Supporting Information (SI) for

Alkali to alkaline earth metals: A DFT study of monolayer $TiSi_2N_4$ for metal ion batteries

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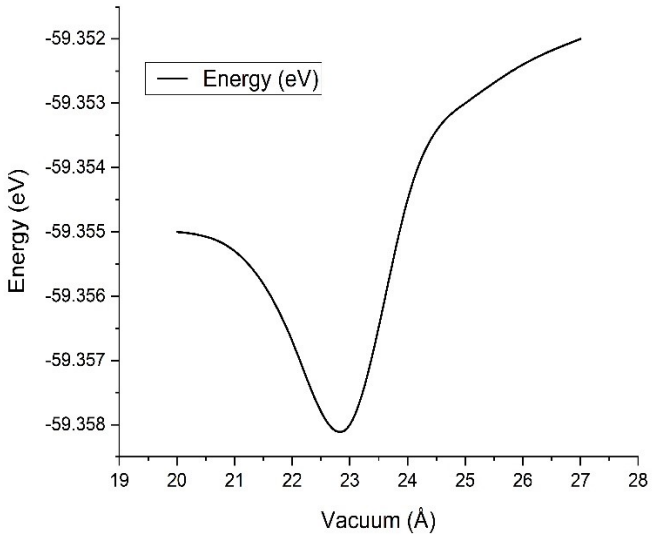

Figure S1. Vacuum optimization of monolayer $TiSi_2N_4$

Table S1. Lattice parameters (a=b in Å), PBE and HSE06 band gaps (E_g), bond lengths (Å), bond angle (θ), Force constants (N/m), Poisson's ratio, Young's Modulus (Y_{2D}), Shear Modulus (G), Formation Enthalpy (eV) and Dipole moment (μ) of monolayer $TiSi_2N_4$.

$TiSi_2N_4$	**Values**
a=b (Å)	2.916
PBE band (E_g)	1.649 (Indirect)
HSE06 band (E_g)	2.611 (Indirect)
N-Ti (Å)	2.063
N-Si (Å)	1.75/1.76
N-Ti-N (θ)	70.63
N-Si-N (θ)	107.07
Ti-N-Si (θ)	125.31
C_{11} (N/m)	725.52
C_{12}(N/m)	232.29
C_{66}(N/m)	247.11
Poisson's ratio	0.319
Young's modulus (Y_{2D})	625.25
Shear Modulus (G)	247.11
Formation Enthalpy	-3.298
Dipole moment (μ)	-1.09

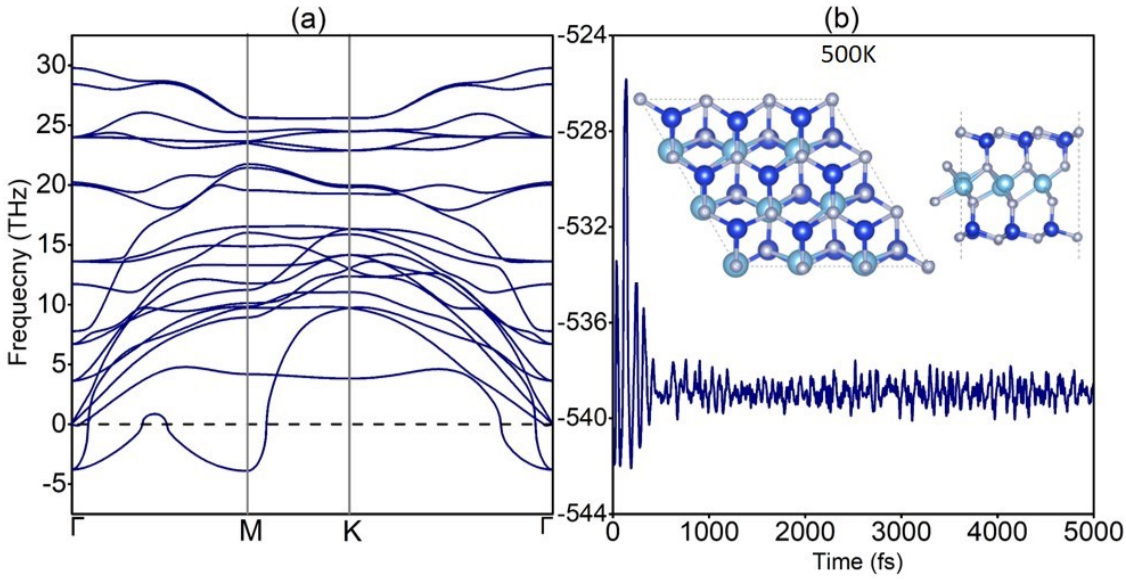

Figure S2. (a) Phonon spectra and (b) AIMD simulation for 1T phase of $TiSi_2N_4$ monolayer at 500K for 5000 time steps with inset display the initial and final structures, respectively.

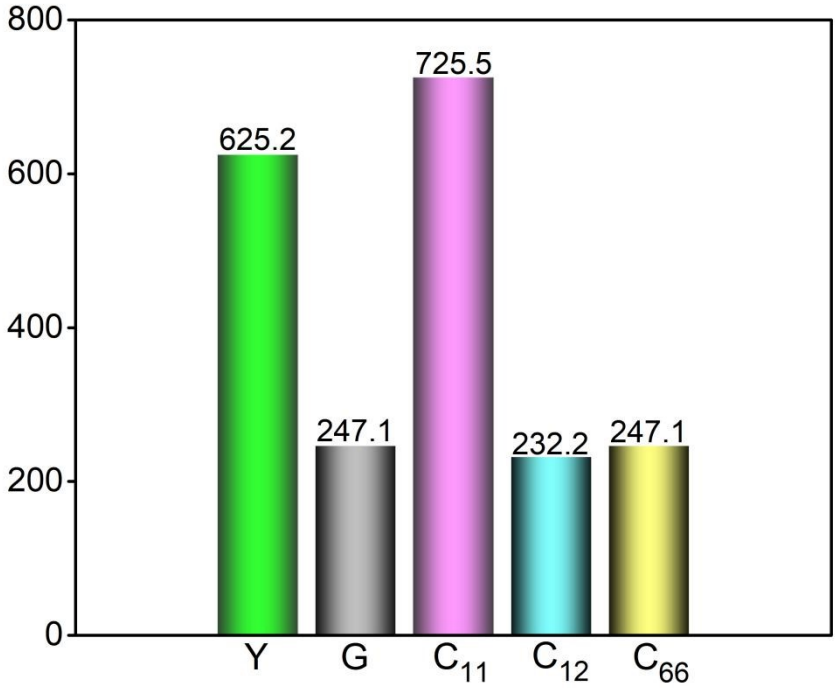

Figure S3. Young's Modulus (Y), Shear Modulus (G), and elastic constants C_{11}, C_{12} and C_{66} for monolayer $TiSi_2N_4$.

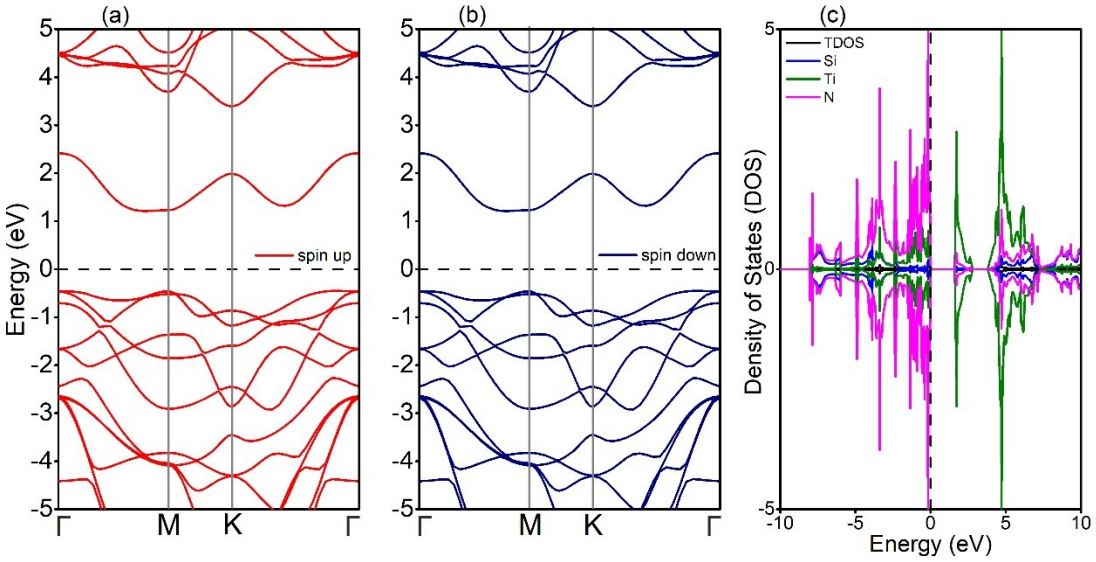

Figure S4. Spin polarized band structure of monolayer $TiSi_2N_4$ (a) spin up (b) spin down and (c) density of states DOS.

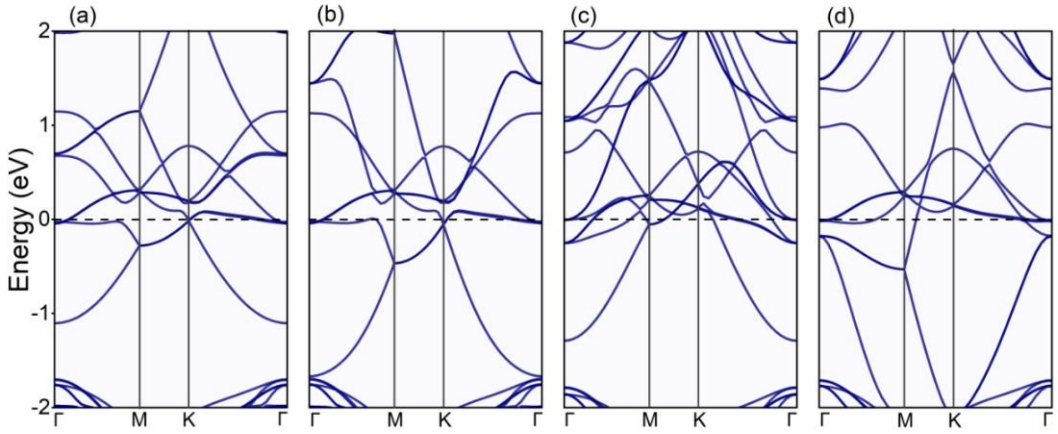

Figure S5. Band structure for single (a) Li, (b) Na, (c) K and (d) Mg atom adsorbed on monolayer $TiSi_2N_4$

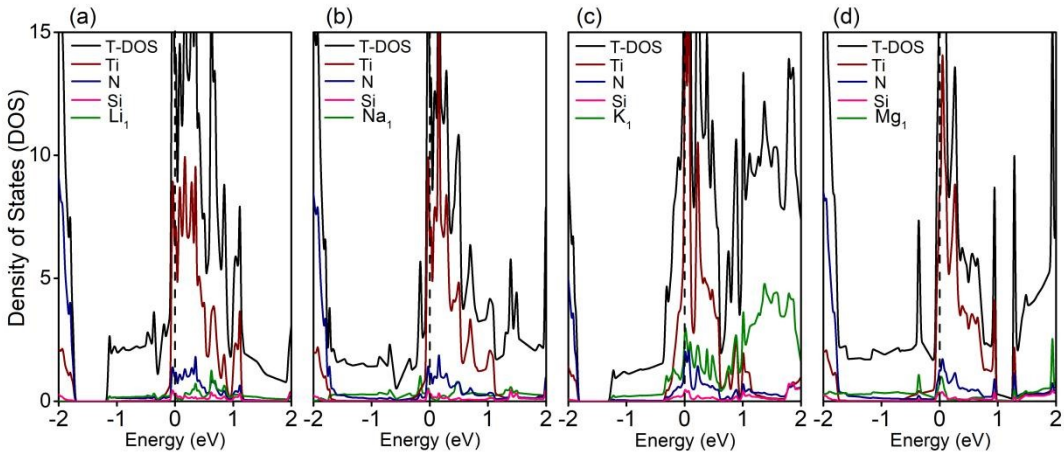

Figure S6. Partial Density of states (DOS) for single (a) Li, (b) Na, (c) K and (d) Mg atom adsorbed on $TiSi_2N_4$ monolayer

Table S2. Change in lattice parameter (a=b) due to adsorption of different layers of metals (Li, Na, K, Mg) atoms of single layer $Ti_4Si_8N_{16}$.

Metals	**Pristine**	**1st layer**	**2nd layer**	**3rd layer**	**4th layer**	**5th layer**	**6th layer**
Li	5.8325	5.8580	5.8754	5.8755	5.8623	5.8675	5.8598
Na	5.8325	5.8510	5.8469	5.9127	5.9335	5.9503	5.9612
K	5.8325	5.8993	5.9780	6.0512	6.1076	----	----
Mg	5.8325	5.7435	5.8708	5.9045	5.9047	5.9224	5.9218

Table S3. Adsorption energy for single alkali atom at different positions, Diffusion barrier energy, Theoretical Specific Capacity and Open Circuit Voltage (OCV) of $Ti_4Si_8N_{16}$ monolayer.

Metals	**Adsorption Energy (eV)**				**Diffusion Barrier (eV)**			**TSC mAh/g**	**OCV_{Avg}**
	Single atom								
	B	**N**	**Si**	**Ti**	**Path-1**	**Path-2**	**Path-3**		
Li	-2.471	-2.4720	-2.11	-2.4722	0.339	0.25	0.369	1004.4	0.55
Na	-1.591	-1.288	-1.443	-1.600	0.146	0.161	0.173	854.7	0.26
Mg	-0.592	-0.593	-0.5153	-0.555	0.189	0.103	0.21	492.3	0.55
K	-1.321	-1.182	-1.325	-1.389	0.074	0.135	0.086	531.5	-1.30

Table S4. Adsorption energy for single and multilayer alkali ion metals on $Ti_4Si_8N_{16}$ monolayer.

Metals	Adsorption Energy (eV)							
	1st layer			2nd layer	3rd Layer	4th Layer	5th Layer	6th layer
	N-site	Si-site	Ti-site					
Li	-2.21	-1.40	-1.981	-4.42	-5.28	-6.08	-5.08	-6.28
Na	-2.07	-1.96	-2.10	-4.19	-4.53	-3.93	-4.60	1.511
Mg	-2.75	-1.43	-1.64	-5.43	-5.08	-4.79	-4.63	-0.83
K	-3.25	-3.88	-4.25	-8.46	-6.08	-8.72	---	---

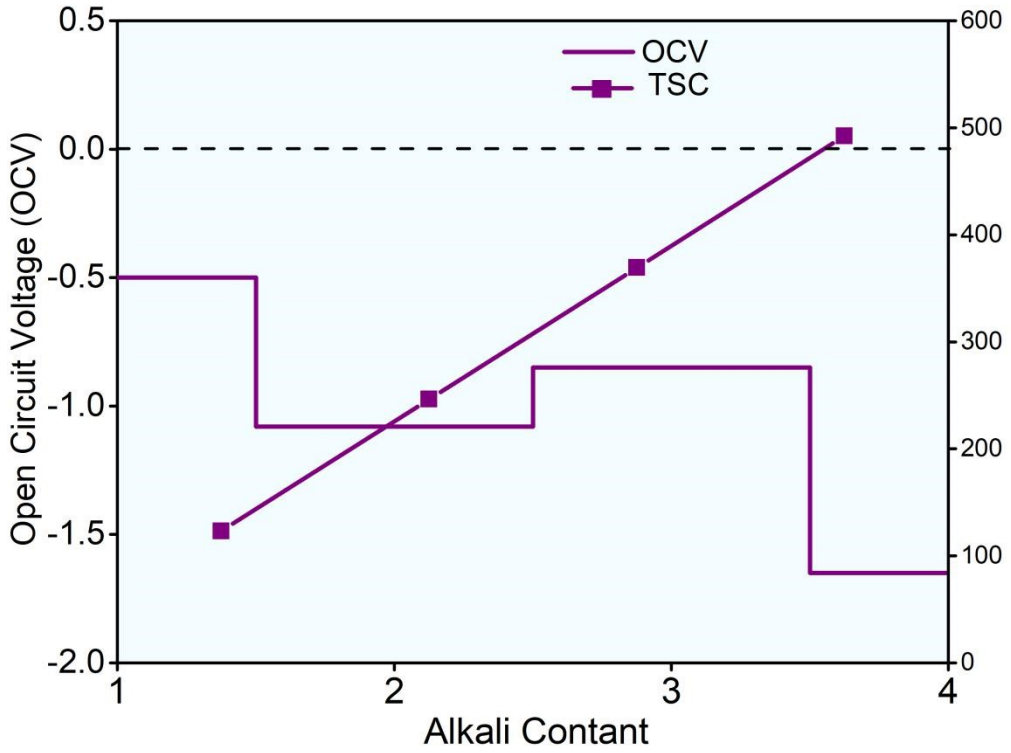

Figure S7. Open Circuit Voltage (OCV) and Theoretical Specific Capacity (TSC) of K adsorption on $TiSi_2N_4$.