Electronic Supplementary Material (ESI) for Materials Advances.

Supporting Information

Exploring Pristine and Transition Metal doped SiP_2 monolayer as a promising anode material for (Li, Na, Mg) Ion Batteries

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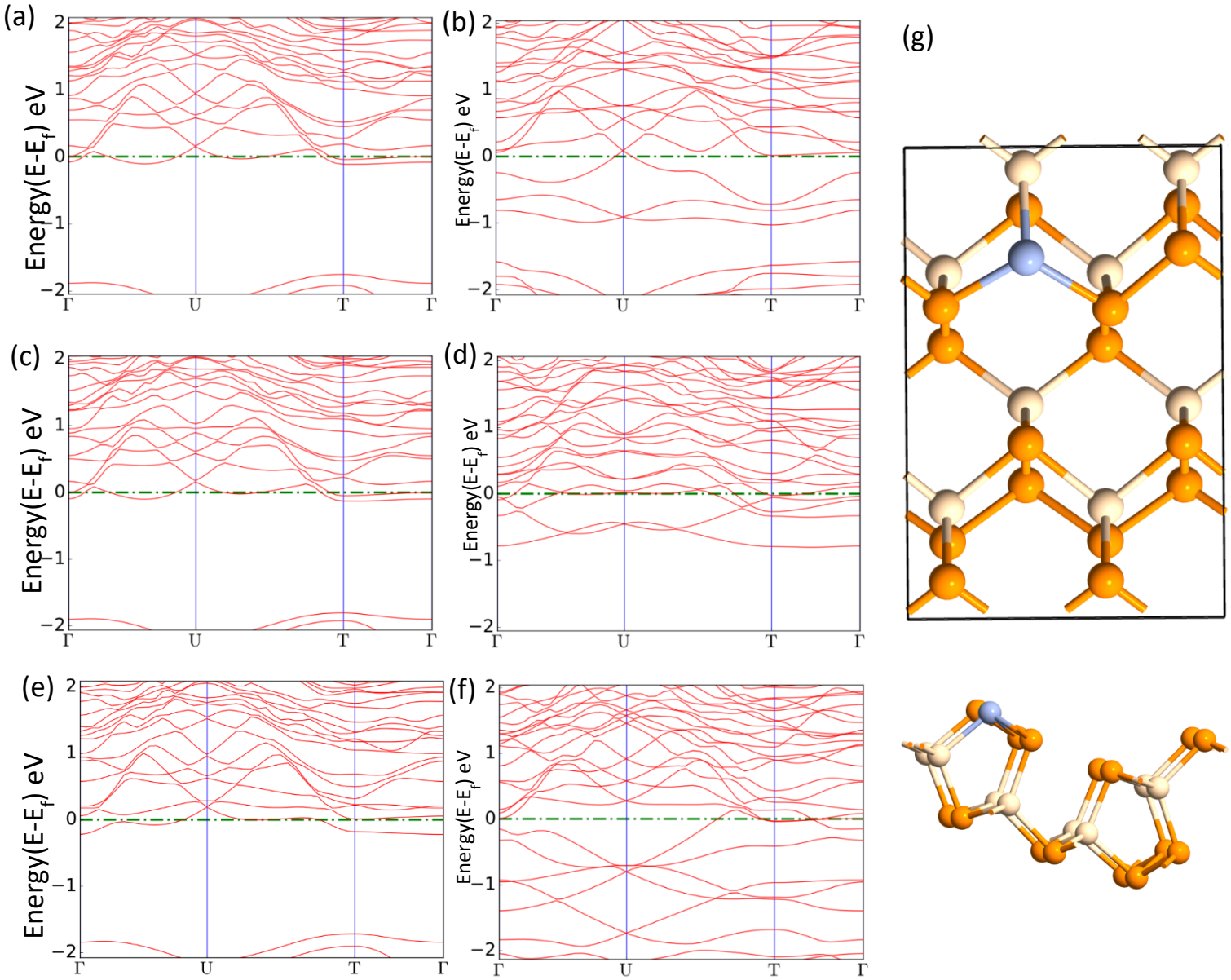

Fig S1: (a),(b) Band structure of single Li and Full Li adsorbed SiP_2 ; (c),(d) and (e),(f) band structure of Na and Mg atom with single and full adsorbed SiP_2 monolayers respectively,(g) doped SiP_2 monolayer

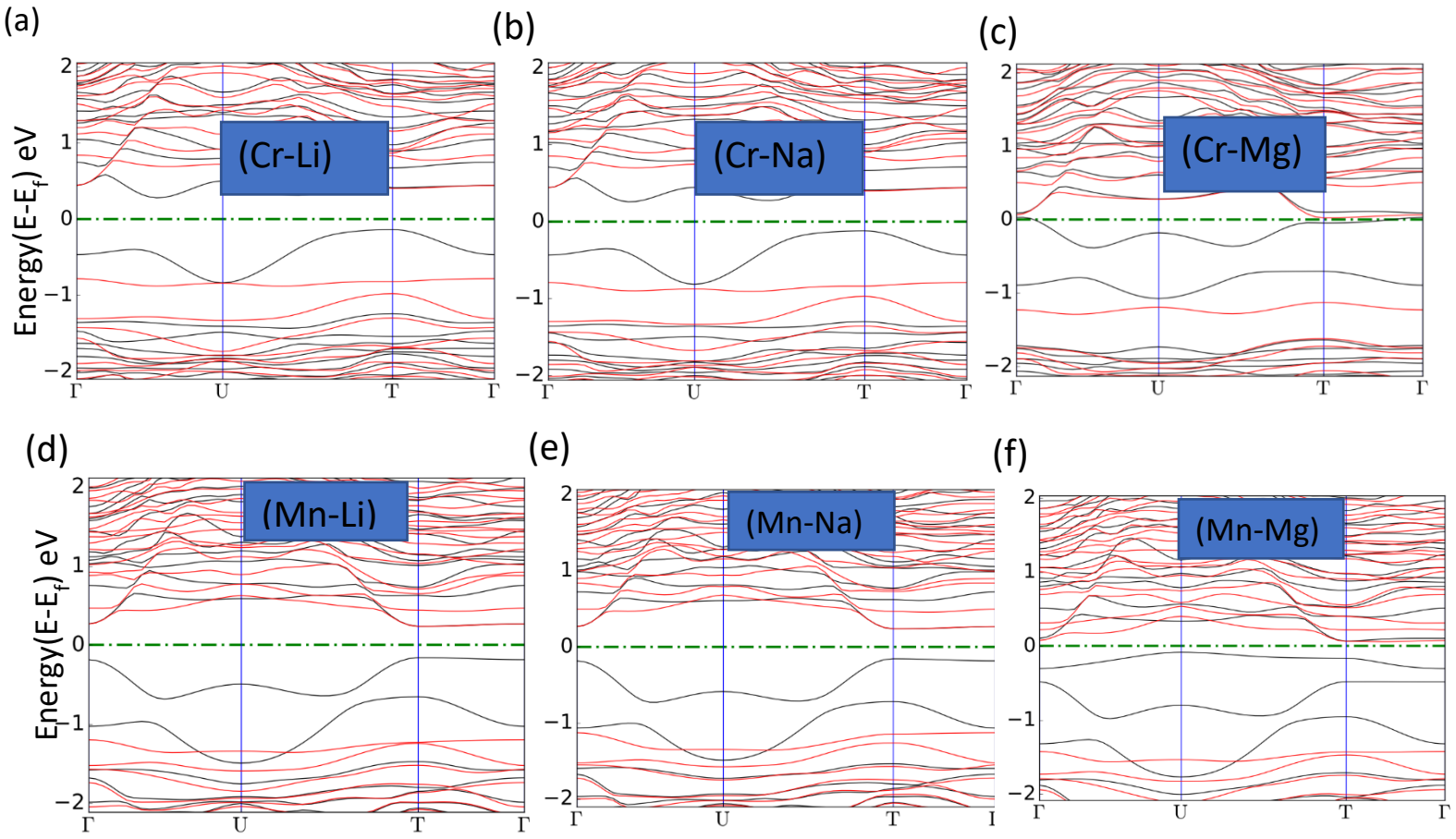

Fig S2: (a),(b),(c) and (d),(e),(f) are band structures of single Li, Na and Mg adsorbed on Cr and Mn-doped SiP_2 monolayers respectively

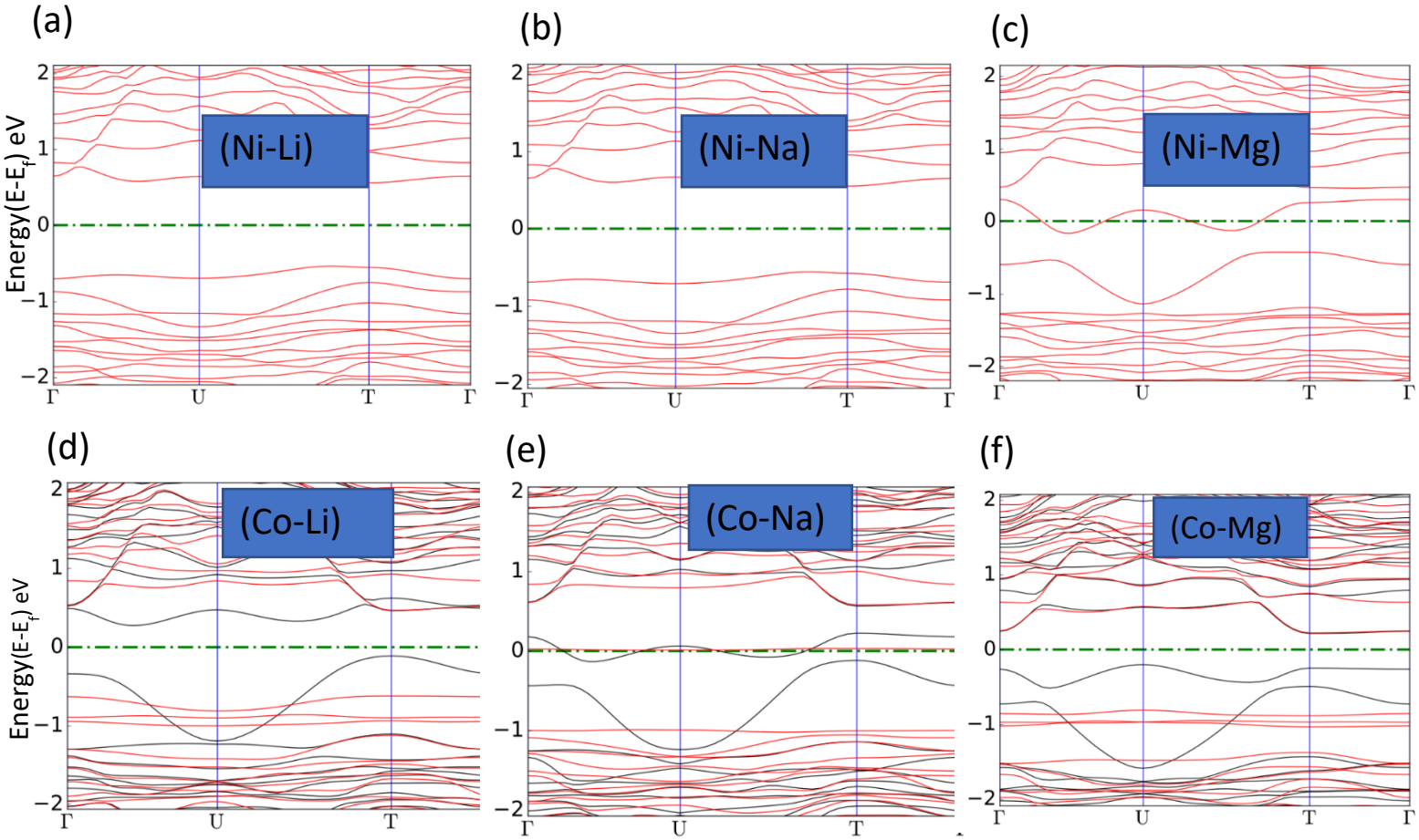

Fig S3: (a),(b),(c) and (d),(e),(f) are band structures of single Li, Na and Mg adsorbed on Ni and Co-doped SiP_2 monolayers respectively

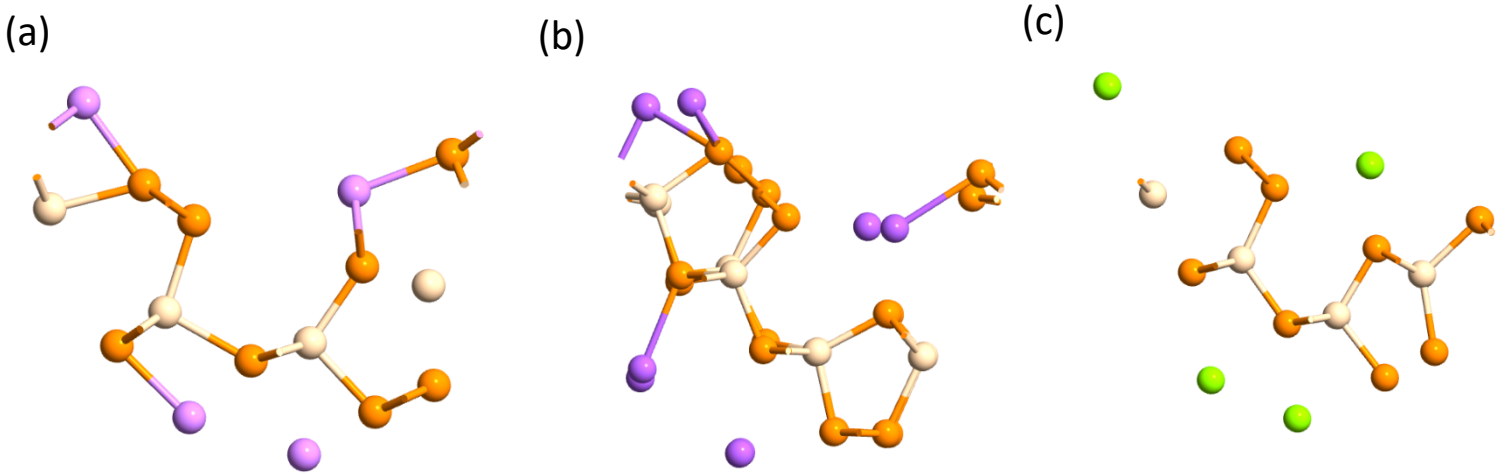

Fig S4: (a),(b),(c) represents 8 Li, Na and Mg atom adsorbed on SiP_2 monolayers respectively

Table S1: Formation energy for P and Si substituted by Transition metal on SiP_2 monolayer

Transition metal	E_{form} (eV) on P – substitution	E_{form} (eV) on Si – substitution
Cr	-2.59	-2.11
Mn	-2.21	-2.02
Ni	-1.91	-1.44
Co	-2.69	-2.09

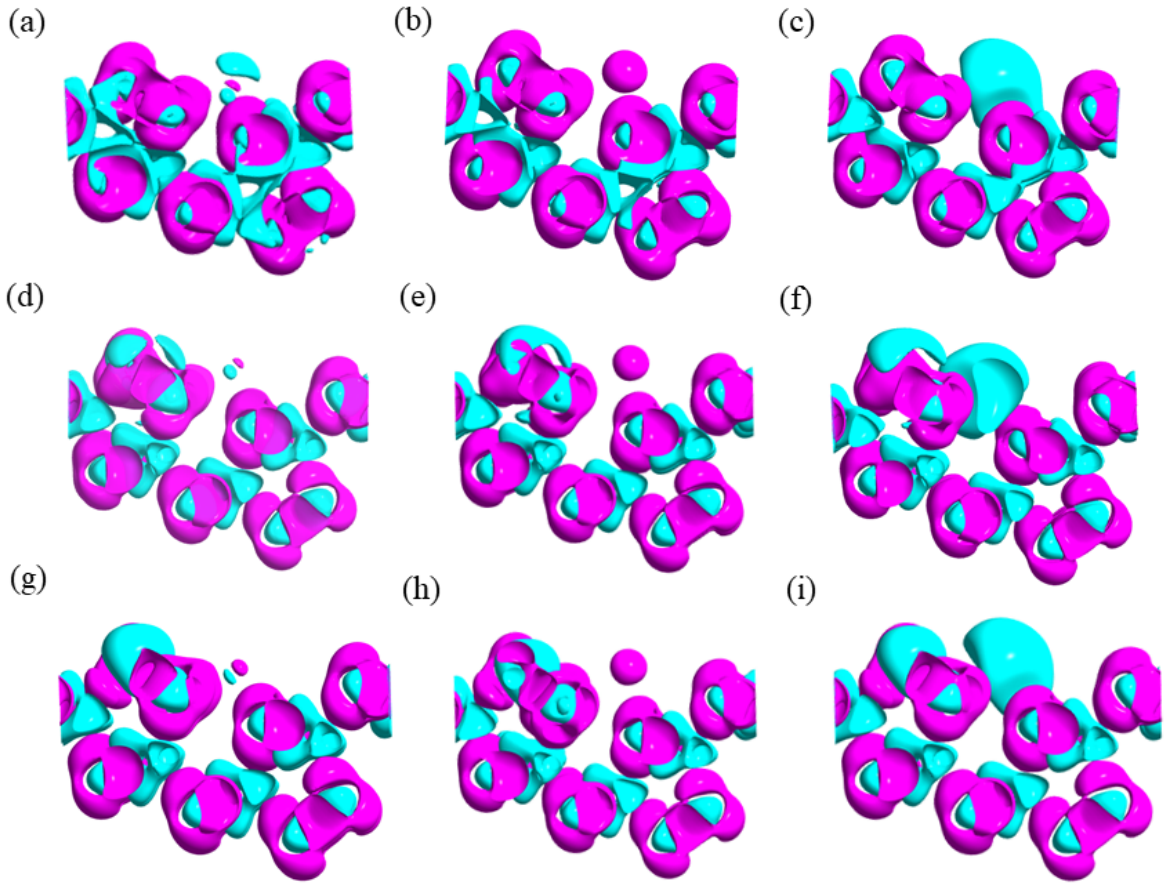

Fig S5: (a), (b) and (c) Isosurface plot for single Li, Na, and Mg adsorbed on pristine SiP_2 monolayer, (d),(e), (f) and(g), (h), (i) Isosurface plot for single Li, Na and Mg adsorbed on Co and Cr doped SiP_2 monolayer respectively.

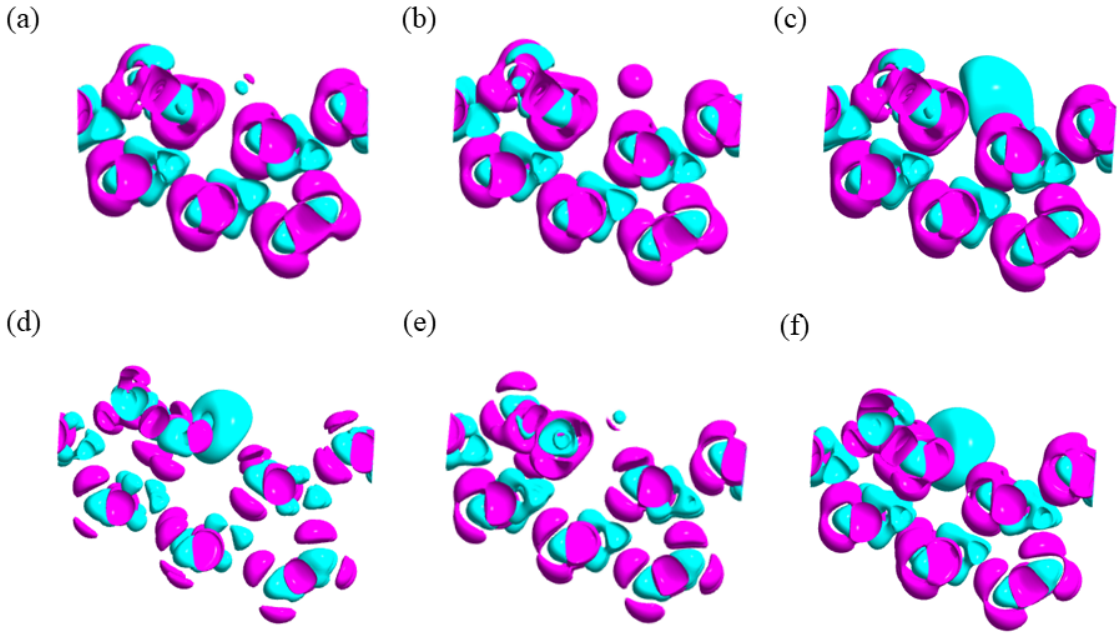

Fig S6: (a), (b),),(c) and (d),(e), (f) Isosurface plot for single Li, Na, and Mg adsorbed on Mn and Ni-doped SiP_2 monolayer respectively.

Brader Charge Analysis:

Table S2: Charge transfer ΔQ in the electronic unit (e) to the pristine and TM-doped SiP_2 monolayer

Metal atom	ΔQ(e) Pristine SiP_2	ΔQ(e) Co-doped SiP_2	ΔQ(e) Cr-doped SiP_2	ΔQ(e) Mn-doped SiP_2	ΔQ(e) Ni-doped SiP_2
Li	0.68	0.39	0.31	0.36	0.31
Na	0.60	0.22	0.34	0.26	0.33
Mg	0.78	0.43	0.41	0.38	0.36

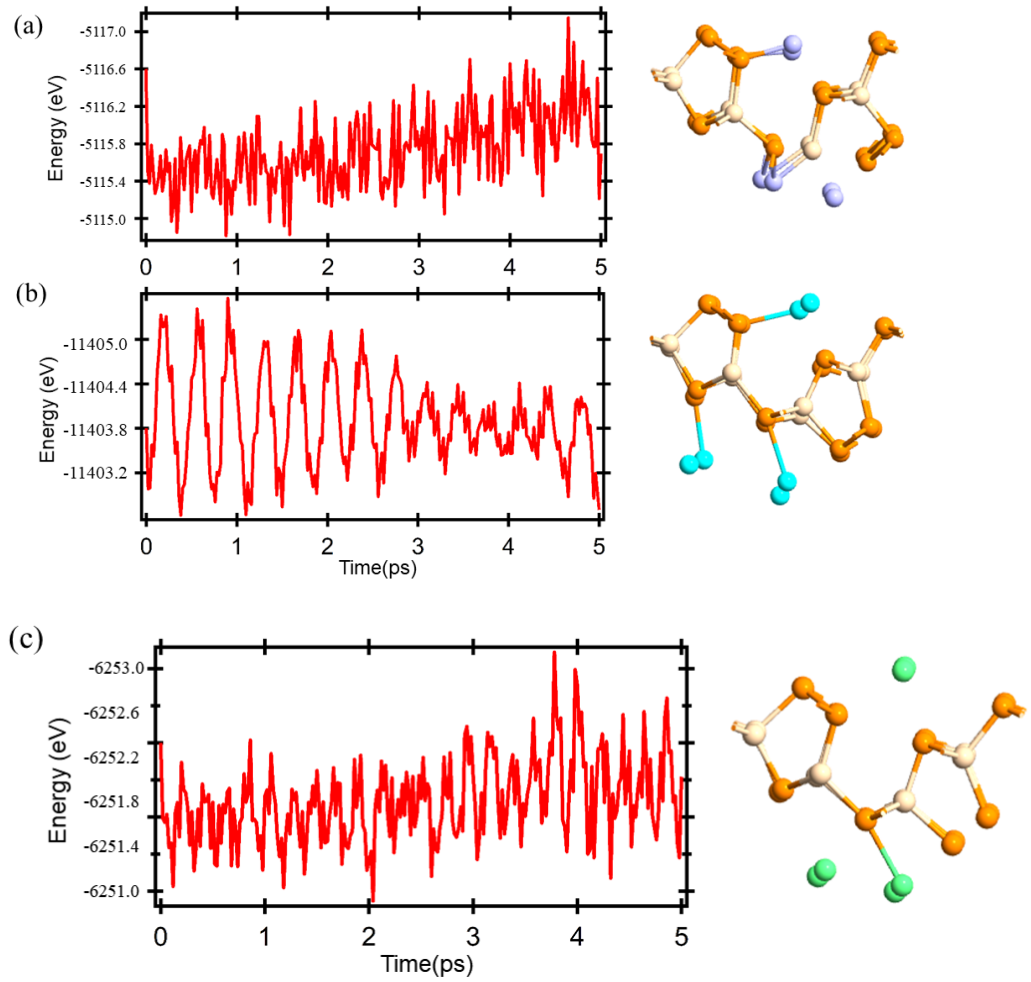

Fig S7: (a) Energy vs Time variation for of lithium adsorbed SiP_2 with the final structure at 300K, (b) and (c) Energy vs Time variation for full sodium and magnesium adsorbed SiP_2 with the final structure at 300K respectively.

Table S3: effective mass and carrier mobility

Carrier type	Effective mass (m*)	Mobility(μ) $cm^2V^{-1}s^{-1}$
Electron (a)	**1.56**	**9554.2**
Hole(a)	**1.99**	**257.5**
Electron (b)	**0.76**	**201.2**
Hole(b)	**1.13**	**2344.3**