Supporting information for:

Potential Applications of MoS_2/M_2CS_2 (M=Ti, V) Heterostructures as Anode Materials for Metal-Ion Batteries

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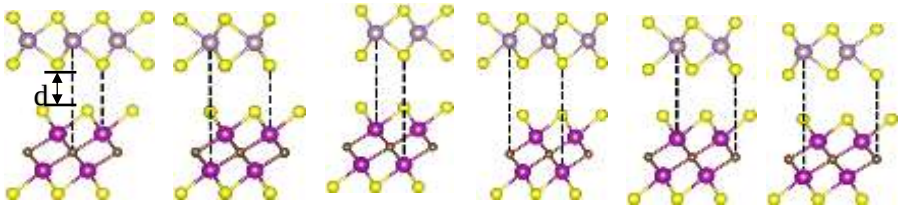
Table S1. Side views, binding energies E_b (eV) and interlayer distance d (Å) of six stacking patterns of MoS_2/M_2CS_2 (M=Ti, V) heterostructures.

System	Pattern					
Mo S C M (Ti, V)						
	Type-1	Type-2	Type-3	Type-4	Type-5	Type-6
E_{b-MoS_2/Ti_2CS_2}	-0.606	-0.607	-0.396	-0.402	-0.609	-0.640
d_{-MoS_2/Ti_2CS_2}	3.002	3.073	3.605	3.604	2.975	3.041
E_{b-MoS_2/V_2CS_2}	-0.173	-0.188	0.042	0.033	-0.127	-0.184
d_{-MoS_2/V_2CS_2}	3.094	3.080	3.656	3.654	3.131	3.080

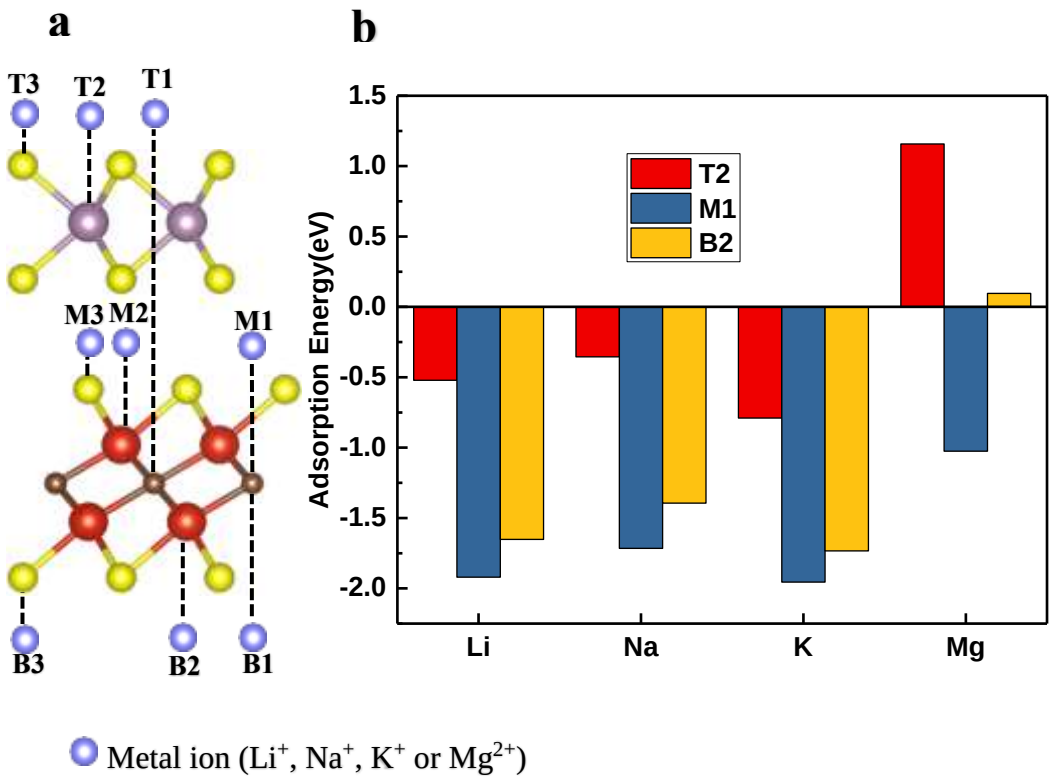


Figure S1. (a) Side view of active adsorption sites of metal ions in MoS_2/V_2CS_2. (b) The most favorable sites and corresponding energies on the surfaces or at the interface in MoS_2/V_2CS_2 for a single ion adsorption.

Table S2. The adsorption energy E_{ad} (eV) of a metal ion at 9 sites (T represents on the top surface, M represent at the interface, B represent on the bottom surface) in MoS_2/M_2CS_2 (M=Ti, V). The # represents that the structure deforms after adsorbing a metal ion or a metal ion moves to adjacent position after optimization of system.

System		E_{ad}								
		T1	T2	T3	M1	M2	M3	B1	B2	B3
MoS_2/Ti_2CS_2	Li	**-0.486**	**-0.686**	#	**-2.159**	**-2.415**	**-1.656**	**-2.148**	**-2.191**	#
	Na	**-0.453**	**-0.502**	**0.039**	**-2.013**	**-2.069**	#	**-1.930**	**-1.933**	#
	K	**-0.884**	**-0.912**	**-0.568**	**-2.300**	**-2.325**	#	**-2.295**	**-2.278**	#
	Mg	**1.075**	**1.052**	**1.464**	**-1.726**	**-1.993**	#	**-0.988**	**-0.954**	#
MoS_2/V_2CS_2	Li	**-0.330**	**-0.521**	**0.404**	**-1.920**	**-1.804**	**-1.401**	**-1.499**	**-1.652**	**-0.602**
	Na	**-0.322**	**-0.355**	**0.097**	**-1.715**	**-1.531**	**-1.310**	**-1.357**	**-1.394**	**-0.716**
	K	**-0.763**	**-0.790**	**-0.497**	**-1.955**	#	#	**-1.709**	**-1.733**	**-1.295**
	Mg	**1.190**	**1.157**	**1.517**	**-1.025**	#	**-0.247**	**0.161**	**0.096**	**0.978**

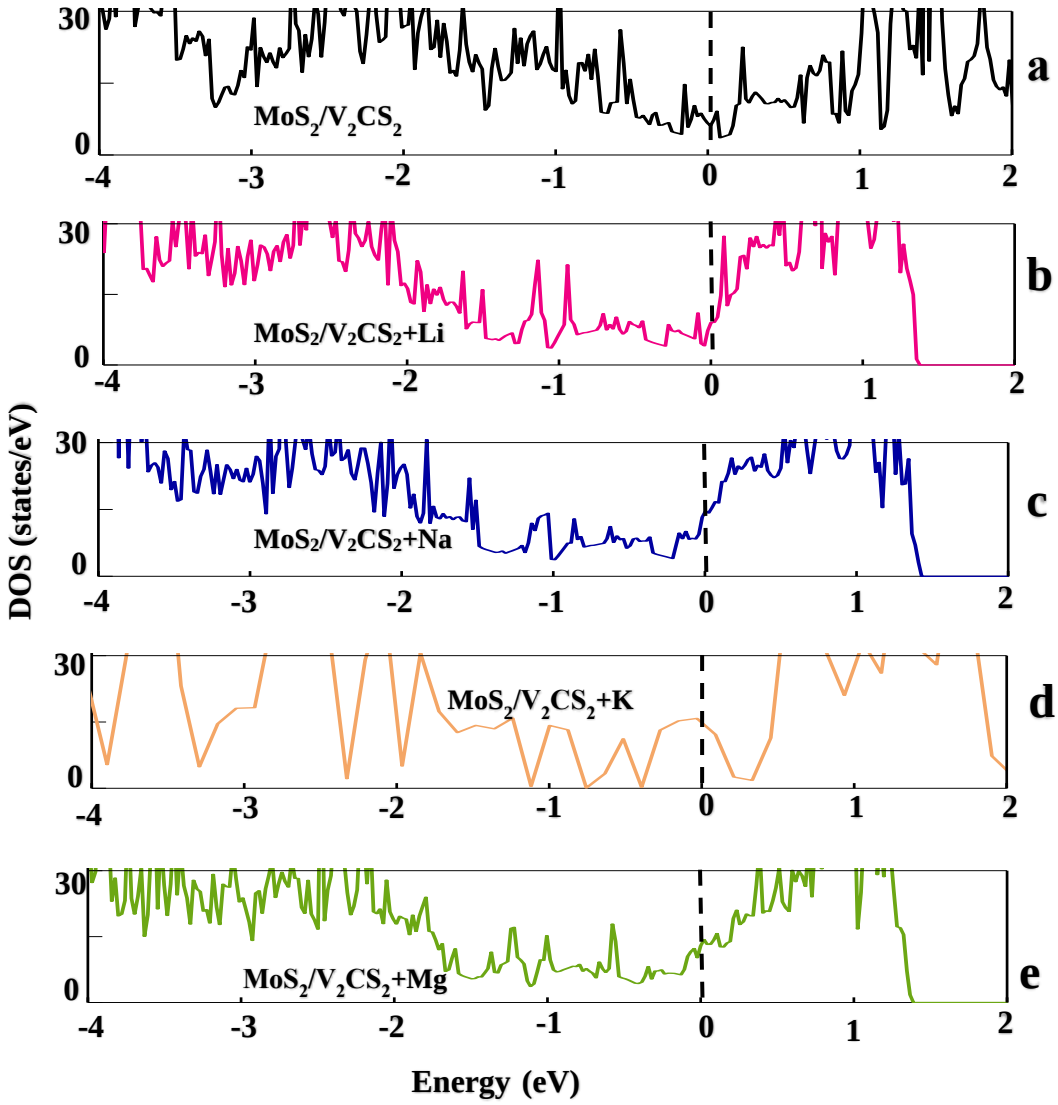


Figure S2. Total DOS of (a) pristine MoS_2/V_2CS_2 and the MoS_2/V_2CS_2 with a metal atom adsorption of (b) Li-ion, (c) Na-ion, (d) K-ion or (e) Mg-ion. The Fermi levels are set to zero and are indicated by black dashed lines.

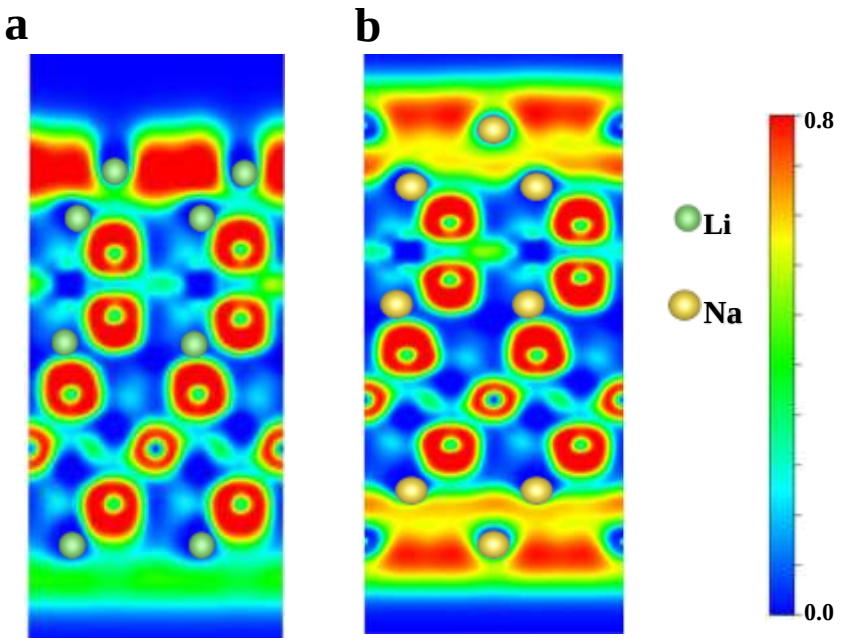


Figure S3. The ELF plots of the (110) slices for a MoS_2/V_2CS_2 with four layers of (a) Li and five layers of (b) Na adatoms.

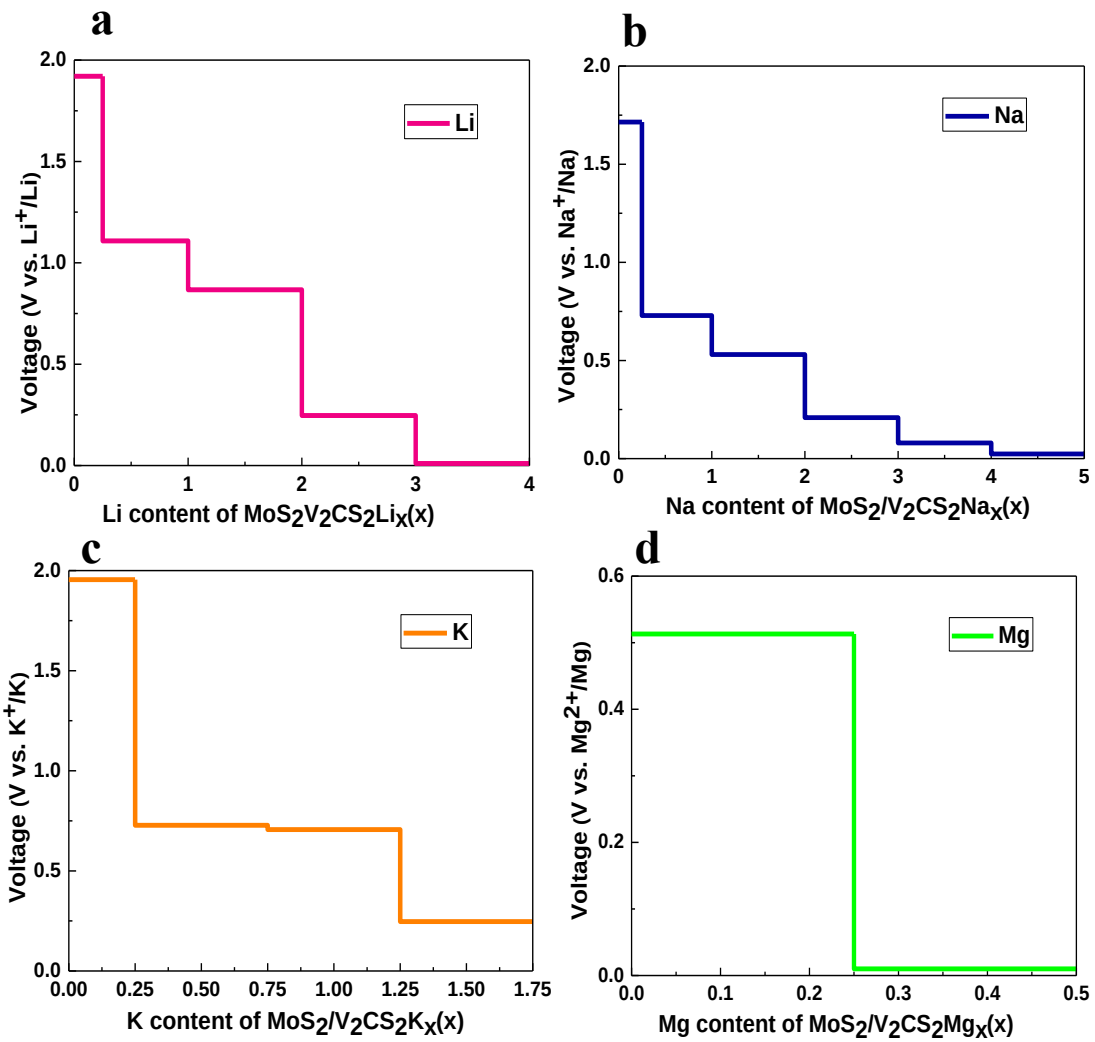


Figure S4. The voltage profiles of MoS_2/V_2CS_2 as a function of concentration of (a) Li-ion, (b) Na-ion, (c) K-ion and (d) Mg-ion.

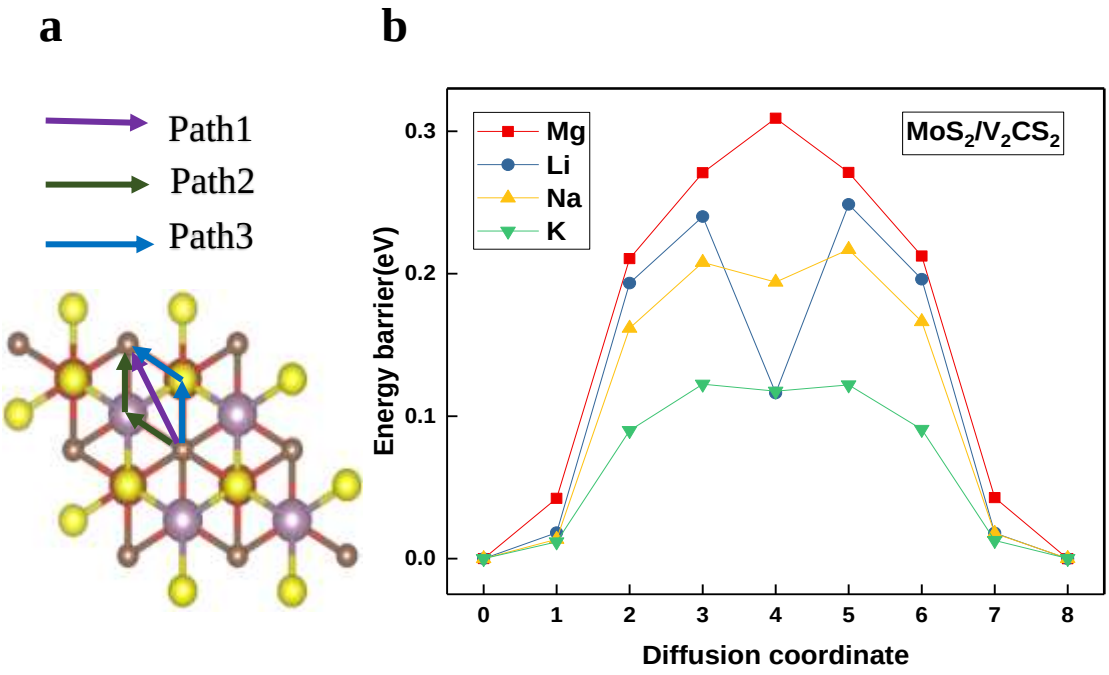


Figure S5. (a) Top view of three diffusion paths of metal ions between adjacent M1 sites in MoS_2/V_2CS_2. (b) Diffusion barrier profiles of MoS_2/V_2CS_2 for Mg/Li/Na/K ions along path 3.