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Supporting Information

Insight into the potential of M–NbS_2 (M = Pd, Ti and V) monolayer as anode materials for alkali ion (Li/Na/K) batteries

Meixia Xiao,*[a] Shuling Xu,[b] Haiyang Song,[a] Zhifei Sun,[c] Jiaying Bi[a] and Beibei Xiao[d]

[a]College of New Energy, Xi'an Shiyou University, Xi'an 710065, China.

[b]School of Materials Science and Engineering, Xi'an Shiyou University, Xi'an 710065, China.

[c]Oil Production Plant No. 11, PetroChina Changqing Oil feld Company, Xi'an 710016, China.

[d]College of Energy and Power Engineering, Jiangsu University of Science and Technology, Zhenjiang 212003, China.

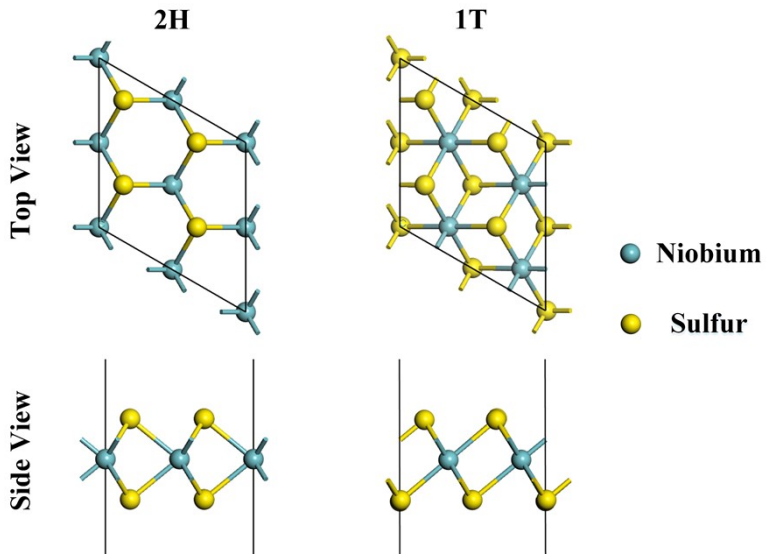

Fig. S1. Ball-and-stick representations of the 2H and 1T phases of NbS_2.

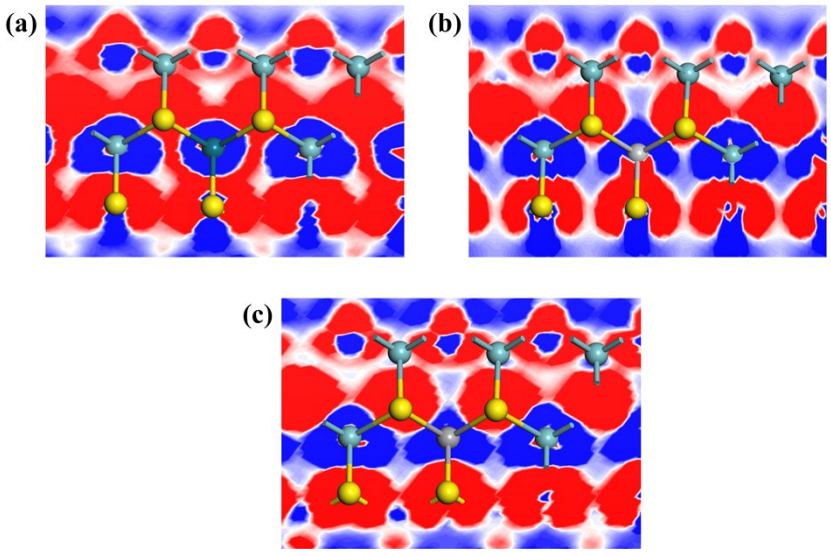

Fig. S2. The charge density difference of (a) Pd-NbS_2, (b) Ti-NbS_2 and (c) V-NbS_2 monolayers. The red- and blue-colored regions indicate the electron accumulation and loss, respectively.

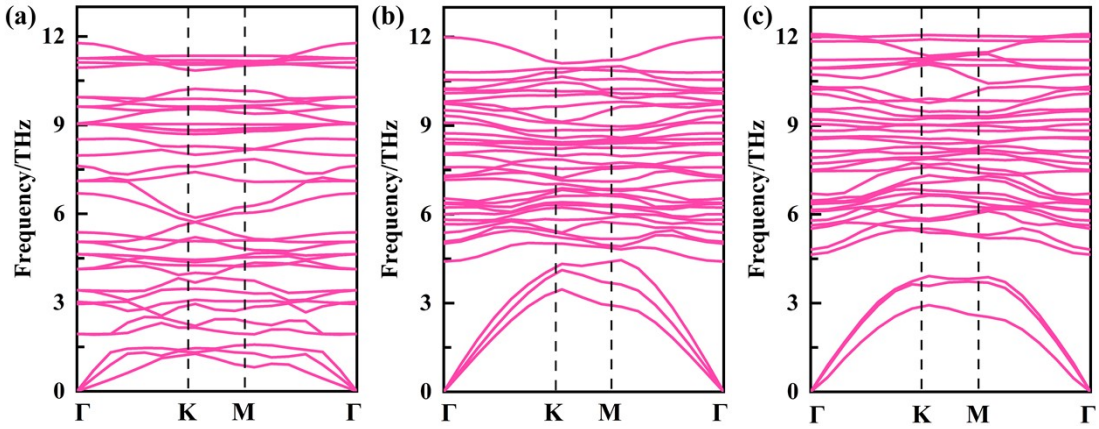

Fig. S3. The Phonon spectrums of (a) Pd-NbS_2, (b) Ti-NbS_2 and (c) V-NbS_2 monolayers.

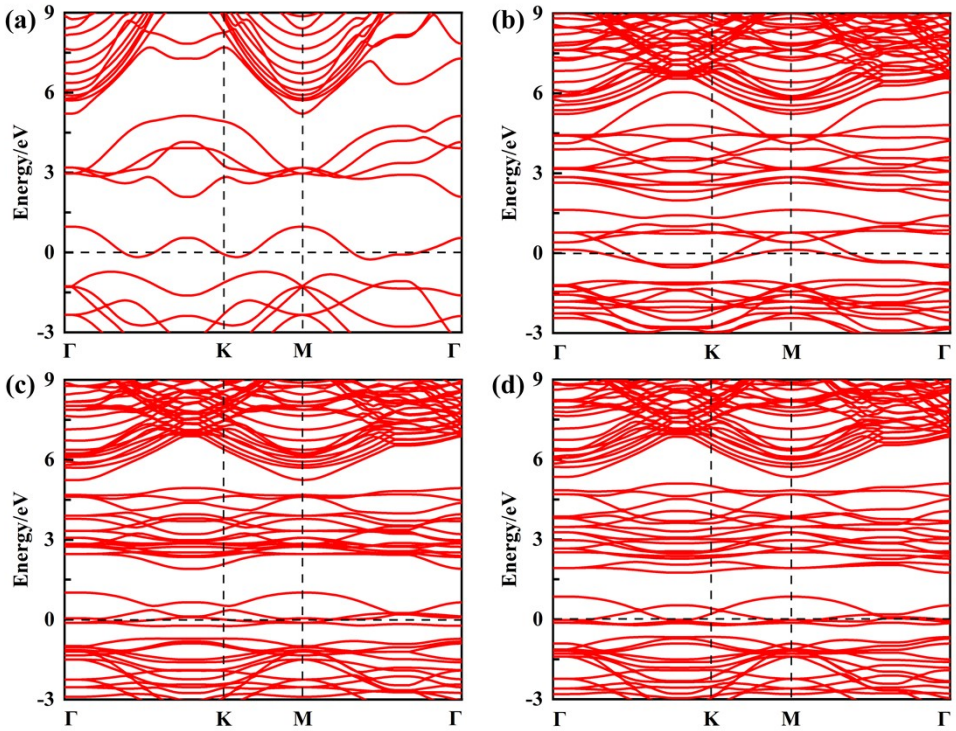

Fig. S4. Electronic band structures of (a) pristine-NbS_2, (b) Pd-NbS_2, (c) Ti-NbS_2 and (d) V-NbS_2 monolayers, where the Fermi energy is set to 0 eV.

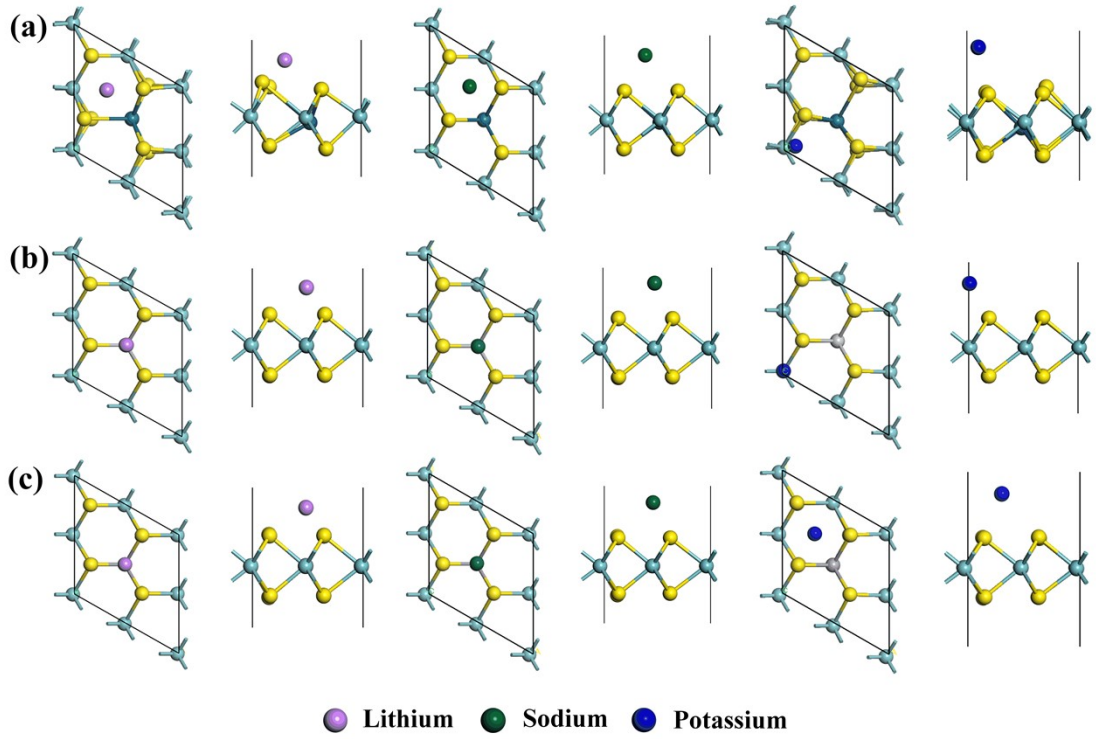

Fig. S5. Main and side views of alkali ion migration from the "T_S" site to the hollow, "T_{Ti}", "T_V", or "T_{Nb}" sites on (a) Pd-NbS_2, (b) Ti-NbS_2 and (c) V-NbS_2 monolayers.

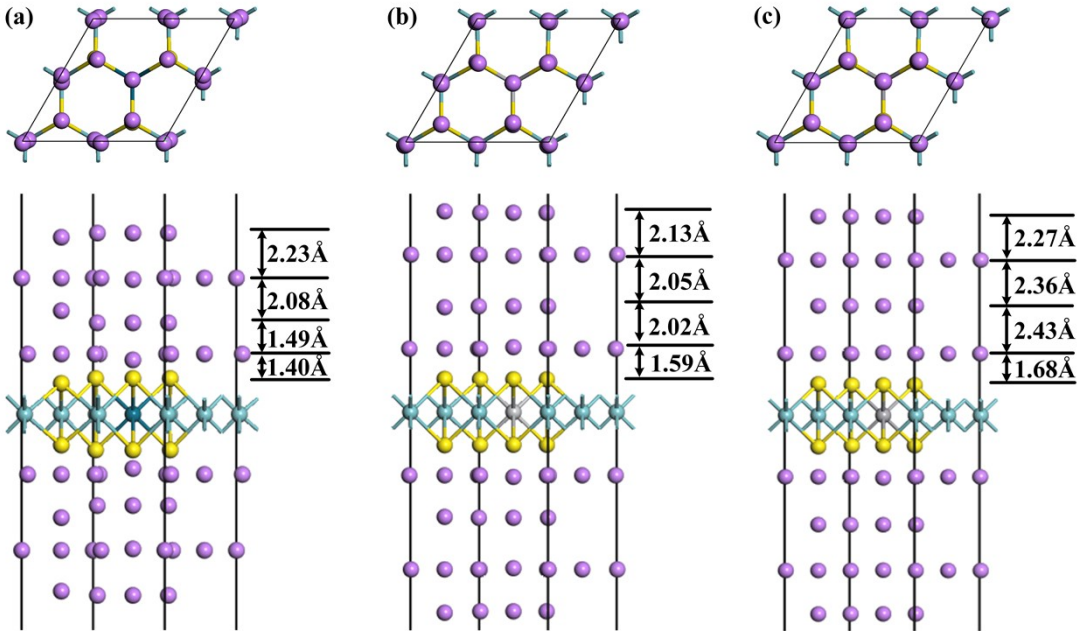

Fig. S6. Top and side views of (a) Pd-NbS_2, (b) Ti-NbS_2 and (c) V-NbS_2 monolayers with Li-ions multi-layer adsorption.

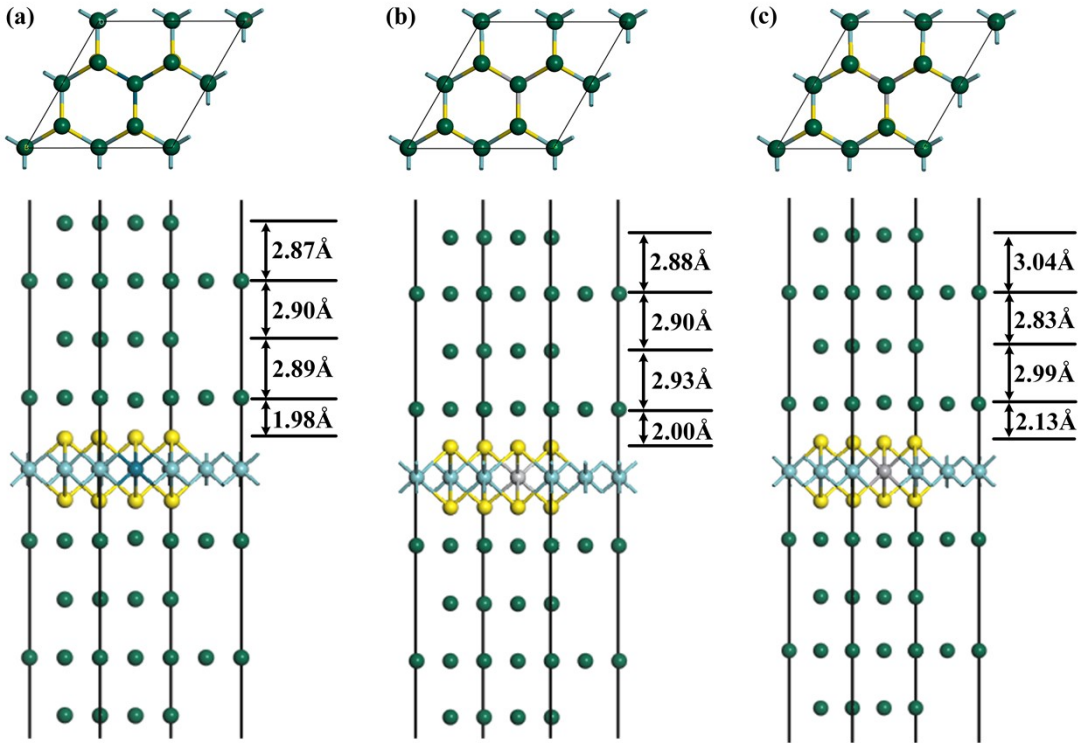

Fig. S7. Top and side views of (a) Pd-NbS_2, (b) Ti-NbS_2 and (c) V-NbS_2 monolayers with Na-ions multi-layer adsorption.

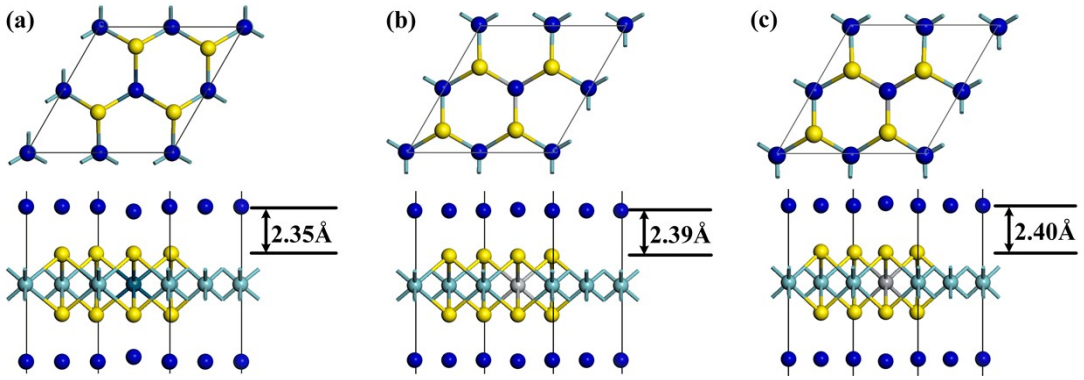

Fig. S8. Top and side views of (a) Pd-NbS_2, (b) Ti-NbS_2 and (c) V-NbS_2 monolayers with K-ions monolayer adsorption.

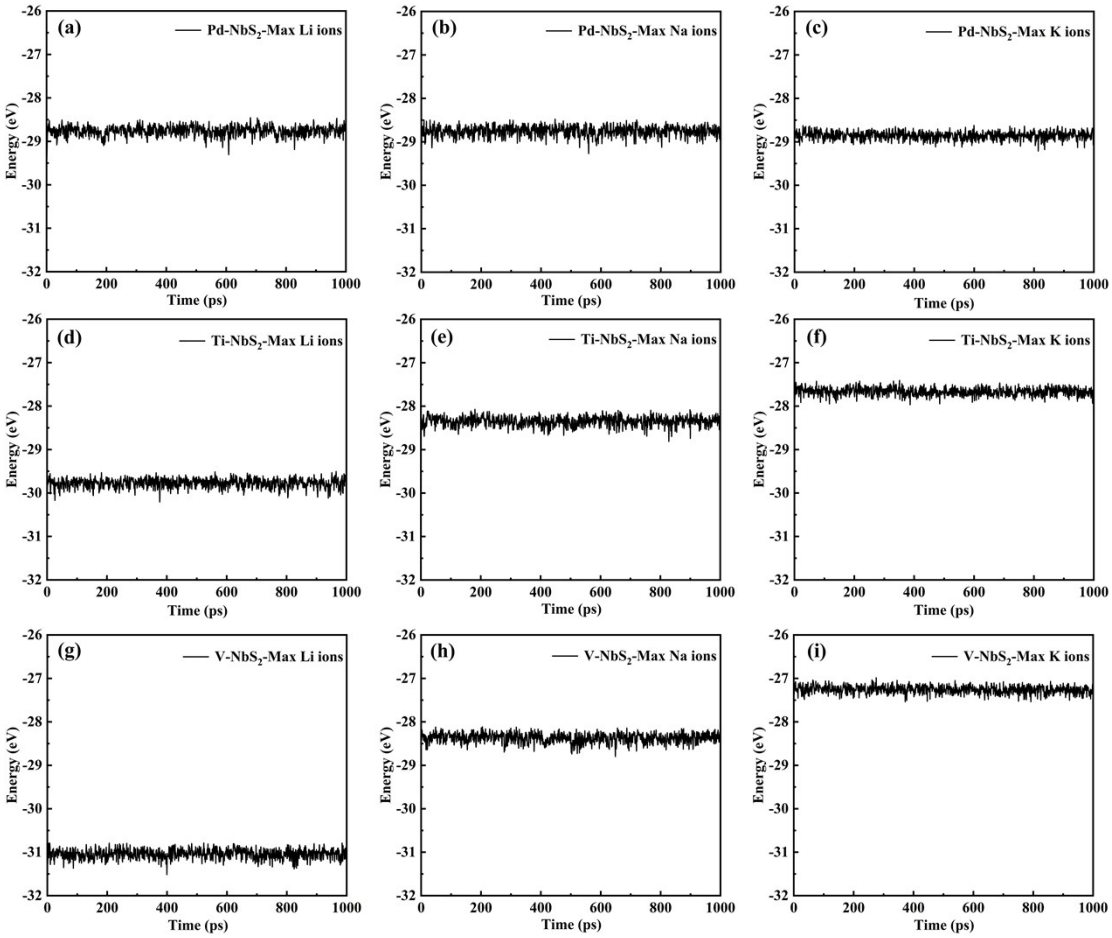

Fig. S9. Total energy evolution as a function of times over 1000 ps at 300 K for (a-c) Pd-NbS_2, (d-f) Ti-NbS_2, and (g-i) V-NbS_2 monolayers with the maximum Li/Na/K adsorption.

Table S1. Calculated diffusion barrier (ΔE_a) and the reaction energy (ΔE_r) in eV of Li, Na and K diffusion on pristine NbS_2 and M-NbS_2 monolayers.

	Diffusion	Li diffusion		Na diffusion		K diffusion	
	pathways	ΔE_a	ΔE_r	ΔE_a	ΔE_r	ΔE_a	ΔE_r
pristine NbS_2	$T_{Nb} \rightarrow H$	0.26	0.07	0.15	0.01	0.09	-0.01
	$H \rightarrow T_{Nb}$	0.19	-0.07	0.14	-0.01	0.10	0.01
Pd-NbS_2	$T_{Nb} \rightarrow H$	0.23	0.18	0.15	0.01	0.12	0.02
	$H \rightarrow T_{Nb}$	0.06	-0.18	0.14	-0.01	0.10	-0.02
	$H \rightarrow T_{Pd}$	0.00	-0.08	0.14	0.02	0.13	-0.01
	$T_{Pd} \rightarrow H$	0.04	0.08	0.12	-0.02	0.13	0.01
Ti-NbS_2	$T_{Nb} \rightarrow H$	0.27	0.09	0.16	0.03	0.10	0.01
	$H \rightarrow T_{Nb}$	0.18	-0.09	0.13	-0.03	0.09	-0.01
	$H \rightarrow T_{Ti}$	0.20	-0.06	0.15	0.01	0.12	0.03
	$T_{Ti} \rightarrow H$	0.26	0.06	0.15	-0.01	0.09	-0.03
V-NbS_2	$T_{Nb} \rightarrow H$	0.26	0.09	0.16	0.03	0.11	0.01
	$H \rightarrow T_{Nb}$	0.17	-0.09	0.13	-0.03	0.09	-0.01
	$H \rightarrow T_V$	0.19	-0.08	0.15	0.01	0.11	0.02
	$T_V \rightarrow H$	0.27	0.08	0.14	-0.01	0.08	-0.02

Table S2. Calculated diffusion constants (cm^2/s) of Li, Na and K ions on pristine-NbS_2 and M-NbS_2 monolayers.

	pristine-NbS_2	Pd-NbS_2	Ti-NbS_2	V-NbS_2
Li diffusion	4.87×10^{-7}	1.45×10^{-6}	3.60×10^{-7}	4.84×10^{-7}
Na diffusion	4.60×10^{-5}	7.69×10^{-5}	3.28×10^{-5}	2.77×10^{-5}
K diffusion	5.66×10^{-4}	3.98×10^{-4}	4.93×10^{-4}	3.14×10^{-4}

Table S3. The average open circuit voltage (OCV), adsorption energies E_{1st}, E_{2nd}, E_{3rd} and E_{4th}, and the maximum theoretical capacity C_m of M-NbS_2 monolayers with multilayer alkali ions adsorption.

Structure	Ion battery	OCV (V)	E_{1st} (eV)	E_{2nd} (eV)	E_{3rd} (eV)	E_{4th} (eV)	C_m (mAh·g^{-1})
Pd-NbS_2	Li	0.17	-2.74	-1.74	-1.73	-1.73	1336.69
	Na	0.45	-1.92	-1.41	-1.37	-1.36	1336.69
	K	0.94	-1.69	\	\	\	334.17
Ti-NbS_2	Li	0.23	-2.83	-1.85	-1.75	-1.75	1470.87
	Na	0.50	-2.14	-1.40	-1.40	-1.34	1470.87
	K	0.95	-1.68	\	\	\	367.72
V-NbS_2	Li	0.22	-2.73	-1.87	-1.78	-1.76	1463.16
	Na	0.50	-2.11	-1.41	-1.37	-1.36	1463.16
	K	0.99	-1.64	\	\	\	365.79

Table S4. The change rate of the lattice constants (Δa) for M-NbS_2 monolayers with maximum alkali ions adsorption.

Structure	Pd-NbS_2			Ti-NbS_2			V-NbS_2		
battery	Li	Na	K	Li	Na	K	Li	Na	K
a (Å)	6.631	6.631	6.631	6.697	6.697	6.697	6.640	6.640	6.640
Δa (%)	3.474	5.469	8.844	1.472	3.254	5.797	2.023	3.378	5.675

Pd-NbS_2 CIF

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Nb1	S11	2.467	1_445	S
Nb1	S8	2.512	1_545	S
S2	Pd10	2.549	.	S
S2	Nb7	2.467	.	S
S3	Pd10	2.549	.	S
S3	Nb7	2.467	.	S
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Nb4	S9	2.512	1_545	S
Nb4	S12	2.467	1_545	S
Nb4	S5	2.467	.	S
Nb4	S8	2.512	1_545	S
Nb4	S11	2.467	1_545	S
S5	Nb7	2.467	1_655	S
S5	Pd10	2.549	.	S
S6	Nb7	2.467	1_655	S
S6	Pd10	2.549	.	S
Nb7	S9	2.512	.	S
Nb7	S6	2.467	1_455	S
Nb7	S8	2.512	.	S
Nb7	S5	2.467	1_455	S
S8	Nb4	2.512	1_565	S
S8	Nb1	2.512	1_565	S
S9	Nb4	2.512	1_565	S
S9	Nb1	2.512	1_565	S
Pd10	S12	2.549	.	S
Pd10	S11	2.549	.	S
S11	Nb1	2.467	1_665	S
S11	Nb4	2.467	1_565	S
S12	Nb1	2.467	1_665	S
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Ti-NbS_2 CIF

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S6    S    0.66456    0.33544   0.54199   0.00000   Uiso   1.00
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Nb1	S11	2.487	1_445	S
Nb1	S8	2.509	1_545	S
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S2	Nb7	2.487	.	S
S3	Ti10	2.471	.	S
S3	Nb7	2.487	.	S
Nb4	S6	2.487	.	S
Nb4	S9	2.509	1_545	S
Nb4	S12	2.487	1_545	S
Nb4	S5	2.487	.	S
Nb4	S8	2.509	1_545	S
Nb4	S11	2.487	1_545	S
S5	Nb7	2.487	1_655	S
S5	Ti10	2.471	.	S
S6	Nb7	2.487	1_655	S
S6	Ti10	2.471	.	S
Nb7	S9	2.509	.	S
Nb7	S6	2.487	1_455	S
Nb7	S8	2.509	.	S
Nb7	S5	2.487	1_455	S
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Ti10	S12	2.471	.	S
Ti10	S11	2.471	.	S
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S11	Nb4	2.487	1_565	S
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Nb1	S11	2.486	1_445	S
Nb1	S8	2.490	1_545	S
S2	V10	2.425	.	S
S2	Nb7	2.486	.	S
S3	V10	2.425	.	S
S3	Nb7	2.486	.	S
Nb4	S6	2.486	.	S
Nb4	S9	2.490	1_545	S
Nb4	S12	2.486	1_545	S
Nb4	S5	2.486	.	S
Nb4	S8	2.490	1_545	S
Nb4	S11	2.486	1_545	S
S5	Nb7	2.486	1_655	S
S5	V10	2.425	.	S
S6	Nb7	2.486	1_655	S
S6	V10	2.425	.	S
Nb7	S9	2.490	.	S
Nb7	S6	2.486	1_455	S
Nb7	S8	2.490	.	S
Nb7	S5	2.486	1_455	S
S8	Nb4	2.490	1_565	S
S8	Nb1	2.490	1_565	S
S9	Nb4	2.490	1_565	S
S9	Nb1	2.490	1_565	S
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S11	Nb4	2.486	1_565	S
S12	Nb1	2.486	1_665	S
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