Supporting Information

BC_2N/Graphene Heterostructure as a Promising Anode Material for Rechargeable Li Ion Batteries by Density Functional Calculations

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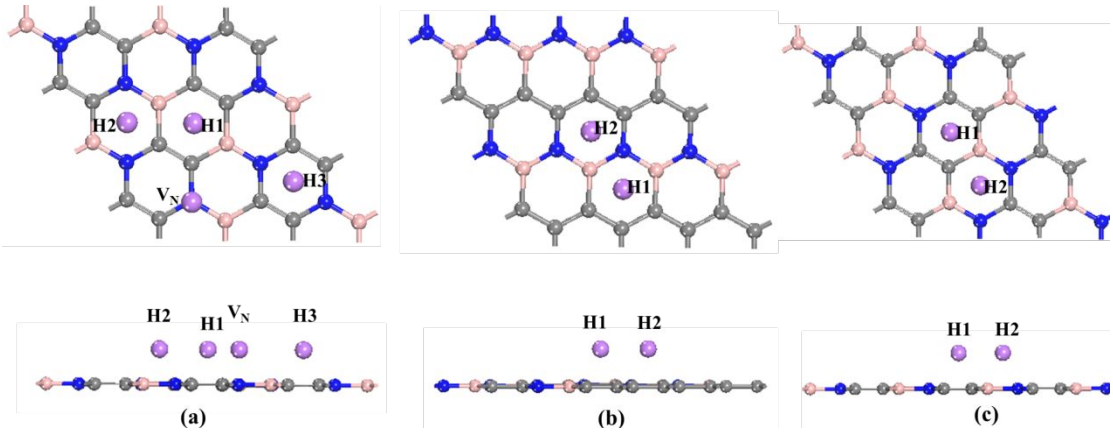

Figure S1. Top and side views of stable adsorption sites for Li-ion adsorption in (a) BC_2N-I, (b) BC_2N-II, (c) BC_2N-III.

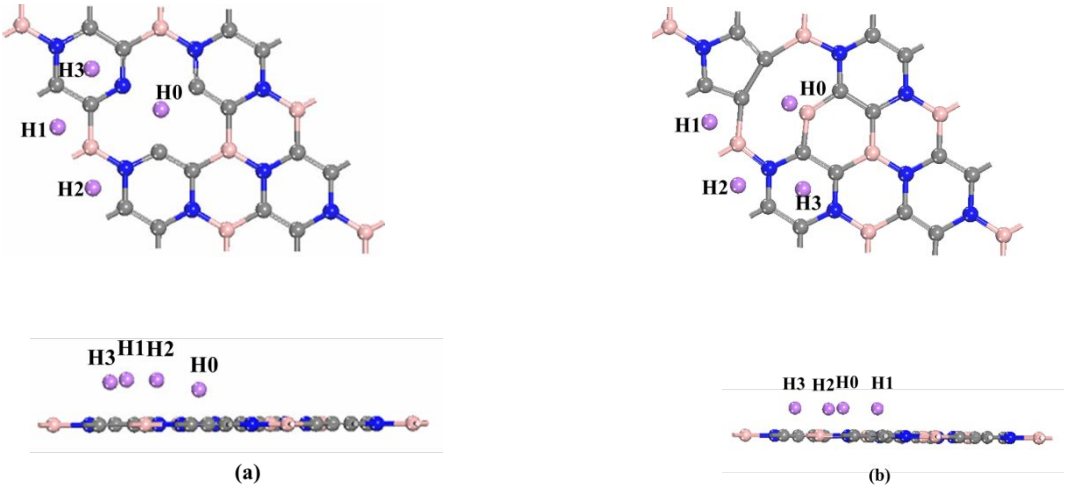

Figure S2. Top and side views of stable adsorption sites for Li-ion adsorption in (a) defective I-B_d monolayer, (b) defective I-N_d monolayer

Table S1. Calculated adsorption energy (E_{ad}) and the height from the Li atom to monolayer at the energetically most favorable adsorption sites of the I-B_d and I-N_d.

system	**Li site**	E_{ad} (eV)	Height (Å)
I-B_d	H0	-2.36	1.39
	H1	-0.96	1.79
	H2	-0.55	1.78
	H3	-0.61	1.71

$I\text{-}N_d$	H0	-1.0	1.75
	H1	-1.14	1.74
	H2	-0.77	1.73
	H3	-0.63	1.74

Table S2. Average net atomic charges for BC_2N-I monolayer.

Atom	B	C	N
Net charge	1.87	-0.17	-1.53

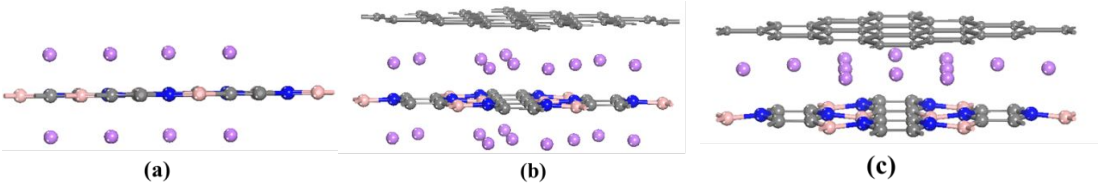

Figure S3. Side views of theoretical maximum Li storage in optimized (a) BC_2N-1, (b) I-BN, (c) I-HH.