A facile synthesis of FePS₃@C nanocomposites and their enhanced performance in lithium-ion batteries

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Figure S1: SAED pattern of the FePS₃@C nanocomposite.

Fig. S2a shows that except the peaks of copper foil, Li₂S 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$_3$P from XRD. **Fig. S2b** 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. S2c** 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](image_url)

**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, shiny 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 C2/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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