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

Supporting Information

Blue-AsP monolayer as a promising anode material for lithium- and sodium-ion batteries: a DFT study

Jing Zhang,[a] *Yong-Fan Zhang,*[a] *Yi Li,*[a] *Yu-Rong Ren,*[b]

Shu-Ping Huang[a], Wei Lin*[a,c] Wen-Kai Chen*[a,c,d]*

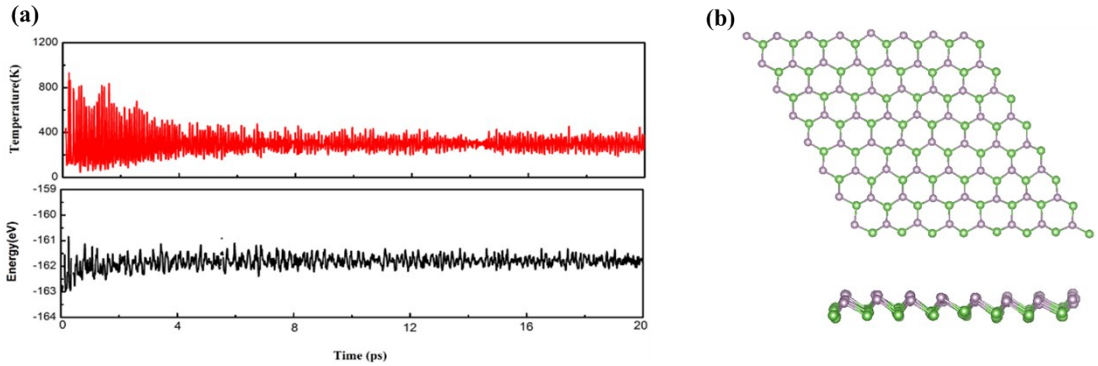

Fig. S1 (a) Variations of temperature and energy in the AIMD simulations of *b*-AsP monolayer; (b) Top and side views of 8 × 8 × 1 supercells of the *b*-AsP monolayer after dynamics simulation at 300K.

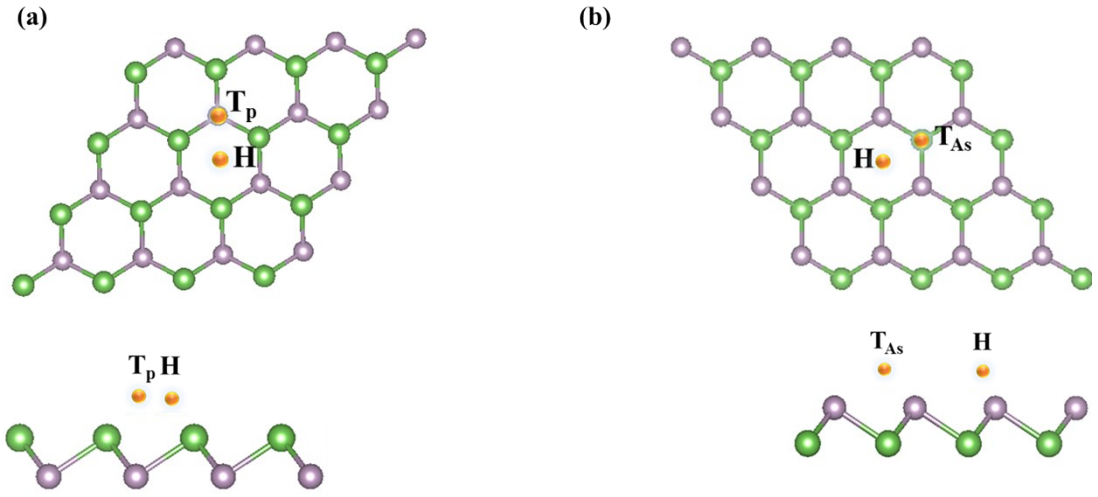

Fig. S2 Top and side views of the table sites when Li/Na-ion is adsorbed (a) on the As side and (b) on the P side.

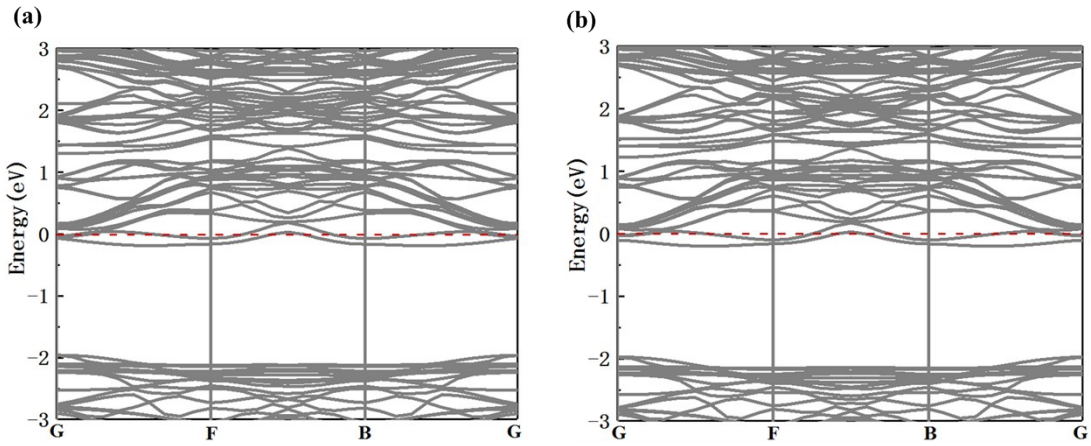

Fig. S3 The electronic bands were calculated by using PBE functional of *b*-AsP monolayer adsorbing a (a) Li atom, (b) Na atom. The Fermi level is set to zero energy.

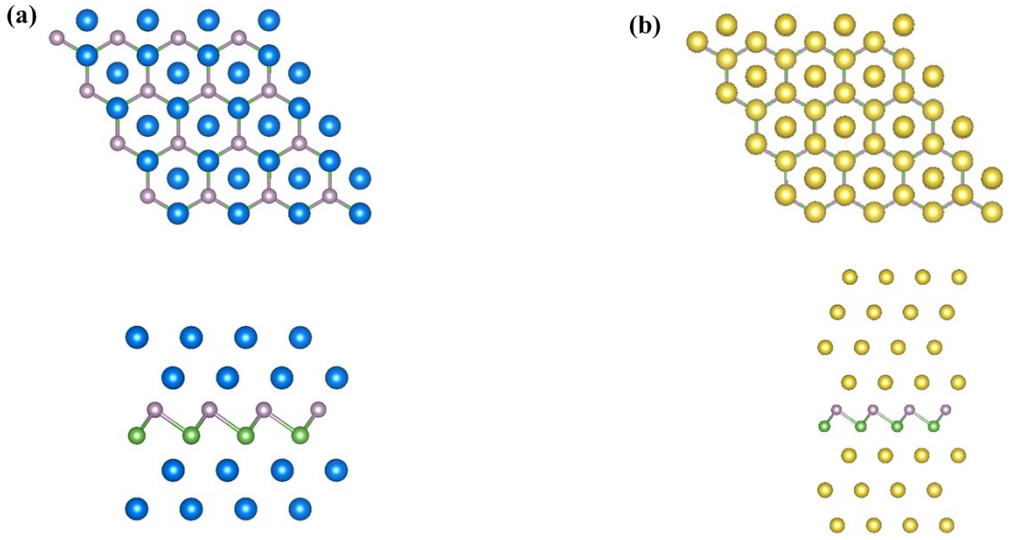

Fig. S4 Top and side views of theoretical maximum Li storage in optimized (a) Li_4AsP, (b) Na_7AsP

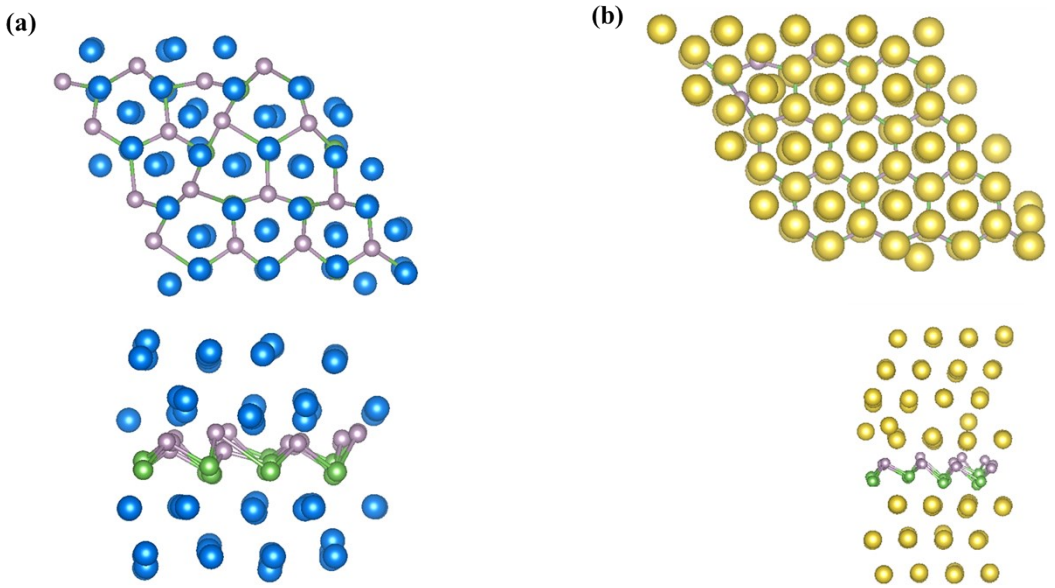

Fig. S5 Top and side views of the last snapshots about Li/Na-saturated supercell models from the AIMD simulations at 300 K: (a) Li-AsP (Li_4AsP); (b) Na-AsP (Na_7AsP).