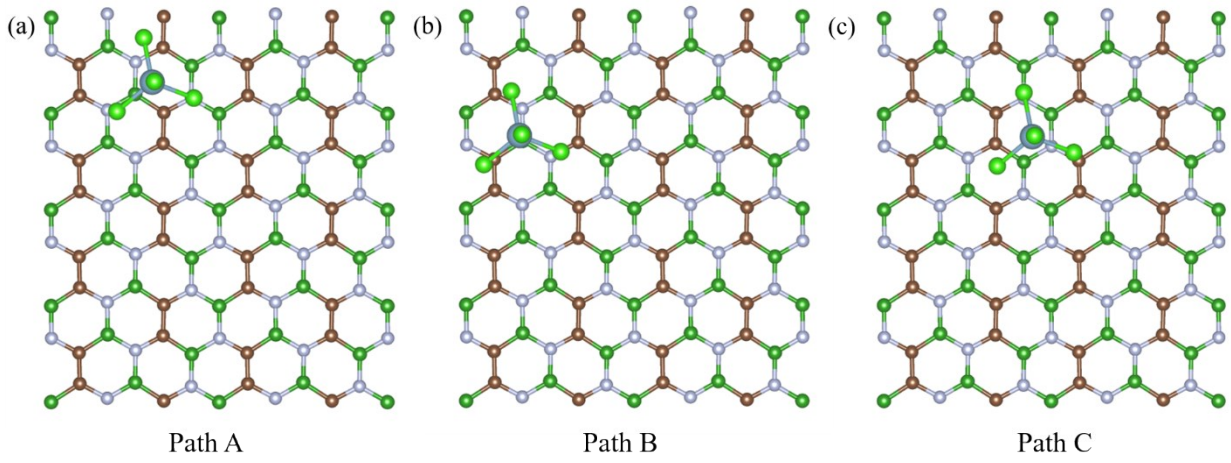

Fig. S6 The optimized highest energy transition states for different possible pathways, (a) Path A, (b) Path B, (c) Path C, available for $AlCl_4$ diffusion.