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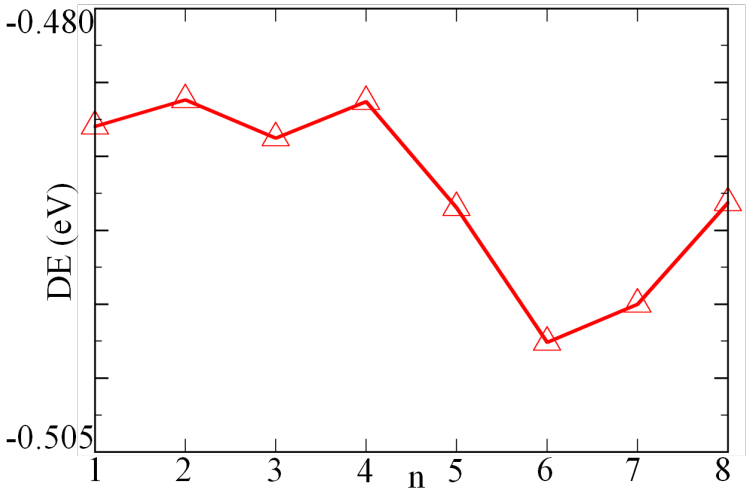
Supporting Information

Possible application of 2D-Boron sheets as Anode Material in Lithium Ion Battery: A DFT and AIMD study

Swastika Banerjee, [a] *Ganga Periyasamy*[b] *and Swapan K. Pati**[a,b]

Figure S1. Average Dispersion energy (DE) per Li are plotted with respect to number of Li atom (n) for lithium adsorbed monolayer (α_1) at various adsorbates'(Li) concentration.



This Average Dispersion energy (DE) per Li vs. n plot says the increment of stabilization of Li adsorption at higher concentration is not only due to the charge transfer interaction as discussed in the main text but also influenced by the intermolecular interaction between sheet and adsorbed Li caused by instantaneous fluctuation of electron density responsible for London dispersion.

Table S1. Relative adsorption energy (Emax – E), distance of adsorbed Li on the surface (D_S) in Å, partial positive charges on surface adsorbed Li (q_s) are given at . Coverage has been mentioned in the term of percentage coverage on H site for lithium adsorbed monolayer (α_1).

No. of Li Atoms	% Coverage	Emax – E	D_S	$q_{S\,(e)}$
1	12.5	0.203	1.66	0.53
2	25	0.00	1.69	0.52
3	37.5	0.034	1.73	0.50
4	50	0.035	1.66	0.47
5	62.5	0.037	1.49,1.62(4:1)	0.44
6	75	0.070	1.60	0.43
7	87.5	0.108	1.76	0.42
8	100	0.181	1.69	0.37

Emax is the highest adsorption energy per Li; E is the adsorption energy per Li for various extent of lithiation.

[a] *New Chemistry Unit, Jawaharlal Nehru Center for Advanced Scientific Research, Jakkur P. O., Bangalore 560064, India; E-mail: pati@jncasr.ac.in*
[b] *Theoretical Science Unit, Jawaharlal Nehru Center for Advanced Scientific Research, Jakkur P. O., Bangalore 560064, India; E-mail: pati@jncasr.ac.in*