Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

S-functionalized 2D V_2B as promising anode materials for rechargeable lithium ion batteries

Yuhang Wang,[a] Ninggui Ma,[a] Yaqin Zhang,[a] Bochun Liang,[a] Jun Zhao,[a] and Jun Fan[a, b,*]

[a] *Department of Materials Science and Engineering, City University of Hong Kong, Hong Kong, China.*

[b] *Center for Advance Nuclear Safety and Sustainable Department, City University of Hong Kong, Hong Kong, China*

*Corresponding author

Email address: junfan@cityu.edu.hk (Jun Fan)

Fig. S1

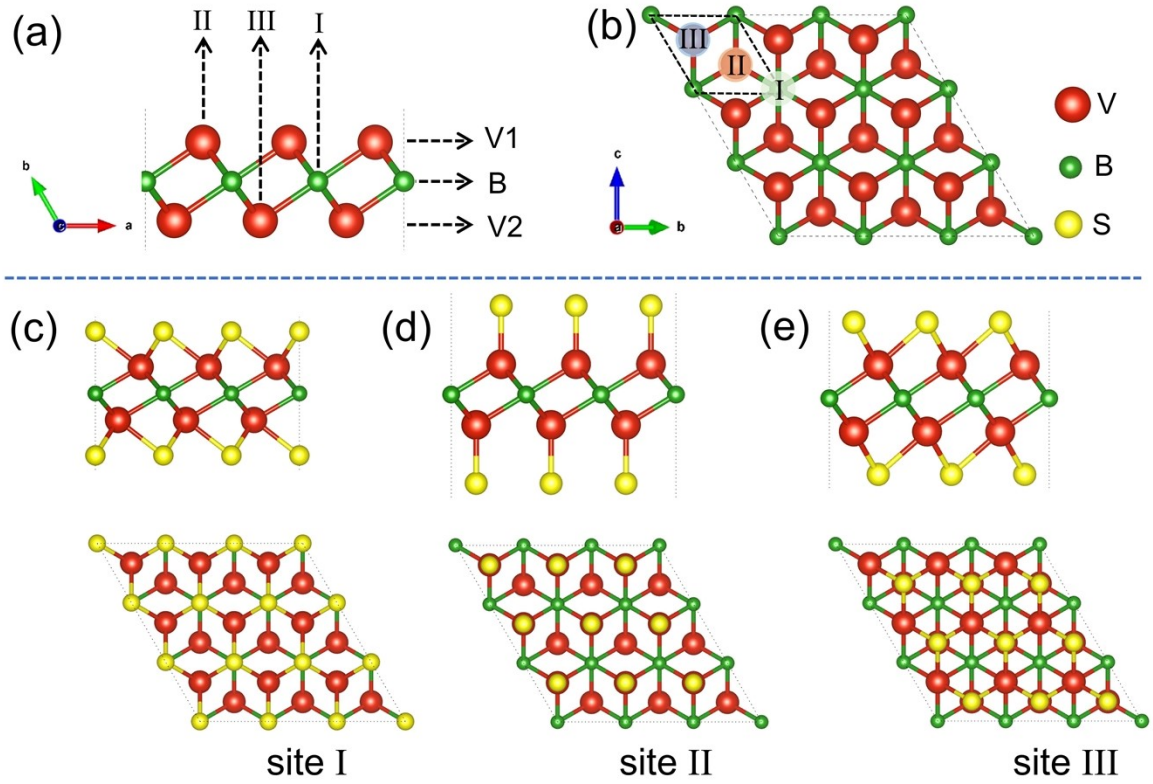

Fig. S1 Top (a) and side (b) view of pristine V_2B. Possible sites for functional atoms are labelled as I (c), II (d), and III (e).

Fig. S2

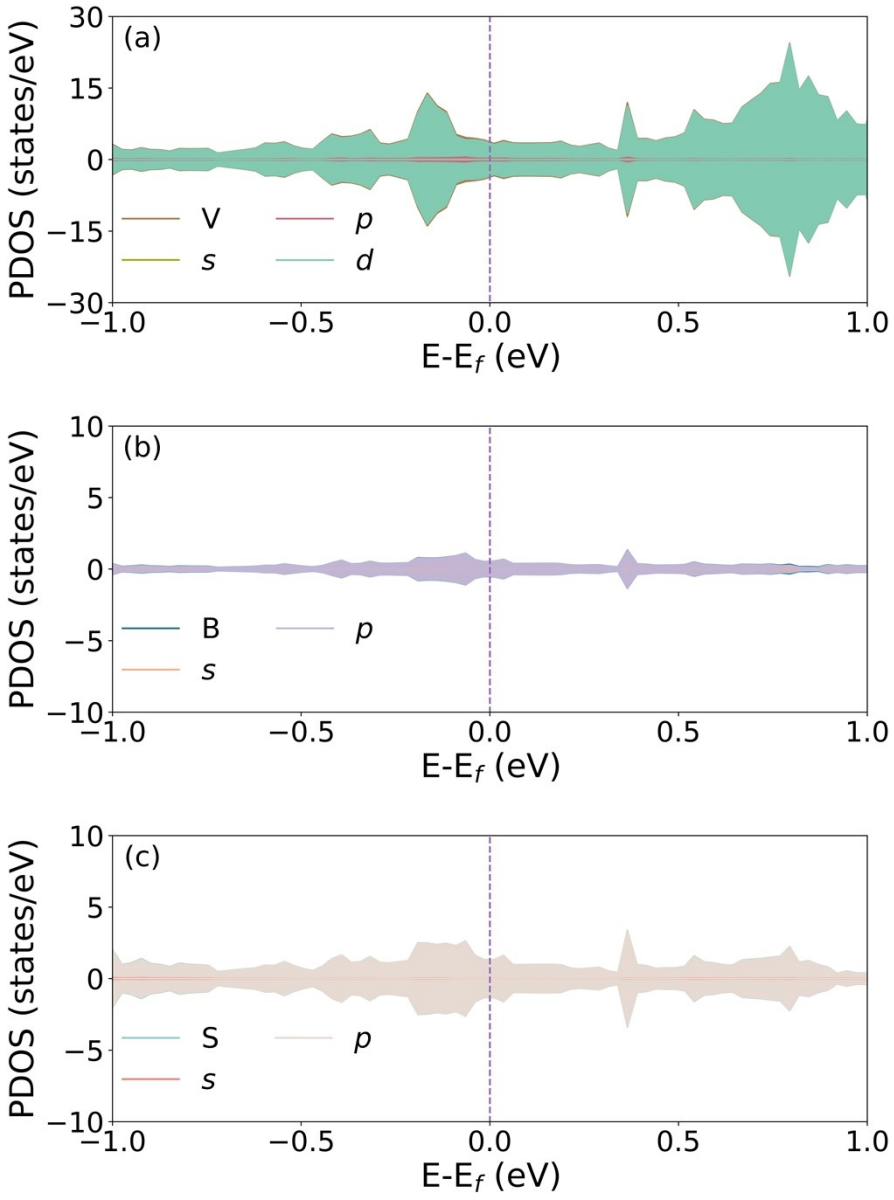

Fig. S2 The partial density of states (PDOS) for V (a), B (b), and S (c) in V_2BS_2.

Fig. S3

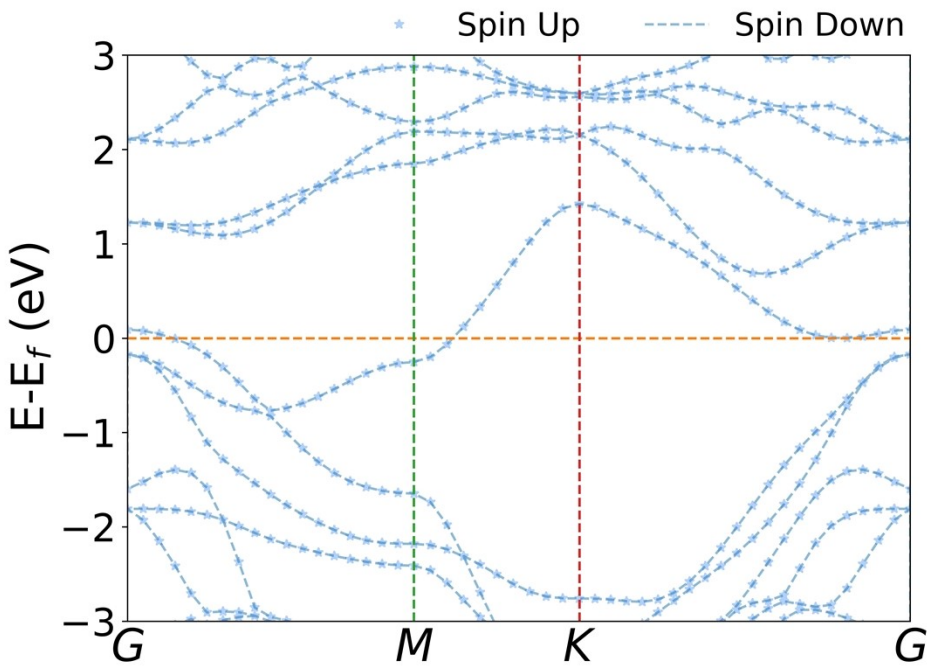

Fig. S3 Band structure of V_2BS_2 using HSE06 functional.

Fig. S4

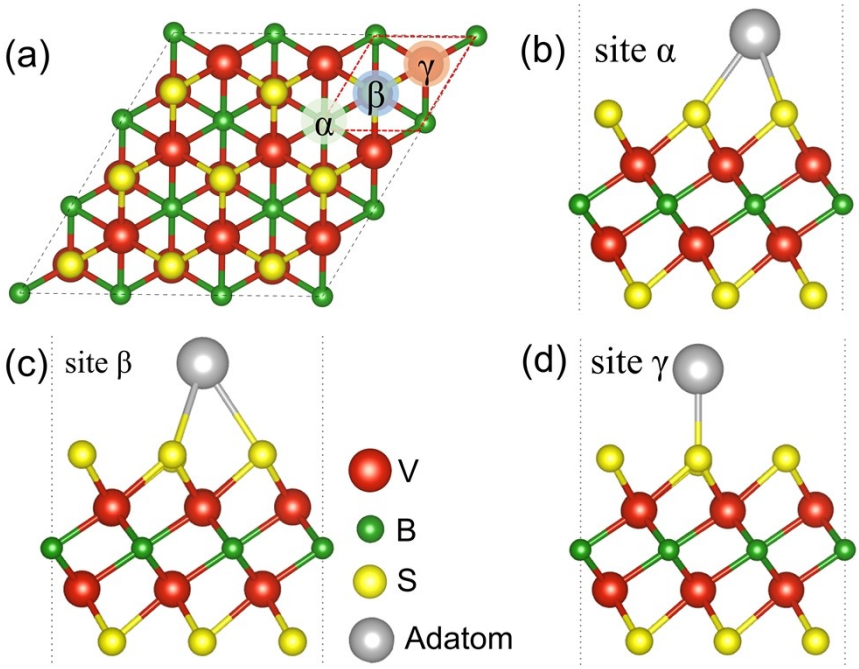

Fig. S4 Top view of possible adsorption sites for metal ions (a), side view for adatom at different sites: (b) on the top of B atom, (c) on the top of V1 atom, (c) on the top of V2 atom.

Fig. S5

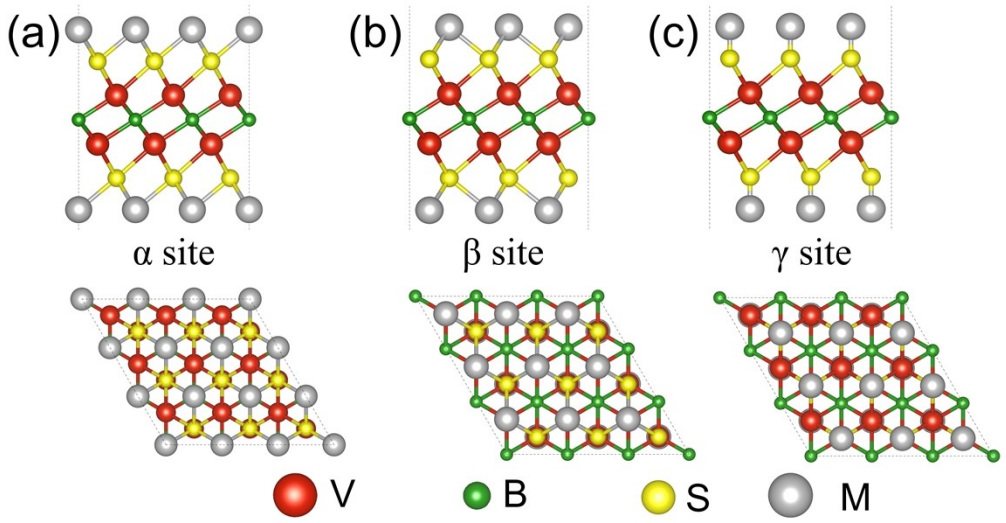

Fig. S5 Adsorption configurations side view and top view for one M layer on V_2BS_2 monolayer: (a) α site, (b) β site, and (c) γ site.

Fig. S6

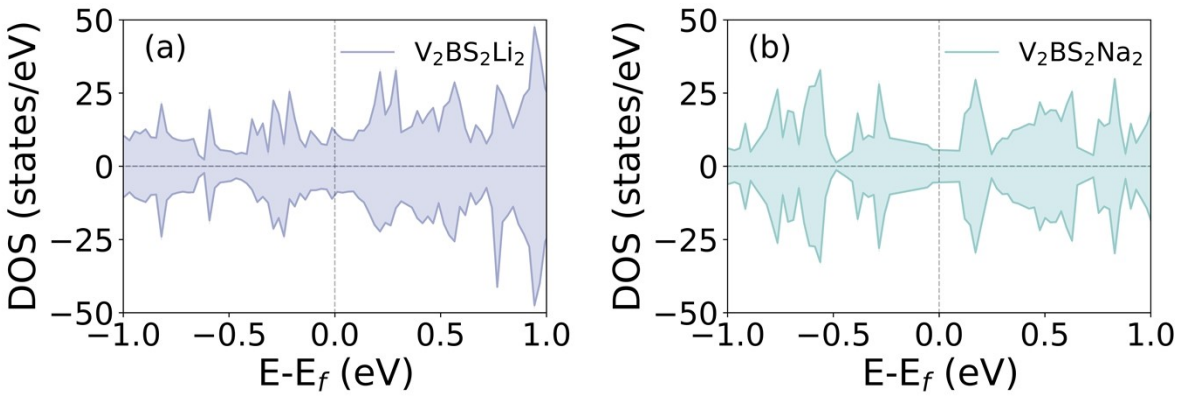

Fig. S6 Density of states (DOS) of stoichiometry of (a) $V_2BS_2Li_2$ and (b) $V_2BS_2Na_2$.

Fig. S7

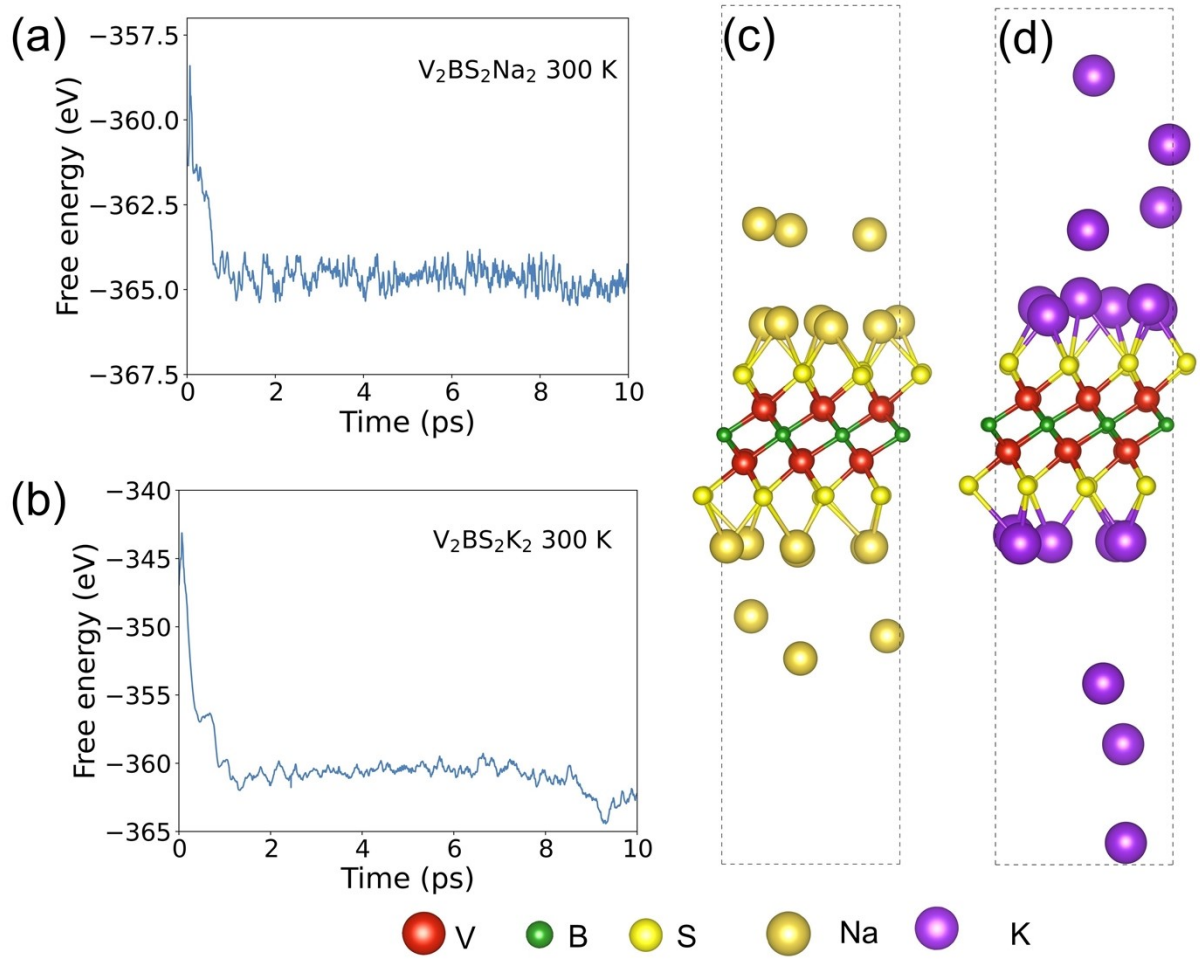

Fig. S7 The variation of the free energy during AIMD simulation at 300 K for stoichiometry of (a) $V_2BS_2Na_2$ and (b) $V_2BS_2K_2$. Side views of (c) $V_2BS_2Na_2$ and (d) $V_2BS_2K_2$ after simulation.

Table S1

Table S1 Comparison of the lattice constant, bond length, layer thickness of V_2BS_2 with other related materials.

	Lattice constant (Å)	**Bond length (V-C/N/B) (Å)**	**Bond length (V-S) (Å)**	**Thickness**	**Ref.**
V_2BS_2	3.05	2.13	2.34	5.47	**This work**
V_2CS_2	3.06	2.08	2.37	5.34	[1]
V_2NS_2	3.09	2.06	2.35	/	[2]
Ti_2NS_2	3.17	2.07	2.39	/	[3]
Ti_2CS_2	3.197	2.211	2.406	/	[4]
Ti_2BS_2	3.50	2.306	2.392	4.78	[5]

Table S2

Table S2 Summary of adsorption energy (unit: eV) for Li, Na, and K at different sites on V_2BS_2.

Adatoms	Adsorption sites	E_{ad}^{1st}	E_{ad}^{2nd}	E_{ad}^{3rd}
Li	α	-0.530	-0.023	0.030
	β	-0.702	0.058	0.035
	γ	-0.166	-0.044	0.132
Na	α	-0.306	0.113	\
	β	-0.327	0.122	\
	γ	-0.099	0.112	\
K	α	0.469	\	\
	β	0.426	\	\
	γ	0.889	\	\

[a] "\" means the corresponding V_2BS_2 can't adsorb full layer of Li/Na/K.

References

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