Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

A First Principle Study of 2D Single-layer SiP as Anode Material for Lithium-ion Battery and Sodium-ion Battery

Yingying Xing [a], Chihao Cao [a], Zhong Huang [a], Liang Huang[*, a], Haijun Zhang[*, a], Quanli Jia [b]

[a] *The State Key Laboratory of Refractories and Metallurgy, School of Materials and Metallurgy, Wuhan University of Science and Technology, Wuhan 430081, China*

[b] *Henan Key Laboratory of High Temperature Functional Ceramics, Zhengzhou University, Zhengzhou 450052, China*

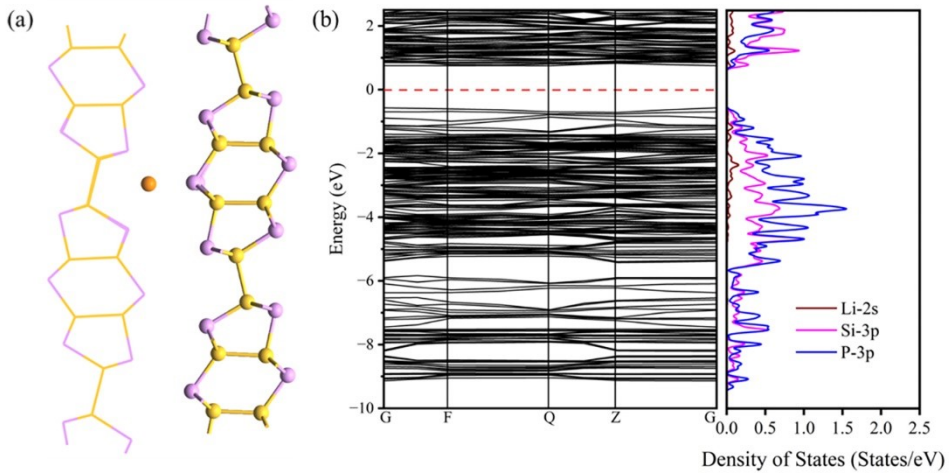

Fig. S1 (a) The optimized structure, (b) the band structure and density of states (DOS) of bulk SiP when Li is intercalated at site 2. The yellow, orange, and purple balls denote Si atoms, Li atoms, and P atoms, respectively.

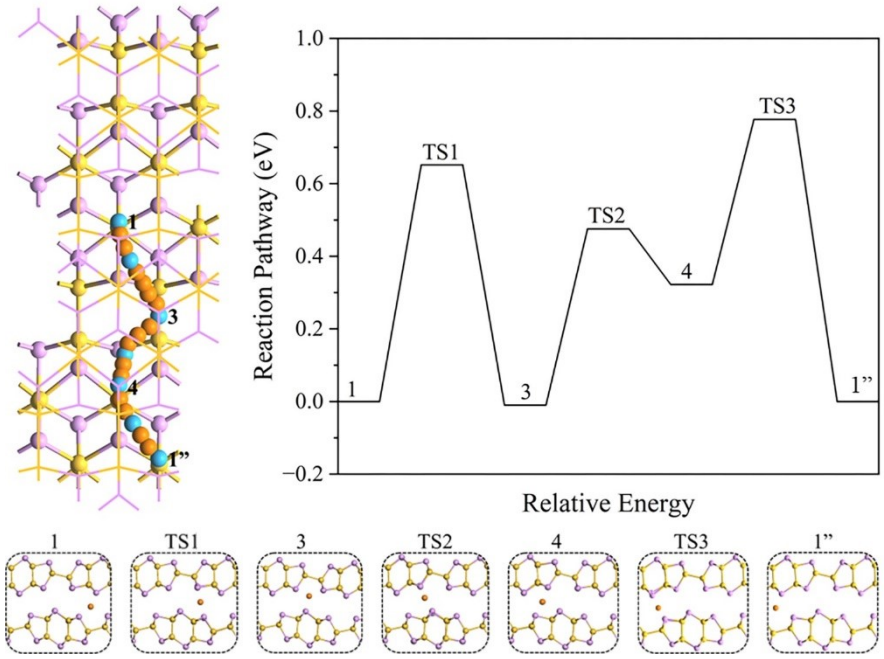

Fig. S2 The reaction coordinates and energy barriers for path 2 of Li diffusion along Y axis in bulk SiP. The blue ball represents initial state, transition state (TS), intermediate and final state.

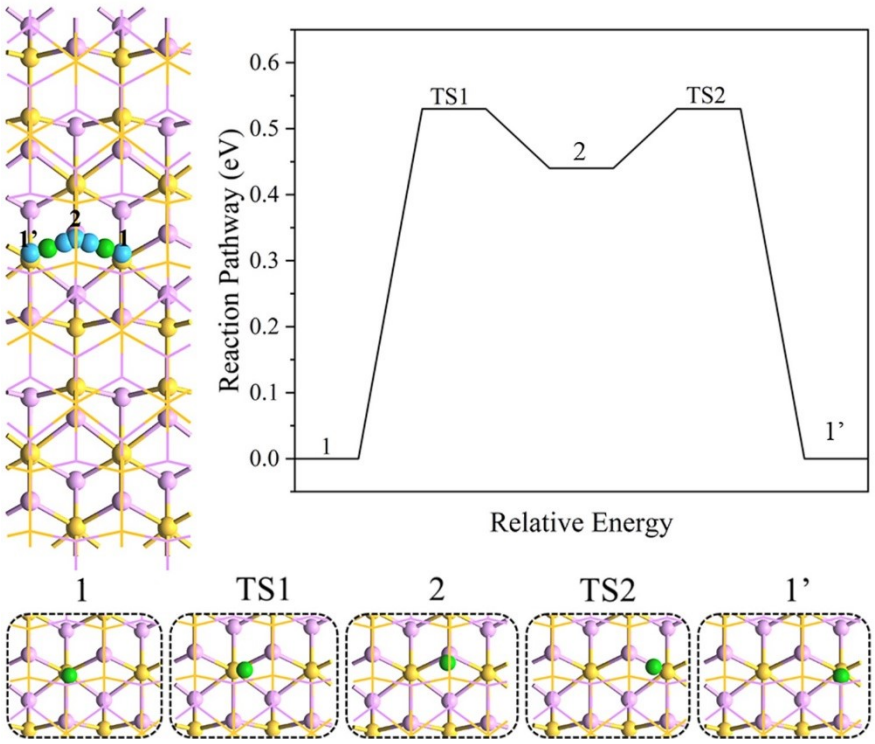

Fig. S3 The reaction coordinates and energy barriers for Na diffusion along the X axis in bulk SiP. The green balls denote Na atoms.

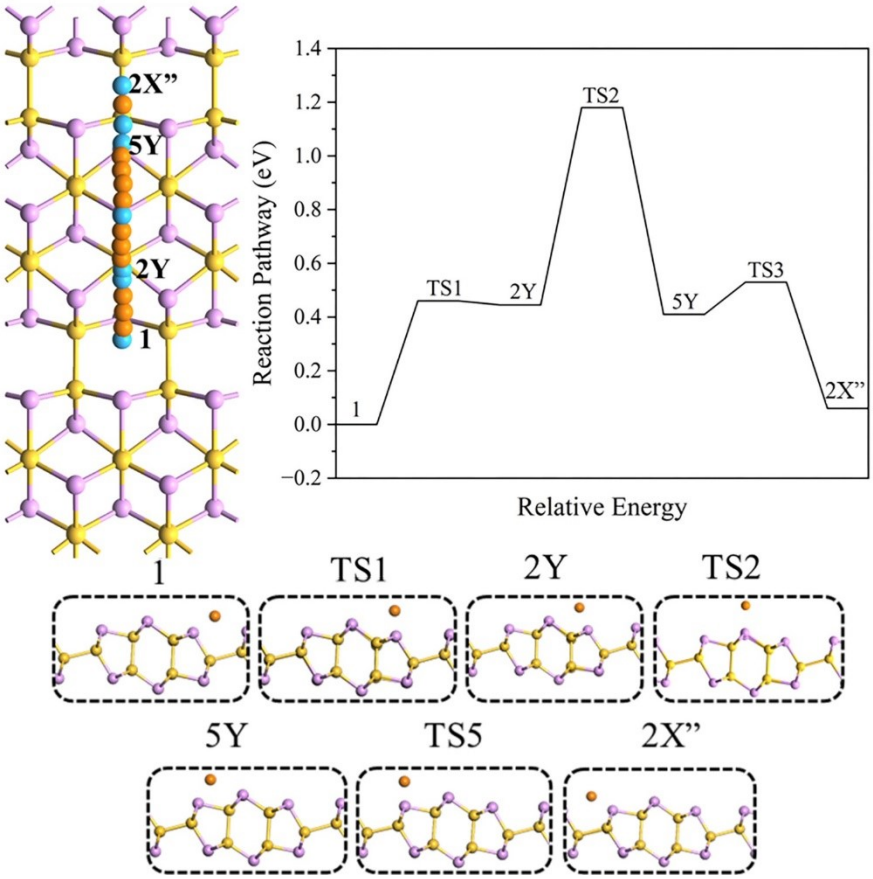

Fig. S4 The reaction coordinates and energy barriers for path 2 of Li diffusion along Y axis on 2D single-layer SiP.

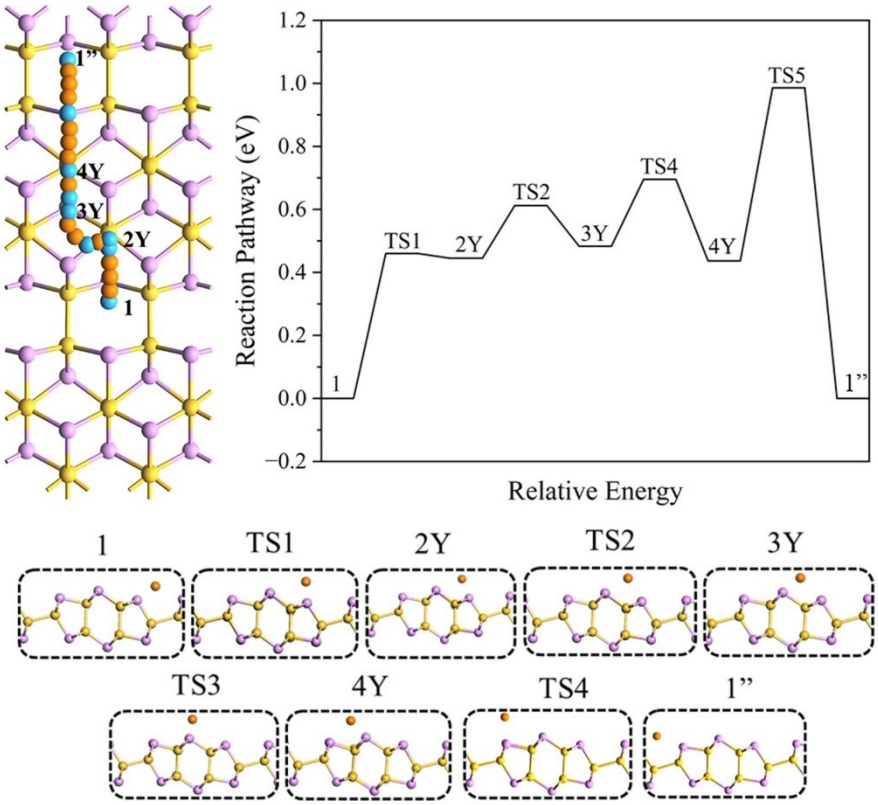

Fig. S5 The reaction coordinates and energy barriers for path 3 of Li diffusion along Y axis on 2D single-layer SiP.

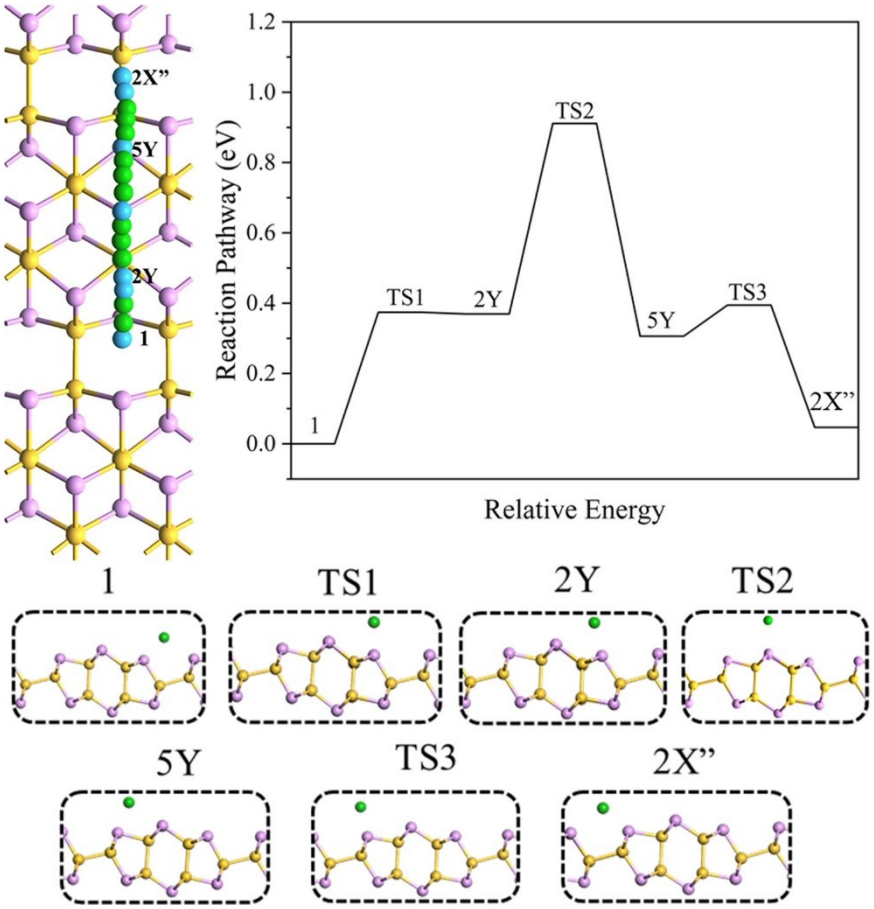

Fig. S6 The reaction coordinates and energy barriers for path 2 of Na diffusion along Y axis on 2D single-layer SiP.

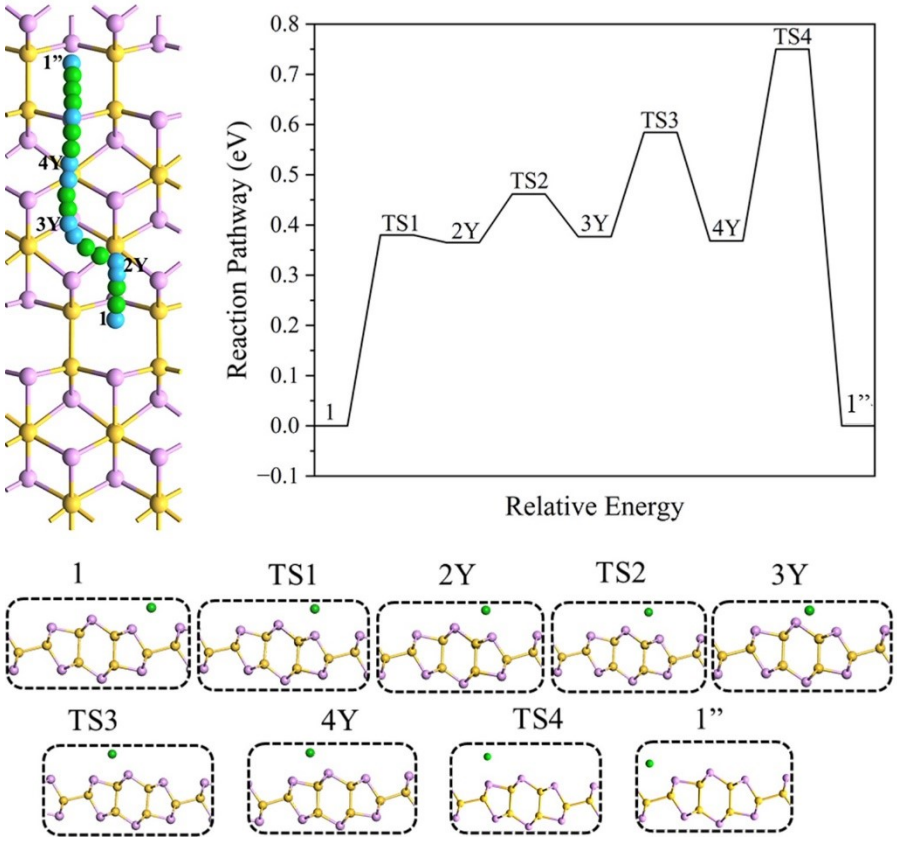

Fig. S7 The reaction coordinates and energy barriers for path 3 of Na diffusion along Y axis on 2D single-layer SiP.

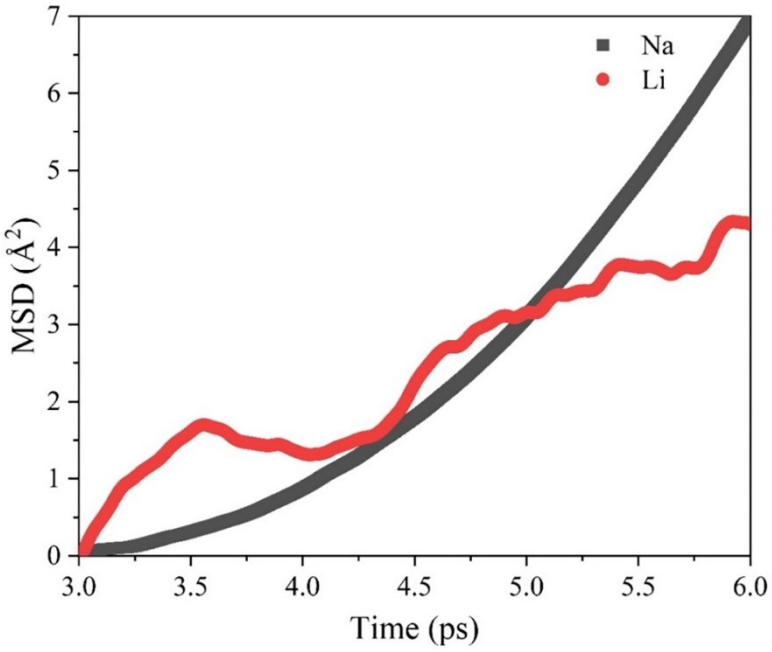

Fig. S8 The mean squared displacement (MSD) of Li or Na atom on 2D Single-layer SiP during MD from 3 to 6 ps at 400 K

Table S1 Adsorption energy of Li/Na on the 2D single-layer SiP or in bulk SiP at different K points

K-point	Li on 2D single-layer SiP	Na on 2D single-layer SiP	Li in bulk SiP
2×1×1	-1.946 eV	-1.392 eV	-2.305 eV
6×3×1	-1.857 eV	-1.296 eV	-2.231 eV
6×3×2	-1.857 eV	-1.296 eV	-2.190 eV
8×4×1	-1.858 eV	-1.295 eV	-2.188 eV
8×4×2	\	\	-2.187 eV

Table S2 The diffusion coefficient of Li/Na atom on 2D single-layer SiP

	Li	Na
Diffusion coefficient ($\mathcal{D}$ 10^{-5} $cm^2 \cdot s^{-1}$)	2.12	5.97

Table S3 System energy of 2D single-layer SiP under the vacuum layer of 15 Å and 20 Å.

Vacuum layer (Å)	15	20
Energy (eV)	-6896.4836	-6896.4829

Table S4 The lattice parameters of 2D single-layer SiP

a	b	c	α	β	γ
6.98 Å	20.56 Å	19.72 Å	90°	90°	90°

Table S5 The fractional coordinate of each atom for 2D single-layer SiP

Element	Atom Number	Fractional coordinates of atoms		
		u	v	w
Si	1	0	0.170732	0.261034
Si	2	0	0.059857	0.220858
Si	3	0	0.435417	0.318389
Si	4	0	0.432405	0.149999
Si	5	0	0.795446	0.165344

Si	6	0	0.798105	0.333262
Si	7	0.25	0.670732	0.261034
Si	8	0.25	0.559857	0.220858
Si	9	0.25	0.935417	0.318389
Si	10	0.25	0.932405	0.149999
Si	11	0.25	0.295446	0.165344
Si	12	0.25	0.298105	0.333262
Si	13	0	0.829268	0.761034
Si	14	0	0.940143	0.720858
Si	15	0	0.564583	0.818389
Si	16	0	0.567595	0.649999
Si	17	0	0.204554	0.665344
Si	18	0	0.201895	0.833262
Si	19	0.25	0.329268	0.761034
Si	20	0.25	0.440143	0.720858
Si	21	0.25	0.064583	0.818389
Si	22	0.25	0.067595	0.649999
Si	23	0.25	0.704554	0.665344
Si	24	0.25	0.701895	0.833262
Si	25	0.5	0.170732	0.261034
Si	26	0.5	0.059857	0.220858
Si	27	0.5	0.435417	0.318389
Si	28	0.5	0.432405	0.149999
Si	29	0.5	0.795446	0.165344
Si	30	0.5	0.798105	0.333262
Si	31	0.75	0.670732	0.261034
Si	32	0.75	0.559857	0.220858
Si	33	0.75	0.935417	0.318389
Si	34	0.75	0.932405	0.149999

Si	35	0.75	0.295446	0.165344
Si	36	0.75	0.298105	0.333262
Si	37	0.5	0.829268	0.761034
Si	38	0.5	0.940143	0.720858
Si	39	0.5	0.564583	0.818389
Si	40	0.5	0.567595	0.649999
Si	41	0.5	0.204554	0.665344
Si	42	0.5	0.201895	0.833262
Si	43	0.75	0.329268	0.761034
Si	44	0.75	0.440143	0.720858
Si	45	0.75	0.064583	0.818389
Si	46	0.75	0.067595	0.649999
Si	47	0.75	0.704554	0.665344
Si	48	0.75	0.701895	0.833262
P	1	0	0.000158	0.360796
P	2	0	0.231032	0.122028
P	3	0	0.344786	0.411032
P	4	0	0.540852	0.119716
P	5	0	0.689422	0.362302
P	6	0	0.885819	0.072281
P	7	0.25	0.500158	0.360796
P	8	0.25	0.731032	0.122028
P	9	0.25	0.844786	0.411032
P	10	0.25	0.040852	0.119716
P	11	0.25	0.189422	0.362302
P	12	0.25	0.385819	0.072281
P	13	0	0.999842	0.860796
P	14	0	0.768968	0.622028
P	15	0	0.655214	0.911032

P	16	0	0.459148	0.619716
P	17	0	0.310578	0.862302
P	18	0	0.114181	0.572281
P	19	0.25	0.499842	0.860796
P	20	0.25	0.268968	0.622028
P	21	0.25	0.155214	0.911032
P	22	0.25	0.959148	0.619716
P	23	0.25	0.810578	0.862302
P	24	0.25	0.614181	0.572281
P	25	0.5	0.000158	0.360796
P	26	0.5	0.231032	0.122028
P	27	0.5	0.344786	0.411032
P	28	0.5	0.540852	0.119716
P	29	0.5	0.689422	0.362302
P	30	0.5	0.885819	0.072281
P	31	0.75	0.500158	0.360796
P	32	0.75	0.731032	0.122028
P	33	0.75	0.844786	0.411032
P	34	0.75	0.040852	0.119716
P	35	0.75	0.189422	0.362302
P	36	0.75	0.385819	0.072281
P	37	0.5	0.999842	0.860796
P	38	0.5	0.768968	0.622028
P	39	0.5	0.655214	0.911032
P	40	0.5	0.459148	0.619716
P	41	0.5	0.310578	0.862302
P	42	0.5	0.114181	0.572281
P	43	0.75	0.499842	0.860796
P	44	0.75	0.268968	0.622028

P	45	0.75	0.155214	0.911032
P	46	0.75	0.959148	0.619716
P	47	0.75	0.810578	0.862302
P	48	0.75	0.614181	0.572281
Si	1	0	0.170732	0.261034
Si	2	0	0.059857	0.220858