Supplementary information for

Towards a new packing pattern of Li adsorption in two-dimensional pentagonal BCN†

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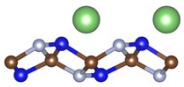
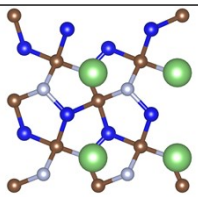
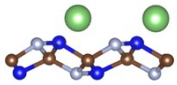
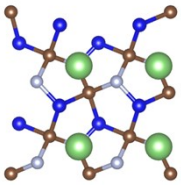
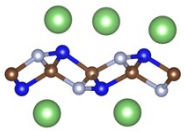
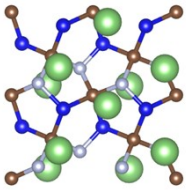
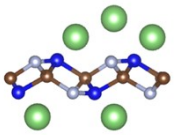
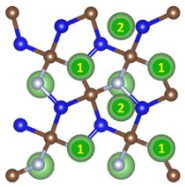
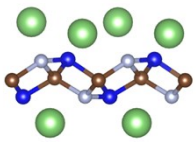
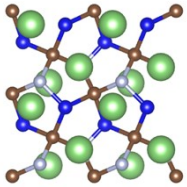
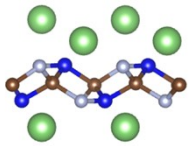
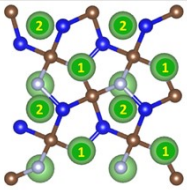
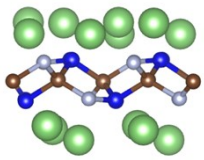
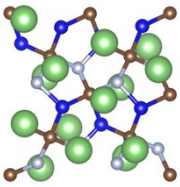
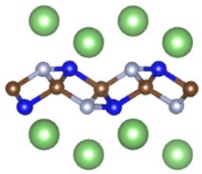
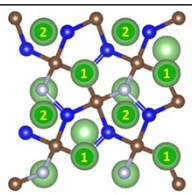
TABLE S1. Adsorption Energies (E_{ad} in eV), Adsorption Height (h in Å) of Single Li-Adsorbed Penta-BCN

Site	E_{ad}^{Li}	h^{Li} (Å)
1	0.05	2.26
2	0.06	2.30
3	0.81	2.85
4	-0.14	1.87
5	0.33	2.62
6	-0.20	1.87
1	0.13	2.38
2	-0.03	2.08
3	0.68	2.55
4	0.12	2.18
5	0.14	2.38
6	0.07	2.17
7	0.65	2.55
8	-0.01	2.14
9	0.54	2.74
10	-0.15	1.74
1	0.69	2.61
2	0.39	2.38
3	0.12	2.25
4	0.40	2.42
M	-0.24	1.82

TABLE S2. The compared structures of Li_xBCN of this works and Chen's model with side and top views

Composition	This work		Chen's model	
	Side view	Top view	Side view	Top view
$Li_{0.50}BCN$		 Note: Li slightly shifted from on top position (M-site)		 Note: Li is exactly on top position (N2-site)
$Li_{1.25}BCN$				
$Li_{1.50}BCN$				
$Li_{1.75}BCN$				
$Li_{2.00}BCN$