A facile synthesis of $FePS_3$@C nanocomposites and their enhanced performance in lithium-ion batteries

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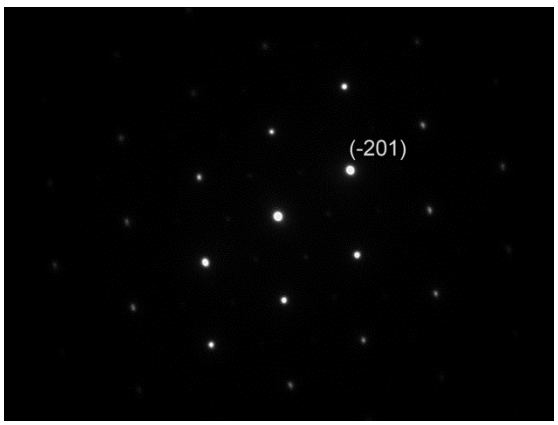

Figure S1: SAED pattern of the $FePS_3$@C nanocomposite.

Fig. S2a shows that except the peaks of copper foil, Li_2S was successfully detected

after the third discharge to 1 V. Because the metallic Fe nanoparticles are presumably smaller than the X-ray coherence length, as there are no diffraction peaks [1]. In addition, we did not detect the presence of Li_3P from XRD. **Fig. S2**b presents an TEM image of the $FePS_3$@C electrode at the 3rd discharged state, which shows that the sample degraded into nano-aggregate. Furthermore, **Fig. S2**c displays the HRTEM image of the $FePS_3$@C electrode after the 3rd discharged reaction, the lattice fringes is 0.182nm, which confirms the existence of iron.

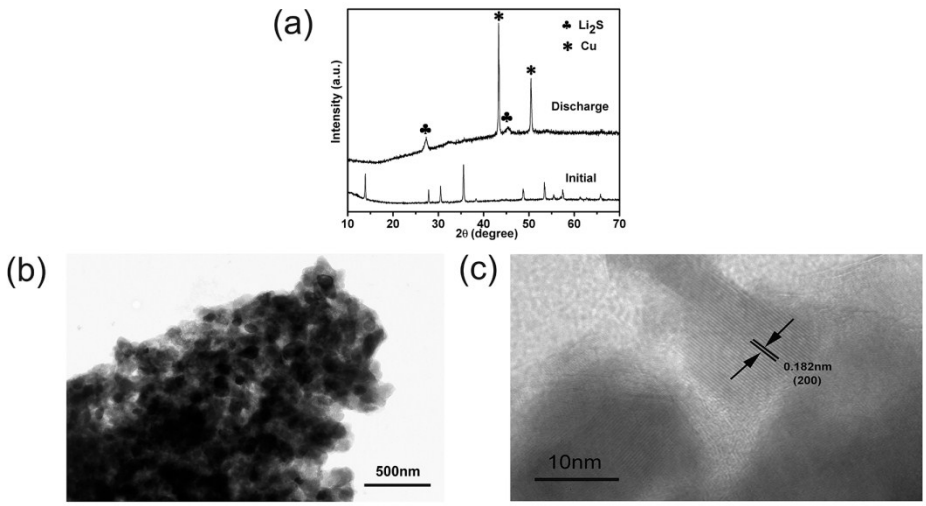

Fig. S2 (a) Cycle testing of an ex situ XRD patterns of the $FePS_3$@C nanocomposite electrode. (b) TEM image of the $FePS_3$@C nanocomposite electrode after 3 cycles at 0.2 A g^{-1}. (c) HRTEM image of the $FePS_3$@C nanocomposite electrode after 3 cycles at 0.2 A g^{-1}.

Bulk $FePS_3$ sample was successfully prepared by a conventional solid state method. Powders of the elements Fe (99%), red phosphorus (99%) and sublimate sulphur (99%), in an atomic ratio of Fe : P : S = 1 : 1 : 3 were thoroughly mixed together, then sealed into

quartz ampoule evacuated. The ampoule was slowly heated up to 923 K, holding for 24 h. Finally, shinny gray-black products for subsequent tests were collected after the furnace cooled down to room temperature naturally. All the peaks of powder XRD pattern can be well indexed based on a monoclinic-type cell with the space group of *C*2/m (JCPDS card no. 33-0672), indicate the single phase of sample. The SEM image of bulk $FePS_3$ sample shows a typical stacked 2D microstructures. The bulk $FePS_3$ electrode exhibits capacity of about 600 mAh g^{-1} over 70 cycles at a current density of 0.2 A g^{-1} and capacity of 400 mAh g^{-1} over 80 cycles at 1 A g^{-1}, as shown in **Fig S3**(c, d).

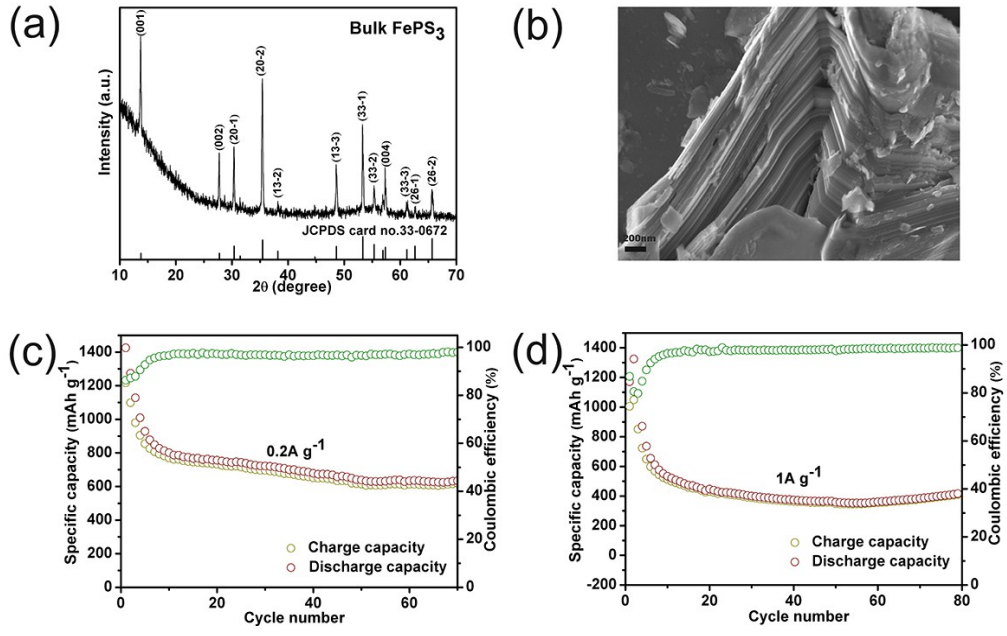

Fig. S3 (a) Powder X-ray diffraction pattern of the bulk $FePS_3$ sample. (b) SEM image of bulk $FePS_3$ sample. (c) Cycling performance and coulombic efficiency (CE) of the bulk $FePS_3$ electrode at a current density of 0.2 A g^{-1}. (d) Cycling performance and coulombic efficiency (CE) of the bulk $FePS_3$ electrode at a current density of 1 A g^{-1}.

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50 **References:**

51 [1] P. Poizot, S. Laurelle, S. Greugon, L. Dupont, J. M. Tarascon, Nature 407 (2000) 496.

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