Supplementary Information

Borophene as an extremely high capacity electrode material for Li-ion and Na-ion batteries

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I. Figure S1

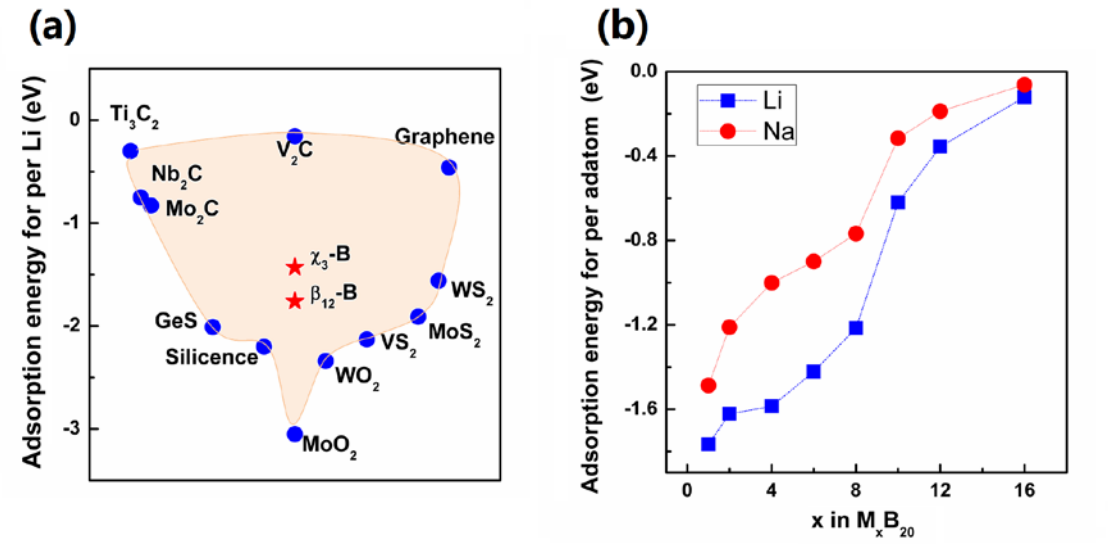

Fig. S1 (a) Comparison of Li adsorption energies between borophene and typical 2D anode materials. The adsorption energies for per Li are calculated from similar size of host materials, and some data are taken from literatures[1-7]. (b) The adsorption energy for per Li (or Na) on borophene as a function of the metal atoms concentration.

II. Tables S1-2 and discussions

For a certain reaction,

$$Host + xM^{+} + xe^{-} \longleftrightarrow M_{x}Host \qquad (1)$$

where *Host* represents the host electrode material, *M* is for the adtom Li or Na, and *x* is the number of adsorbed atoms. The maximum capacity (C_M) of an electrode material is usually estimate as

$$C_M = x_m F / M_{\text{Host}} \qquad (2)$$

Where x_m represents the maximum electrons involving the electrochemical process, *F* derives from the Faraday constant with the value of 26798 mA h mol^{-1}, and M_{Host} is the mass of host material in g mol^{-1}. Meanwhile, there also some works use another calculating formulation:

$$C_M = x_m F / M_{M_{x_m}\text{Host}} \qquad (3)$$

Comparing with equation (2), the only difference is that in equation (3) the mass of adtoms is taken into account.

Here we display the comparisons of Li/Na capacities between borophene and other typical 2D electrode materials by using the equation (2) and (3), respectively. From Tables S1 and S2, we find that: i) most former literatures follow equation (2) to estimate the maximum capacities of the electrode materials, as used in our work; ii) for both calculating strategies, borophenes are several times higher in Li/Na capacities than the typical electrode materials provided.

Table S1 Comparisons of Li capacities between borophene and other typical 2D electrode materials. C_M^a and C_M^b are the maximum capacities calculated from equation (2) and equation (3), and C_M^{ref} are the values used in literatures. The case that literatures follow the values from equation (2) and equation (3) are denoted with light blue and light yellow colors, respectively.

	C_M^a (mA h g^{-1})	C_M^b (mA h g^{-1})	C_M^{ref} (mA h g^{-1})	Reference
β_{12}-borophene	1984	1312	1984	Current work
χ_3-borophene	1240	939	1240	Current work
Silicence	954	768	954	Ref. 6
V_2C	941	765	941	Ref. 2
MnO_2	616	591	616	Ref. 7
Nb_2C	542	454	542	Ref. 3
Mo_2C	526	462	526	Ref. 8
VS_2	466	415	466	Ref. 9
Graphite	372	339	372	Ref. 10
MoS_2	335	308	335	Ref. 11
Ti_3C_2	319	273	273	Ref. 12
TiS_3	279	260	260	Ref. 13
GeS	256	239	256	Ref. 5

Table S2 Similar with Table S1 but for the comparisons of Na capacities.

	C_M^a (mA h g^{-1})	C_M^b (mA h g^{-1})	C_M^{ref} (mA h g^{-1})	Reference
β_{12}-borophene	1984	733	1984	Current work
χ_3-borophene	1240	601	1240	Current work
Ca_2N	1138	576	1138	Ref. 14
Phosphorene	865	496	865	Ref. 15
GeS	512	355	512	Ref. 5
V_2C	470	344	344	Ref. 12
TiS_2	339	268	339	Ref. 16
Ti_3C_2	319	250	250	Ref. 12
Sr_2N	283	228	283	Ref. 14
Nb_2C	271	223	271	Ref. 3
NbS_2	263	219	263	Ref. 16
Mo_2C	132	118	132	Ref. 8
MoS_2	146	128	146	Ref. 17

III. References

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