Electronic Supplementary Material (ESI) for Nanoscale.

Supporting Information for

Few-layer $NiPS_3$ nanosheets as bifunctional materials for Li-ion storage and oxygen evolution reaction

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Figure S1. Raksha Dangol *et al.*

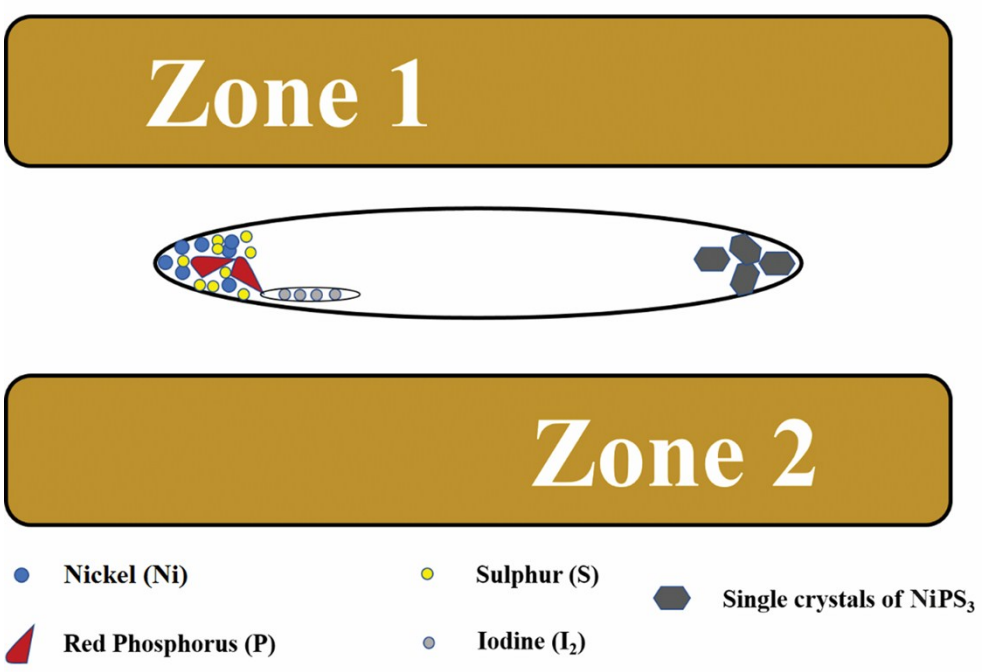

Figure S1 Schemetic of preparation of $NiPS_3$ bulk crystal.

Initially, the source zone (Zone 1) was kept at 650ºC and the growth zone (Zone 2) at 750ºC for 48 hours. This was done to allow the constituents to react completely as well as prevent the back transport or formation of undesired additional phases. After this duration, the temperature of Zone 1 was gradually increased to 750ºC and that of Zone 2 was lowered to 700ºC. This arrangement continued for next 120 hours. Further, the temperatures of both the zones were lowered to room temperature and ampoules were taken out to obtain the compounds for characterization and subsequent processes.

Figure S2. Raksha Dangol *et al.*

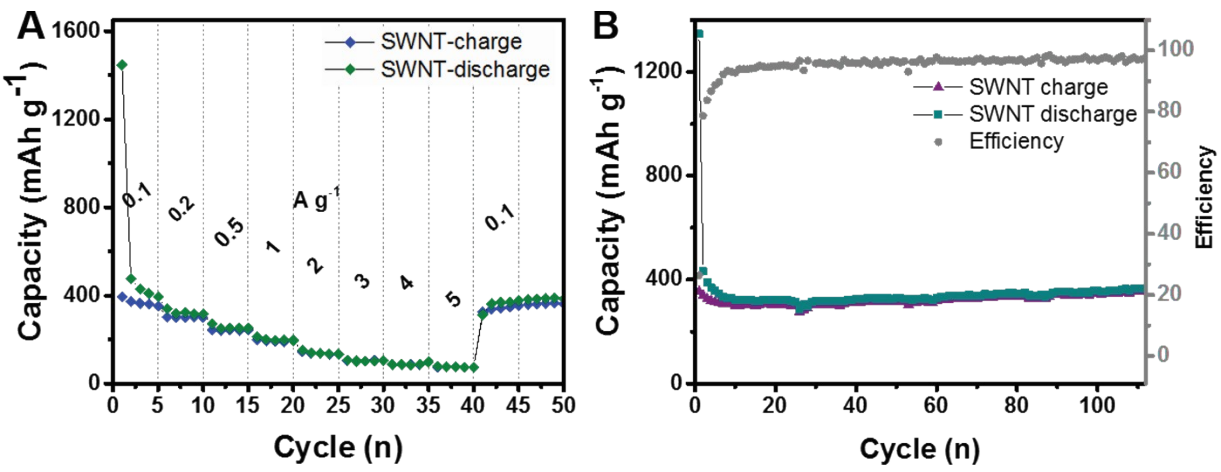

Figure S2 (A) Charge and discharge specific capacities at different current densities of single walled carbon nanotubes and (B) Cycling capacity of single walled carbon nanotubes at 0.1 A g^{-1}.

Figure S3. Raksha Dangol *et al.*

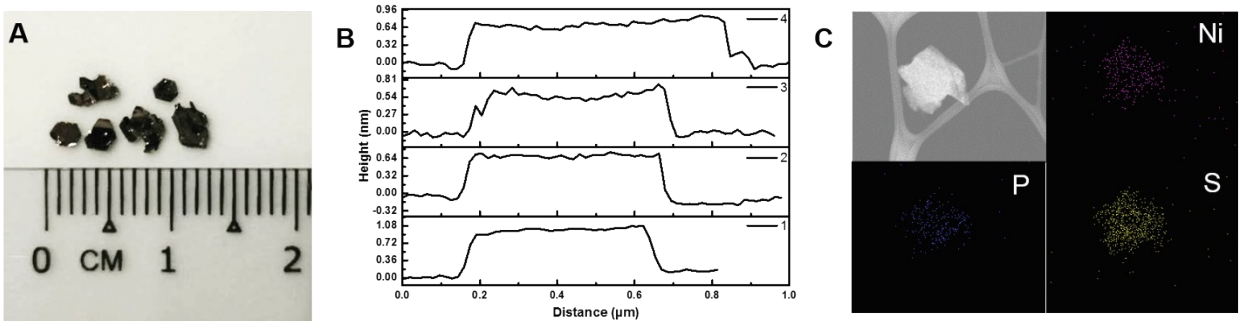

Figure S3 (A) Hexagonal bulk crystals of $NiPS_3$, (B) AFM height profiles of ENPS nanosheets in Figure 3 and (C) Elemental mapping of ENPS nanosheets.

Figure S4. Raksha Dangol *et al.*

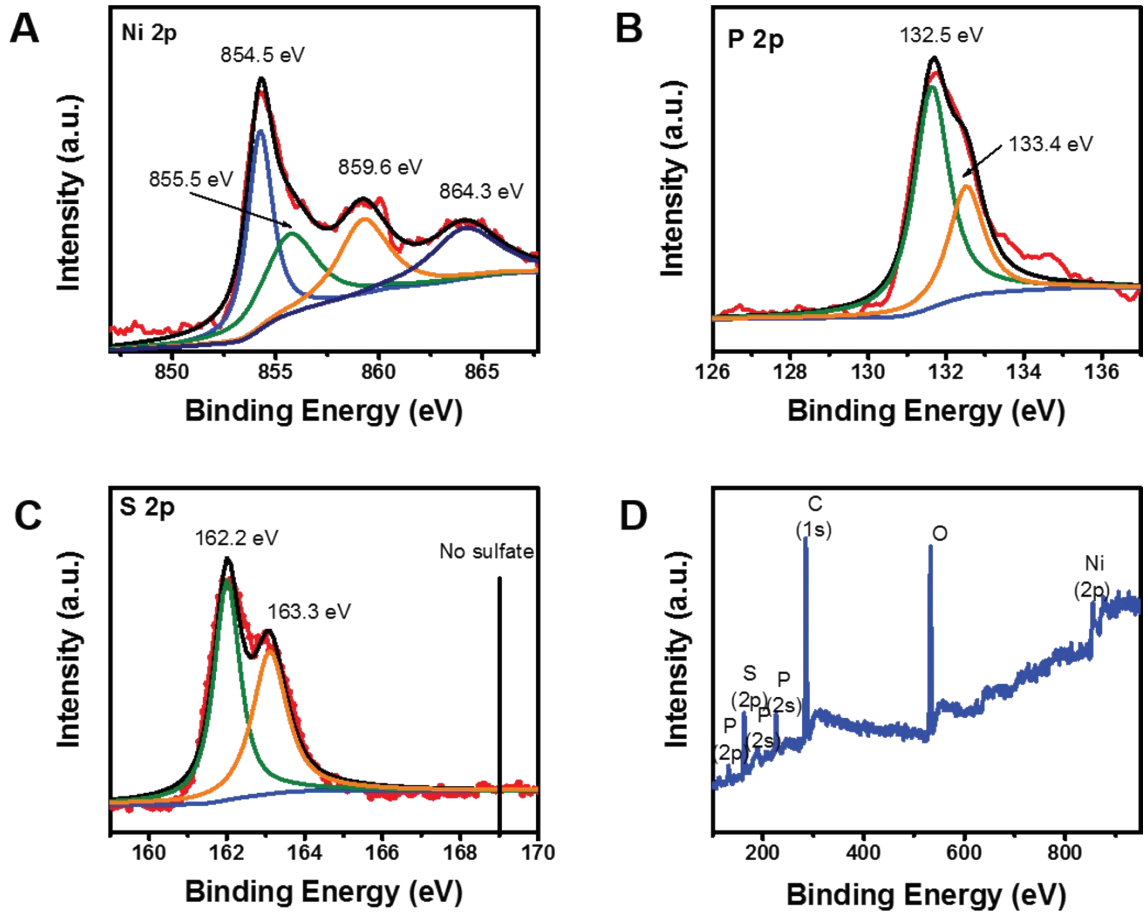

Figure S4 XPS spectra of (A) Ni 2p, (B) P 2p, (C) S 2p, and (D) Survey XPS spectrum.

Figure S5. Raksha Dangol *et al.*

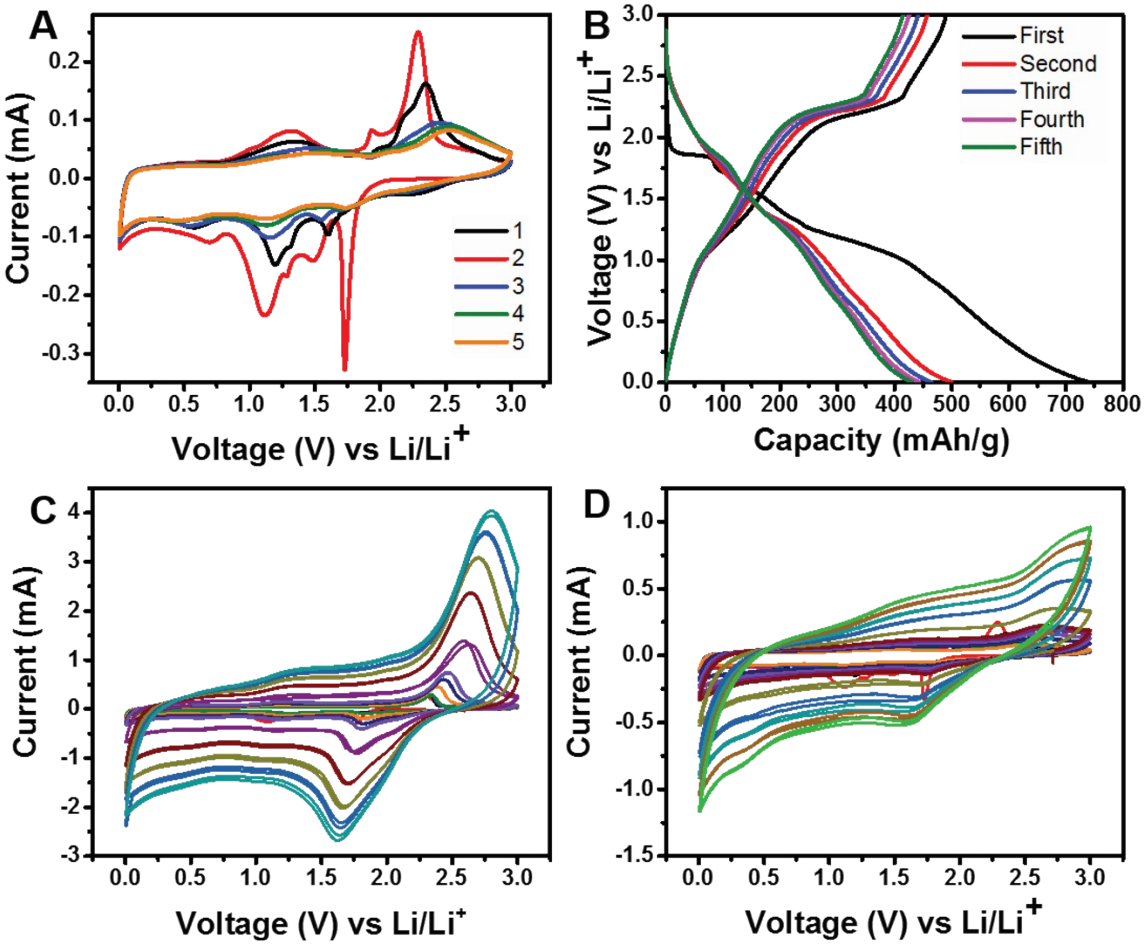

Figure S5 (A) First five CV cycles of BNPS at 0.1 mV s^{-1}, (B) First five charge-discharge cycles of BNPS at 0.1 A g^{-1}, (C) CV cycles of ENPS at various rates (0.1 – 5 mVs^{-1}) and (D) CV cycles of BNPS at various rates (0.1 – 5 mVs^{-1}).

Figure S6. Raksha Dangol *et al.*

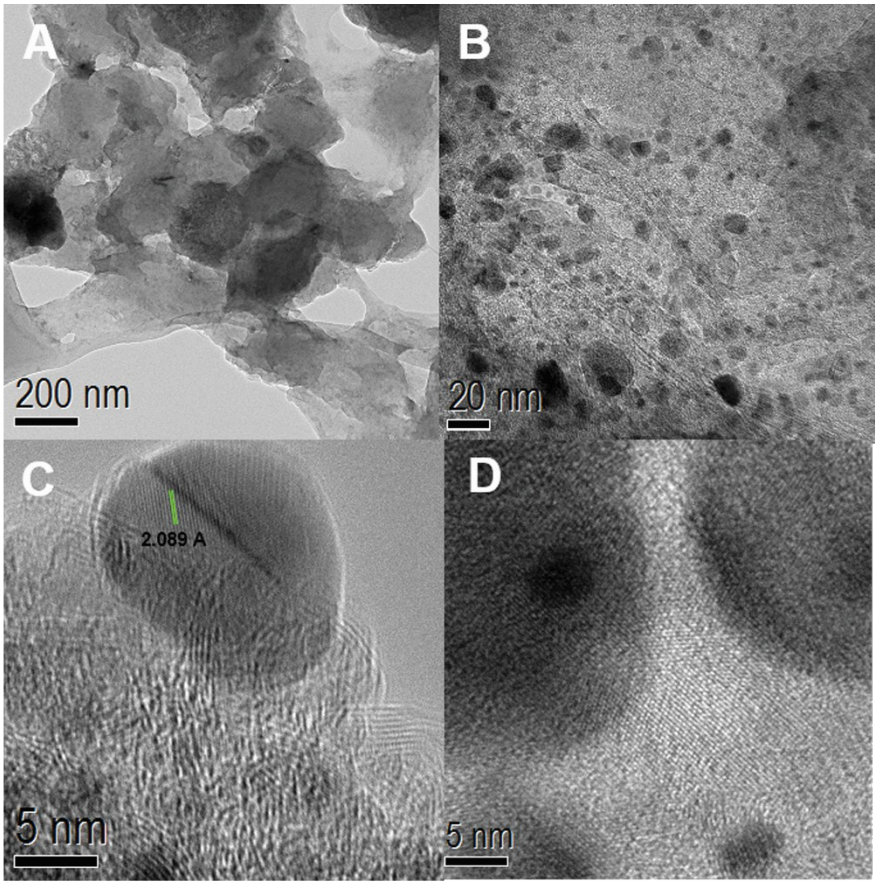

Figure S6 (A) and (B) TEM images, and (C) and (D) HRTEM images of ENPS electrode after first full discharge.

Figure S7. Raksha Dangol *et al.*

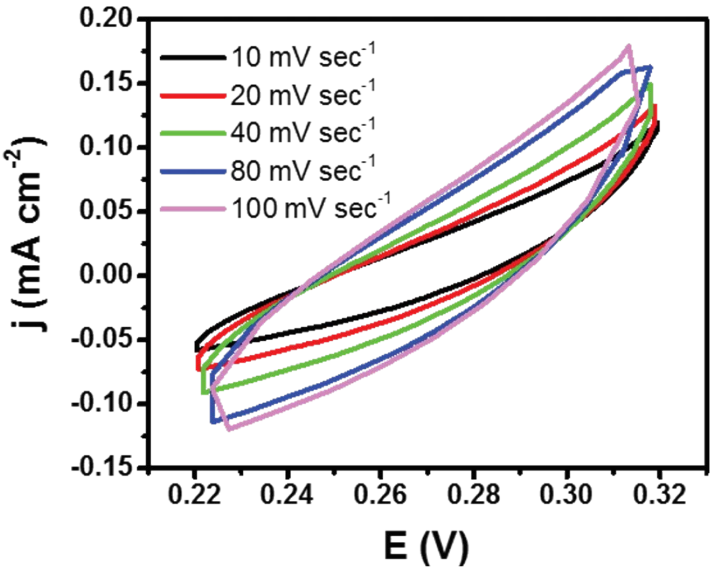

Figure S7 CV in the range of 0.22 V - 0.32 V for the calculation of ECSA of ENPS.

For the ECSA calculation, the CV measurements are first observed at the voltage range where the electrode material is inactive. The CV at this range is obtained at the scan rates of 10, 20, 40, 80 and 100 mV sec^{-1} given in Figure S7. Hence, Δj is calculated by absolute difference between values of j at the mid-point of E at j = 0. Lastly, the plot of Δj *vs*. square root of scan rate is plotted as in Figure 5D and their linear fit i.e. slope was obtained.

Figure S8. Raksha Dangol *et al.*

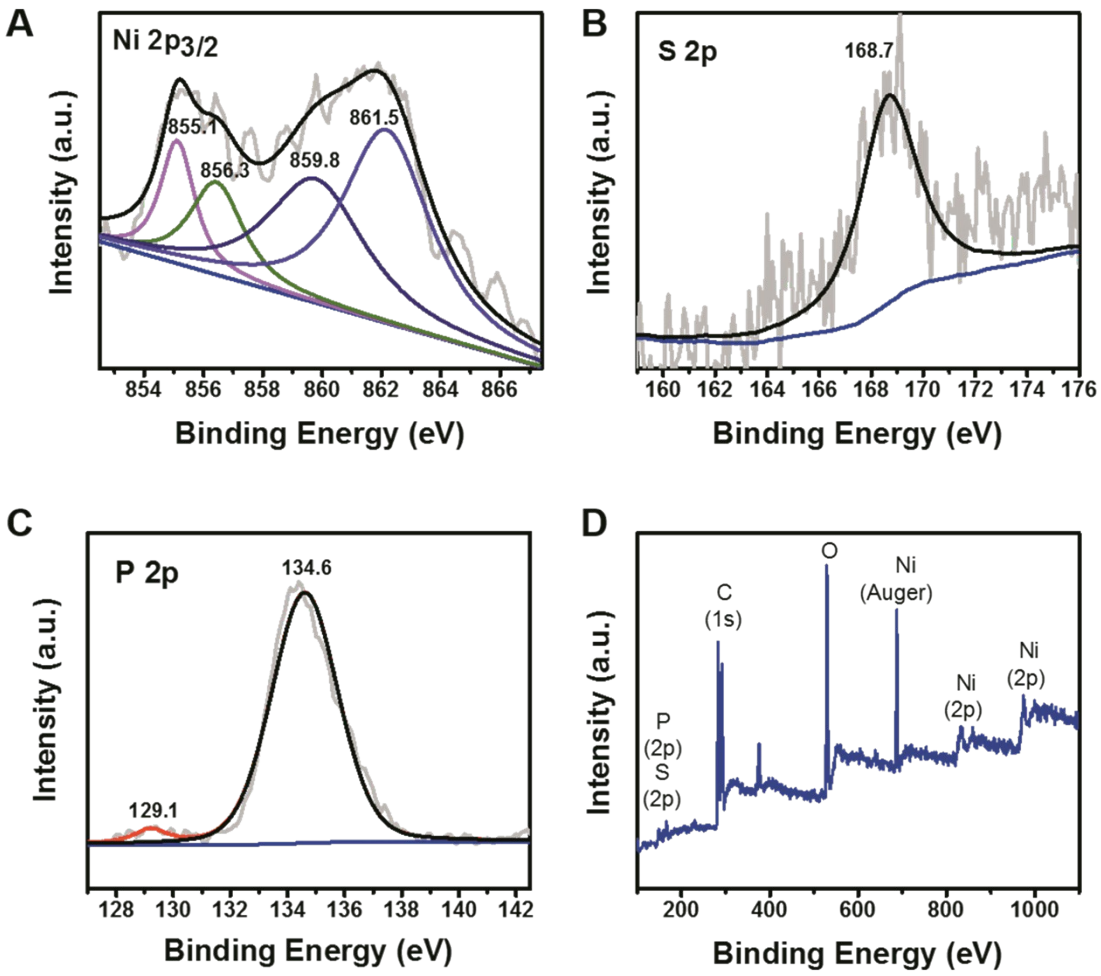

Figure S8 XPS spectra of (A) Ni $2p_{3/2}$, (B) S 2p, (C) P 2p and (D) Survey XPS spectrum of ENPS after OER.

Figure S9. Raksha Dangol *et al.*

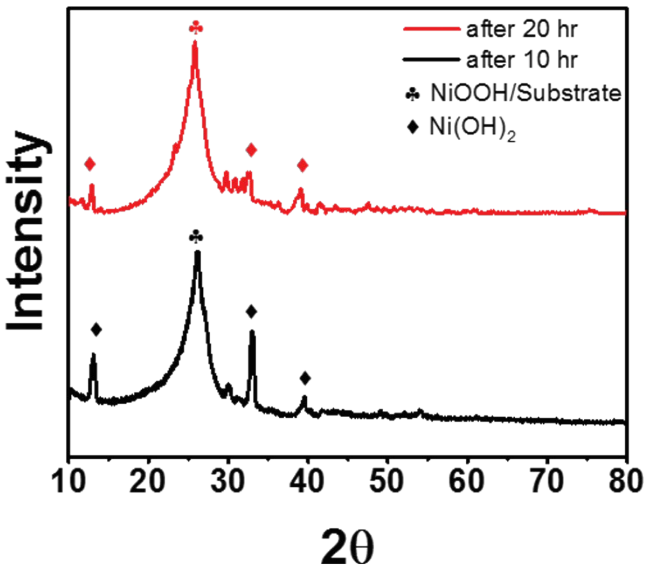

Figure S9 XRD patterns of ENPS after OER durability testing.