Supporting Information

Theoretical investigate of Janus Ti_2BST (T = O, Se) monolayers as anode materials for Na/K-ion batteries

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Table S1 The relative energies per unit cell for different configurations in eV of Ti_2BSO and Ti_2BSSe monolayers.

MBene	I	II	III	IV
Ti_2BSO	0	0.209	0.621	0.232
Ti_2BSSe	0	0.536	0.440	0.132

Table S2 The calculated lattice constant a_0 (Å), bond length l (Å), and Bader charge ΔQ (e) transferred from Ti to S (T) atom of Ti_2BSO and Ti_2BSSe monolayers.

Ti_2BOT	a_0	$l_{Ti\text{-}S}$	$l_{Ti\text{-}T}$	ΔQ_S	ΔQ_T
Ti_2BSO	3.130	2.384	1.998	0.418	1.207
Ti_2BSSe	3.259	2.380	2.541	0.542	0.314

Table S3 The calculated elastic constants C_{ij} (N m^{-1}) and Young's modulus Y (N m^{-1}) of Ti_2BSO and Ti_2BSSe monolayers.

Ti_2BOT	$C_{11}=C_{22}$	C_{12}	C_{66}	Y
Ti_2BSO	132.21	26.88	52.66	126.74
Ti_2BSSe	135.99	19.13	58.43	133.29

Table S4 Diffusion constants (D) of Na and K on two surfaces of Ti_2BSO and Ti_2BSSe monolayers.

Surface	D_{Na} (cm^2 s^{-1})	D_K (cm^2 s^{-1})
Ti_2BSO-S	2.028×10^{-4}	2.889×10^{-3}
Ti_2BSO-O	8.569×10^{-7}	7.048×10^{-5}
Ti_2BSSe-S	1.169×10^{-4}	7.778×10^{-4}
Ti_2BSSe-Se	1.933×10^{-4}	1.237×10^{-3}

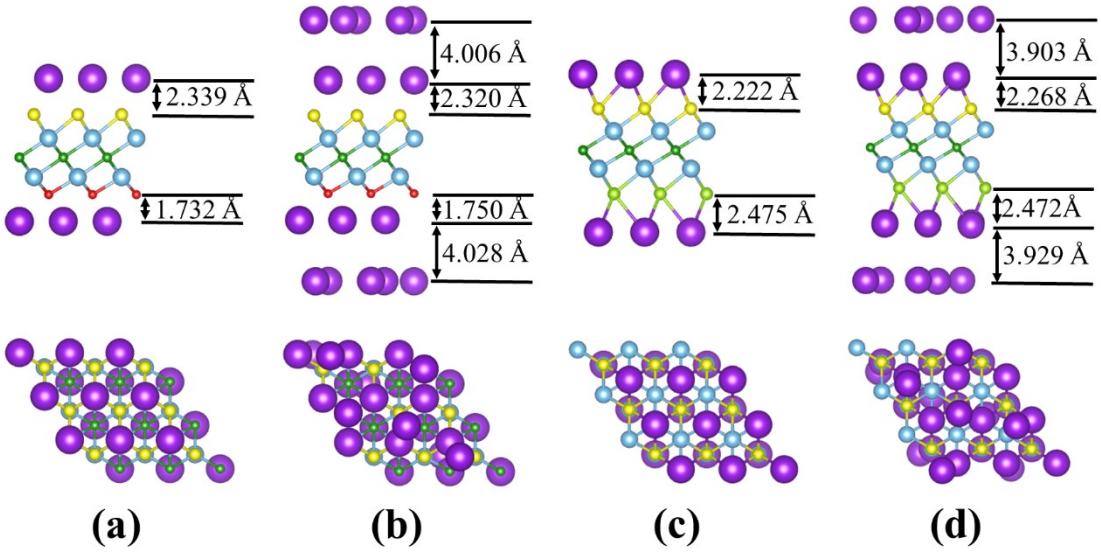

Fig. S1 Side and top views of K adsorbed (a)-(b) Ti_2BSO and (c)-(d) Ti_2BSSe monolayers.

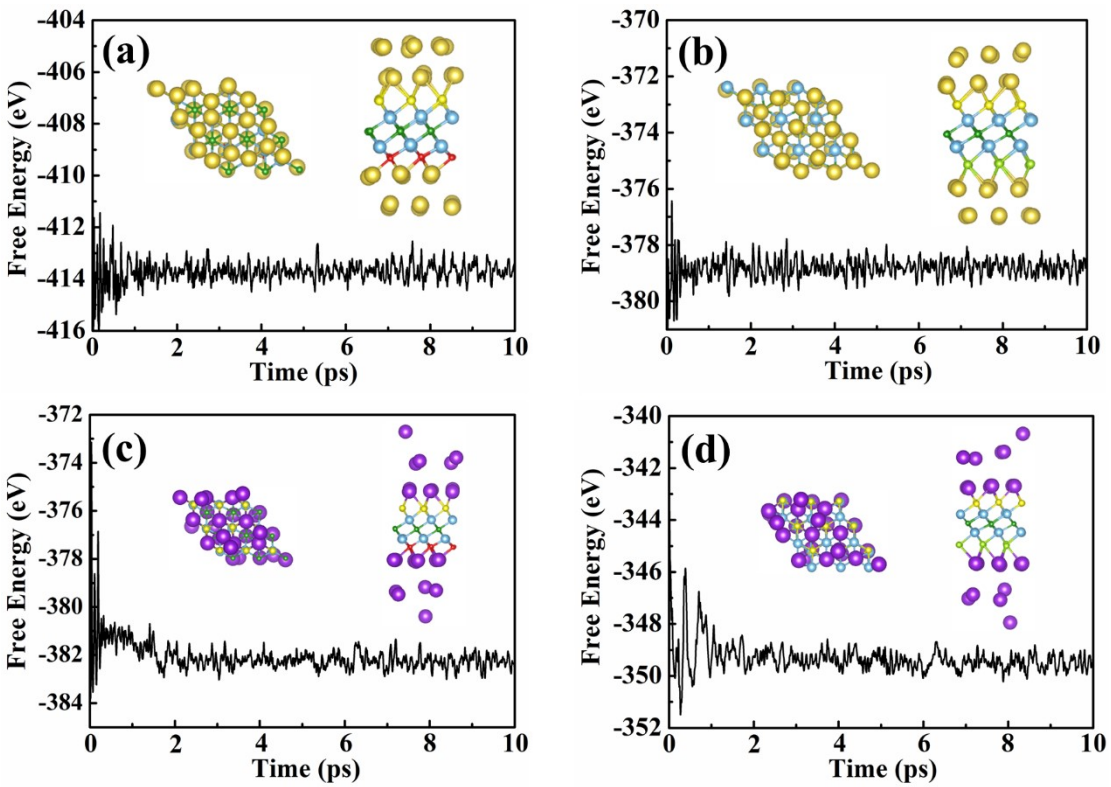

Fig. S2 The variations of free energy for (a) Na_4Ti_2BSO and (b) Na_4Ti_2BSSe (c) $K_{3.11}Ti_2BSO$ (d) $K_{3.11}Ti_2BSSe$ monolayers at 300 K during the AIMD simulations (insets are the final structures after simulations).