Supporting Information

## Black phosphorene/NP heterostructure as a novel anode material for Li/Na-ion batteries

Yanwei Wang<sup>*a*</sup>, Wu Tian<sup>*a*</sup>, Huijuan Zhang<sup>*a*\*</sup>, Yu Wang<sup>*a*, *b*\*</sup>

<sup>a</sup> The School of Chemistry and Chemical Engineering, State Key Laboratory of Power Transmission Equipment & System Security and New Technology, Chongqing

University, 174 Shazheng Street, Shapingba District, Chongqing City, 400044, PR

China

<sup>b</sup> The School of Electrical Engineering, Chongqing University, 174 Shazheng Street, Shapingba District, Chongqing City 400044, PR China

\*E-mail: wangy@cqu.edu.cn; zhanghj@cqu.edu.cn



**Fig. S1.** Density of states (DOS) of Black P/NP heterostructure. The Fermi level is set to zero.



Fig. S2. Band structures of (a) Black P, and (b) NP monolayer.



Fig. S3. Open circuit voltage profiles of Black P/NP\_Li, and Black P/NP\_Na system

as a function of the Li, and Na concentration, respectively.