Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Improved Electrochemical Properties of Tavorite $LiFeSO_4F$ by Surface Coating with Hydrophilic Poly-Dopamine via a Self-Polymerization Process

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Experimental Details

Synthesis of tavorite $LiFeSO_4F$: Tavorite $LiFeSO_4F$ was prepared by the tetraethylene glycol (TEG) assisted solvothermal method. First, 850 mg $FeSO_4 \cdot H_2O$ was prepared by heating $FeSO_4 \cdot 7H_2O$ at 100 °C for 3 h in an Ar/H_2 (93:7) atmosphere. The $FeSO_4 \cdot H_2O$ precursor was mixed with stoichiometric LiF, and then ball-milled for 24 hours in acetone. The mixture was transferred into a Teflon-lined steel autoclave filled with 30 ml TEG. The autoclave was kept at 260 °C for 60 h. After cooling to room temperature, the white-gray powder was washed with acetone and then dried in vacuum-oven at 60 °C.

Synthesis of PDA@Li_xFeSO_4F: The poly-dopamine coating of the material follows a two-step process. For the first step, 400 mg $LiFeSO_4F$ was chemically de-lithiated by 300 mg NO_2BF_4 in 30 ml acetonitrile. Then, the obtained Li_xFeSO_4F powder was dispersed in 20 mL ethanol. After ultrasonic treatment for 30 min, 40 mg dopamine hydrochloride was added into the suspension with constant stirring for 12 hours to complete the polymerization of dopamine. The product was washed with ethanol and collected by centrifugation.

Materials characterizations: The crystal structure of the materials was studied by X-ray diffraction on a Bruker AXS D8 diffractometer with Cu Kα radiation. Fourier transform infrared spectroscopy was carried out using a Thermao Scientific Nicolet 6700 spectrometer with the KBr disk method. X-ray photoelectron spectroscopy was performed on an ESCALAB spectrometer using Mg-Kα light source. Thermogravimetric analysis was performed on an SDTA851E thermoanalyzer with a heating rate of 10 °C min^{-1} under N_2 flow. The morphologies of the materials were observed by a JSM-6700F scanning

electron microscope and a FEI Tecnai G2transmission electron microscope. Mössbauer spectroscopy was collected in the transmission mode using a ^{57}Co/Pd γ-ray source. Velocity calibration was performed with the data of α-Fe at room temperature. The ac impedance spectroscopy was performed on a Solartron 1260 impedance analyzer.

Electrochemical measurements: Electrochemical experiments were conducted on CR2032 coin cells using metallic lithium as the anode. The cathode slurry was composed of 70 wt.% active material, 20 wt.% active carbon and 10 wt.% poly-vinylidenefluoride binder which was pasted on an Al current collector. The anode and cathode were separated by a Celgard 2400 membrane. A 1 mol L^{-1} lithium hexafluorophosphate ($LiPF_6$) solution dissolving in ethylene carbonate (EC) and diethyl carbonate (DEC) (EC : DEC = 1: 1) was used as the electrolyte. Galvanostatic charge-discharge was performed on a LAND-2010 automatic battery tester in the voltage window of 2.5-4.5 V. Cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS) were performed on a Bio-Logic VSP multichannel potentiostatic-galvanostatic system. The CV curves were collected using a voltage scan rate of 0.1 mV s^{-1}. The impedance data were recorded by applying an *ac* voltage of 5 mV in the frequency range from 1 MHz to 1 mHz.

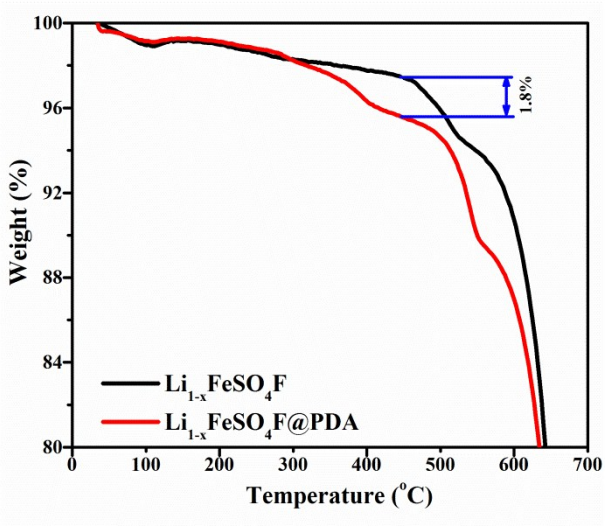

Figure S1. TG curves of the $Li_{1-x}FeSO_4F$ and PDA@$Li_{1-x}FeSO_4F$ samples.

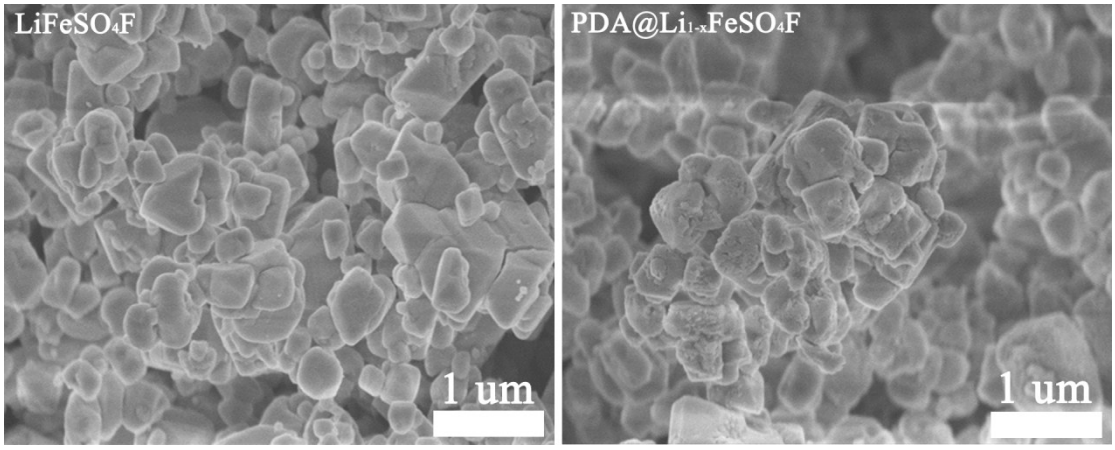

Figure S2. SEM images of the $LiFeSO_4F$ and $PDA@Li_{1-x}FeSO_4F$ samples.

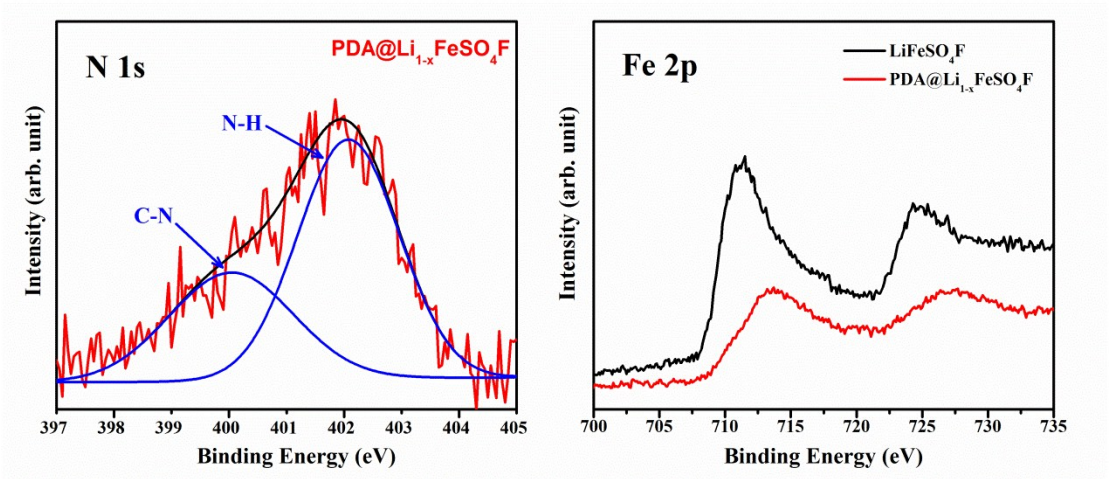

Figure S3. N 1s XPS of PDA@$Li_{1-x}FeSO_4F$, and the Fe 2p XPS of the $LiFeSO_4F$ and PDA@$Li_{1-x}FeSO_4F$ samples.

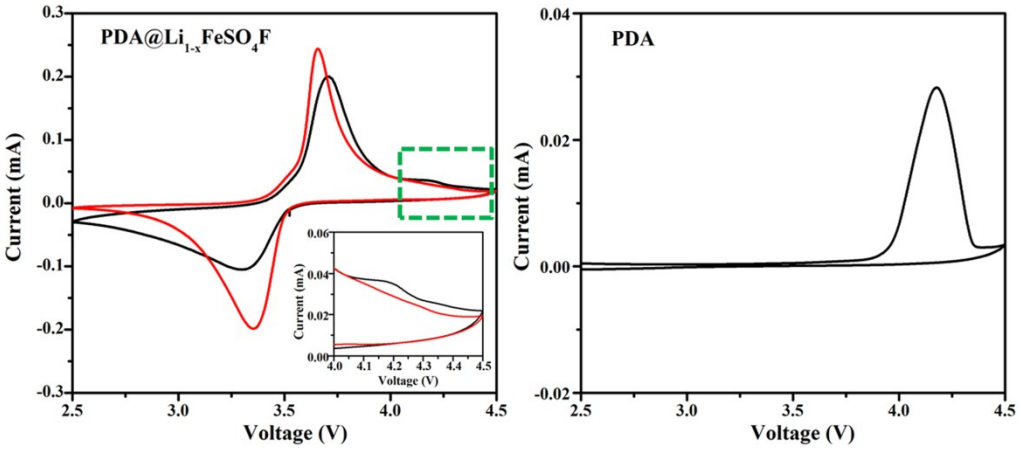

Figure S4. CV curves of the PDA and PDA@$Li_{1-x}FeSO_4F$ materials.

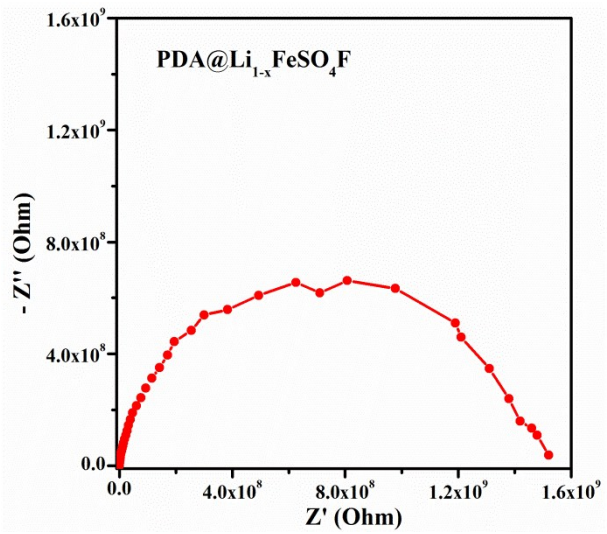

Figure S5. AC impedance spectroscopy of the PDA@$Li_{1-x}FeSO_4F$ material.