Supporting Information for

Ti_2P monolayer as a high performance 2-D electrode material for ion batteries

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Contents of Supporting Information

COMPUTATIONAL DETAILS

The first principles calculations in this work were realized by using the Vienna ab initio Simulation Package (VASP) [1], based on density functional theory (DFT) [2]. For the exchange-correlation potential, we applied the generalized gradient approximation (GGA) of the Perdew-Burke-Ernzerhof (PBE) functional [3, 4]. The cutoff energy was set as 500 eV during the calculations. To avoid artificial interaction between two isolated monolayers, a vacuum with the thickness of 20 Å was built in the bare Ti_2P monolayer. During the calculations, the long-range van der Waals interactions were taken into account by using the DFT-D2 method [5]. For geometrical optimization, a 7×7×1 k-mesh was applied, while a 9×9×1 k-mesh was used in static energy calculations. The force and energy convergence criteria were set as 0.01 eV $Å^{-1}$ and 10^{-6} eV, respectively. To investigate the dynamical stability of Ti_2P monolayer, the phonon spectra were calculated by using the PHONOPY package [6, 7]. The climbing-image nudged elastic band (CI-NEB) method [8, 9] was used to obtain the diffusion barrier height during the ion diffusion process.

References

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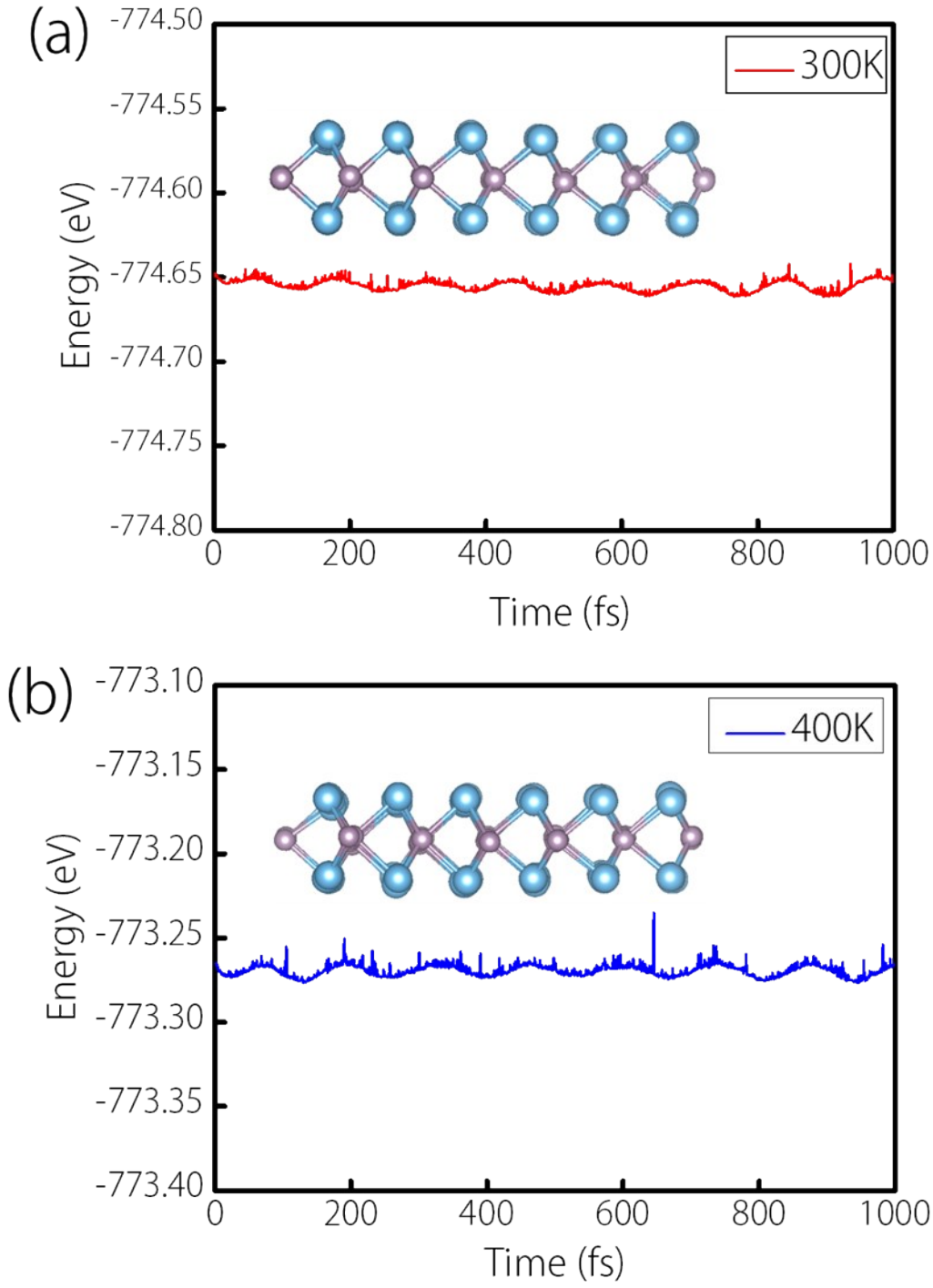

Figure S1 Evolution of the potential energy versus simulation time for Ti_2P monolayer during AIMD simulation at (a) 300K and (b) 400 K. The inset images (side views) are the geometries of Ti_2P monolayer at the end of the simulation.

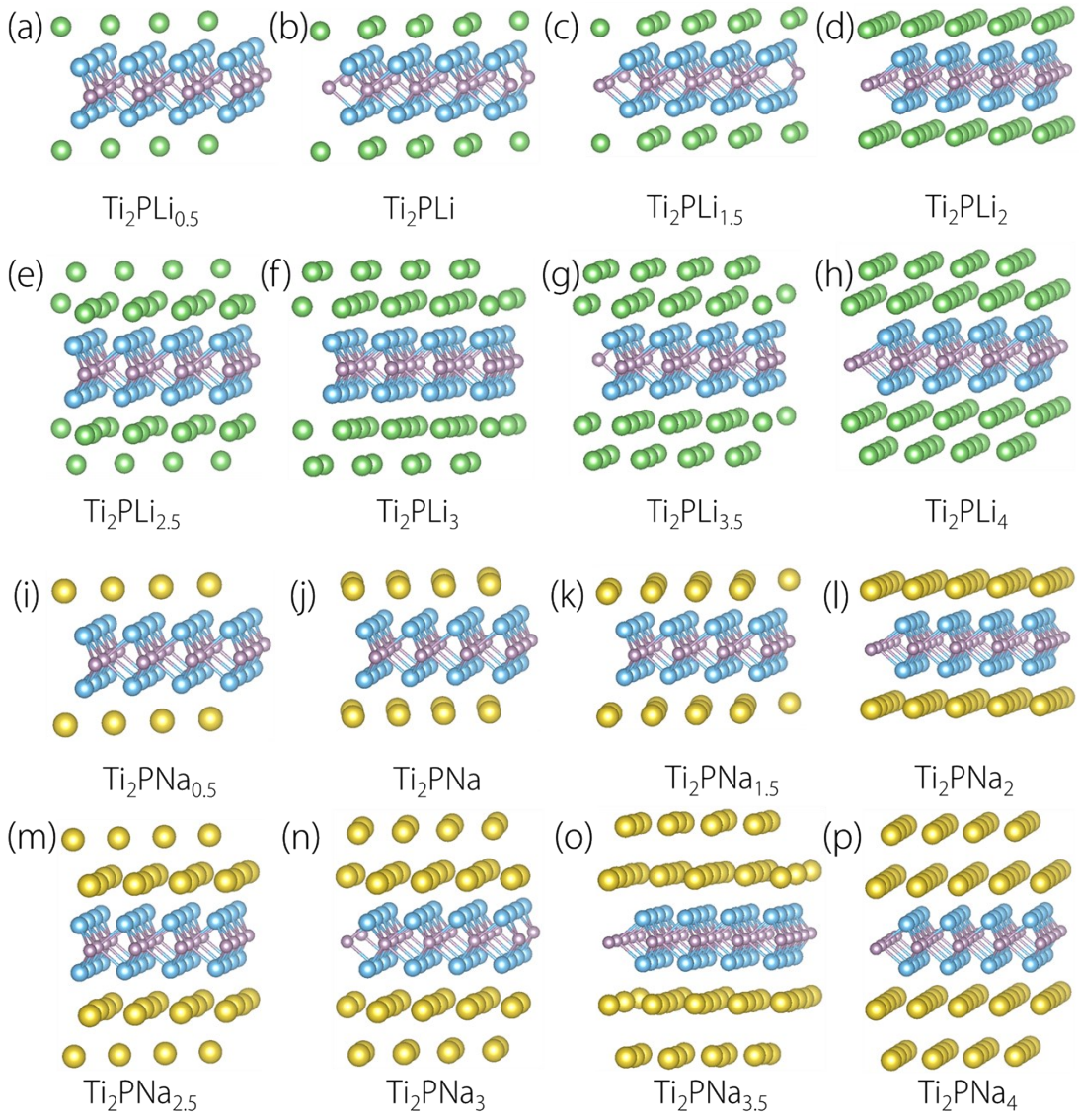

Figure S2 The optimized structures of the increasing of the Li/Na concentrations. The figures (a)–(h) represent the optimized structures of Ti_2PLi_x (x= 0.5–4); and the images (i)–(p) represent the optimized structures of Ti_2PNa_x (x= 0.5–4).

Table S1 Layered adsorption energy at different temperatures. $E_{32Li+sub}$, $E_{64Li+sub}$, $E_{32Na+sub}$, and $E_{64Na+sub}$ represent the layer adsorption energies of the Ti_2P substrate adsorbed one layer of Li, two layers of Li, one layer of Na, and two layers of Na, respectively.

Temperature	$E_{32Li+sub}$ (eV)	$E_{64Li+sub}$ (eV)	$E_{32Na+sub}$ (eV)	$E_{64Na+sub}$ (eV)
0 K	-0.67739	-0.06388	-0.58586	-0.17332
300 K	-0.66492	-0.02757	-0.56916	-0.16144
400 K	-0.66483	-0.02767	-0.56927	-0.16134