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

Supporting Information

Strain Engineered Blue P-MoS_2 van der Waals Heterostructure with Improved Lithiation/Sodiation for LIBs and SIBs

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Fig. S1 Schematic views of the charge density difference of single Li (top line) and Na (bottom line) adsorption on unstrained Blue P-MoS_2 heterostructure. Adsorption on the out-surface of MoS_2 (left); Adsorption at the interlayer of Blue P and MoS_2 (middle) and Adsorption on the out-surface of phosphorene (right). The loss of electrons is indicated in pink and gain of electrons is indicated in blue colour.

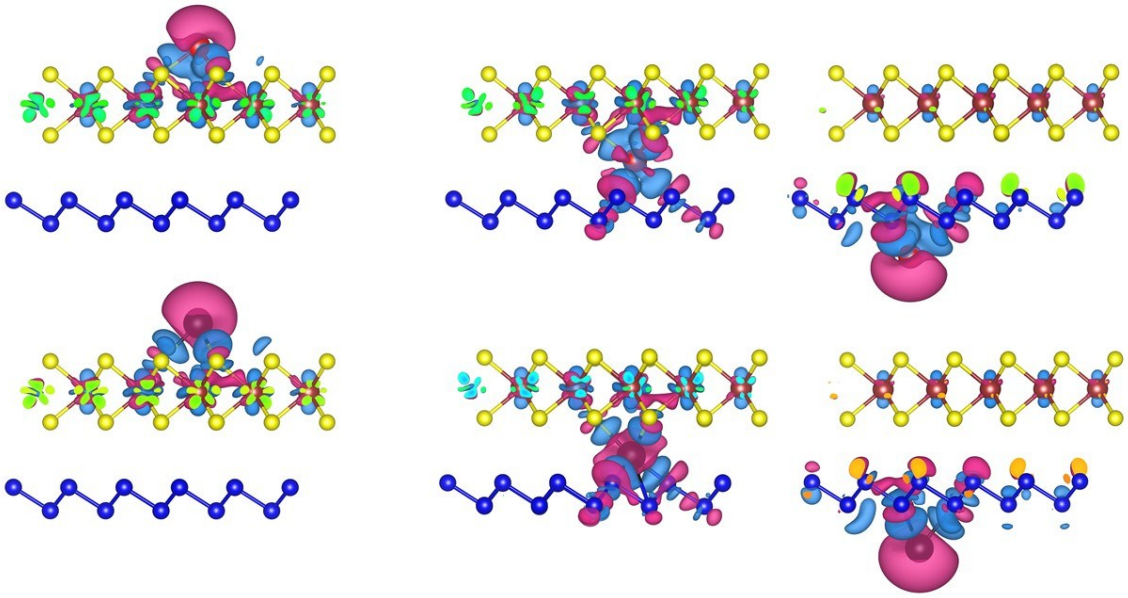

Fig. S2 Schematic views of the charge density difference of single Li (top line) and Na (bottom line) adsorption on Blue P-MoS_2 heterostructure at 10% Tensile strain. Adsorption on the out-surface of MoS_2 (left); Adsorption at the interlayer of Blue P and MoS_2 (middle) and Adsorption on the out-surface of phosphorene (right). The loss of electrons is indicated in pink and gain of electrons is indicated in blue colour.

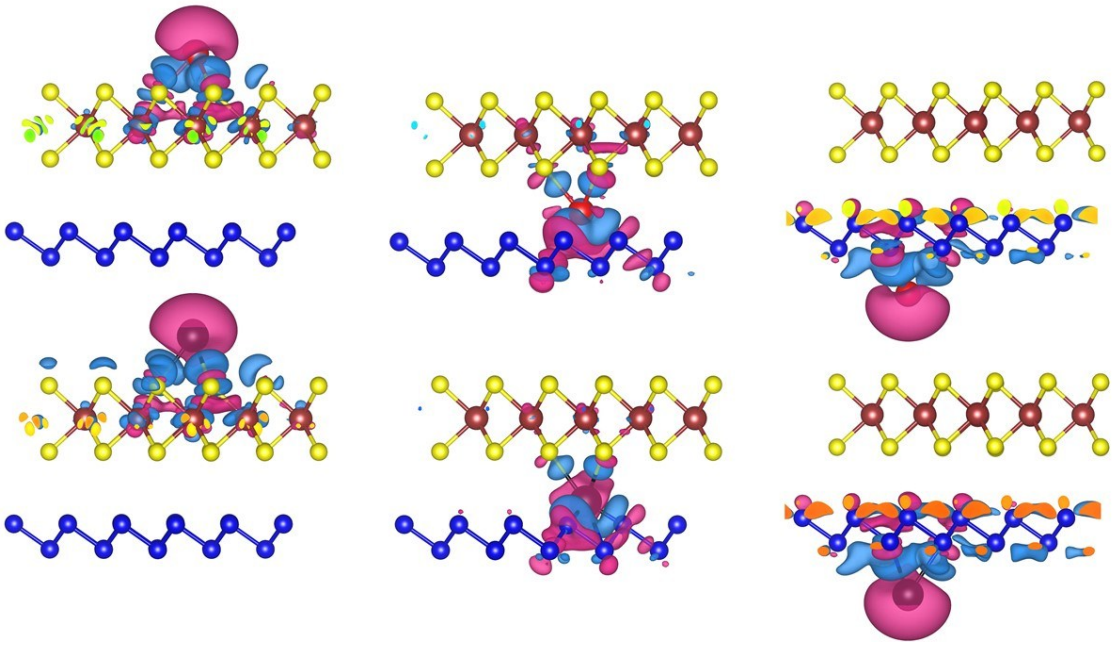

Fig. S3 Schematic views of the charge density difference of single Li (top line) and Na (bottom line) adsorption on Blue P-MoS_2 heterostructure at 10% compressive strain. Adsorption on the out-surface of MoS_2 (left); Adsorption at the interlayer of Blue P and MoS_2 (middle) and Adsorption on the out-surface of phosphorene (right). The loss of electrons is indicated in pink and gain of electrons is indicated in blue colour.

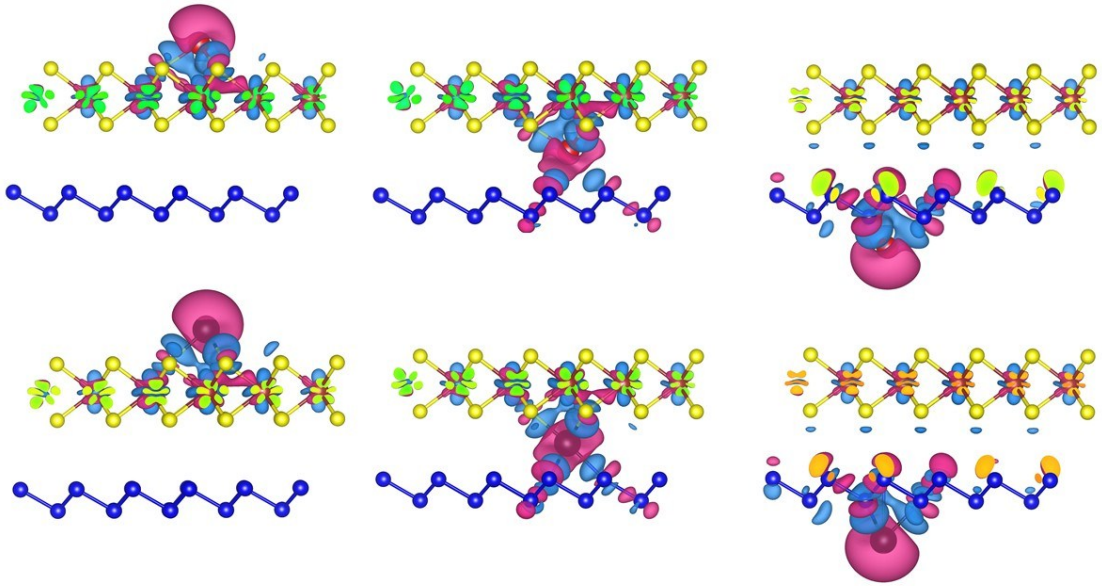

Table S1. Energy difference ΔE_i (meV) and interlayer distance d (Å), between various configurations obtained by subtracting the total energy of most stable configuration in Blue P-MoS_2 vdW heterostructures.

Rotation angle (°)	ΔE_i (meV)	Inter layer distance d (Å)
0	0.00	3.9
60	2.45	3.78
120	32.81	3.45
180	34.85	3.45
240	48.86	3.47
300	20.64	3.77

Table S2. Interatomic distance in unstrained Blue P-MoS_2 van der Waals heterostructure, by the application of 10% compressive strain, 10% tensile strain.

Strain	D_{Mo-Mo}in Å (In-plane)	D_{S-S}in Å (Height)	D_{P-P} in Å (In-plane)	D_{P-P} in Å (Height)	Interlayer distance in Å	Total thickness in Å
Unstrained Blue P-MoS_2	3.28	3.18	2.27	1.25	3.45	7.88
Compressed (10%)	2.95	3.43	2.15	1.32	3.63	8.38
Stretched (10%)	3.60	3.01	2.40	1.20	3.13	7.38

Table S3: Change in structural properties obtained by the application of strain on Blue P-MoS_2 vdW heterostructure.

% of strain	E_{form} in eV	IL distance (Å)	θ_{P-P-P} (°)	D_{P-P} (Å)	θ_{P-P-P} (°)	D_{Mo-S} (Å)
-10	-0.589	3.63	86.31	2.15	75.23	2.41
-8	-0.477	3.65	87.53	2.17	76.76	2.42
-6	-0.371	3.68	88.91	2.20	78.48	2.43
-4	-0.295	3.72	90.20	2.22	80.09	2.45
-2	-0.217	3.74	91.35	2.25	81.54	2.46

0	-0.154	3.45	92.48	2.27	83.01	2.47
2	-0.093	3.39	93.53	2.30	84.33	2.49
4	-0.039	3.34	94.50	2.32	85.60	2.51
6	0.015	3.30	95.47	2.35	86.83	2.53
8	0.053	3.23	96.25	2.38	87.89	2.55
10	0.084	3.16	97.02	2.40	89.07	2.56

Table S4: (a) Strain-induced Li/Na adsorption properties of Blue P-MoS_2 heterostructure when Li/Na adsorption takes place at the interface. Li adsorption energy (E_{ad} (Li)), Na adsorption energy (E_{ad} (Na)), and Bond Lengths between Li-Mo (D_{Li-Mo}), Na-Mo (D_{Na-Mo}), charge transfer from Li, q (|e|) Li and charge transfer from Na, q (|e|) Na.

% of strain	E_{ad} (Li) in eV	D_{Li-Mo} (Å)	q (|e|) Li	E_{ad} (Na) in eV	D_{Na-Mo} (Å)	q (|e|) Na
-10	-2.71	3.62	0.882	-1.69	3.90	0.829
-8	-2.52	3.50	0.881	-1.48	3.83	0.827
-6	-2.42	3.41	0.884	-1.37	3.75	0.822
-4	-2.37	3.33	0.880	-1.32	3.70	0.818
-2	-2.40	3.30	0.882	-1.35	3.65	0.813
0	-2.51	3.26	0.822	-1.46	3.56	0.813
2	-2.70	3.16	0.884	-1.63	3.46	0.810
4	-2.89	3.09	0.883	-1.84	3.42	0.811
6	-3.09	3.04	0.884	-2.03	3.39	0.813
8	-3.25	3.00	0.883	-2.17	3.37	0.815
10	-3.36	2.99	0.883	-2.27	3.35	0.819

Table S4: (b) Strain-induced Li/Na adsorption properties of Blue P-MoS_2 heterostructure when Li/Na adsorption takes place on the surface of MoS_2. Li adsorption energy (E_{ad}(Li)), Na

adsorption energy (E_{ad}(Na)), and Bond Lengths between Li-Mo (D_{Li-Mo}), Na-Mo (D_{Na-Mo}), charge transfer from Li, q (|e|) Li and charge transfer from Na, q (|e|) Na.

% of strain	E_{ad} (Li) in eV	D_{Li-Mo} (Å)	Q (|e|) Li	E_{ad} (Na) in eV	D_{Na-Mo}(Å)	Q (|e|) Na
-10	-2.17	3.38	0.899	-1.31	3.89	0.823
-8	-2.12	3.31	0.896	-1.28	3.87	0.806
-6	-2.09	3.27	0.896	-1.27	3.84	0.791
-4	-2.09	3.23	0.896	-1.29	3.80	0.782
-2	-2.12	3.16	0.895	-1.33	3.76	0.778
0	-2.28	3.09	0.899	-1.42	3.60	0.857
2	-2.54	3.04	0.898	-1.69	3.55	0.870
4	-2.79	3.02	0.899	-1.96	3.51	0.866
6	-3.03	3.00	0.900	-2.21	3.49	0.867
8	-3.21	2.97	0.899	-2.40	3.47	0.868
10	-3.34	2.98	0.902	-2.54	3.44	0.867

Table S4: (c) Strain-induced Li/Na adsorption properties of Blue P-MoS_2 heterostructure when Li/Na adsorption takes place on the surface of Blue P. Li adsorption energy (E_{ad} (Li)), Na adsorption energy (E_{ad} (Na)), and Bond Lengths between Li-P (D_{Li-P}), Na-P (D_{Na-P}), charge transfer from Li, q (|e|) Li and charge transfer from Na, q (|e|) Na.

% of strain	E_{ad} (Li) in eV	D_{Li-P} (Å)	q (|e|) Li	E_{ad} (Na) in eV	D_{Na-P} (Å)	q (|e|) Na
-10	-2.05	3.44	0.896	-1.10	3.70	0.843
-8	-1.89	3.33	0.896	-1.09	3.70	0.843
-6	-1.79	3.25	0.897	-1.06	3.64	0.836
-4	-1.75	3.18	0.895	-1.03	3.61	0.807

-2	-1.77	3.13	0.891	-1.05	3.58	0.789
0	-1.82	3.14	0.895	-1.14	3.56	0.794
2	-1.95	3.10	0.895	-1.26	3.52	0.802
4	-2.10	3.05	0.892	-1.42	3.49	0.806
6	-2.27	3.00	0.895	-1.59	3.47	0.813
8	-2.42	2.95	0.892	-1.75	3.44	0.816
10	-2.56	2.95	0.894	-1.90	3.41	0.820