Supporting Information

Improved and scalable method for the preparation of Sn-doped hexagonal tungsten bronze-type iron fluoride material as cathode for sodium-ion batteries

Keywords: Iron fluoride; Sn-doped; First-principles calculation; Cathode material; Sodium-ion battery

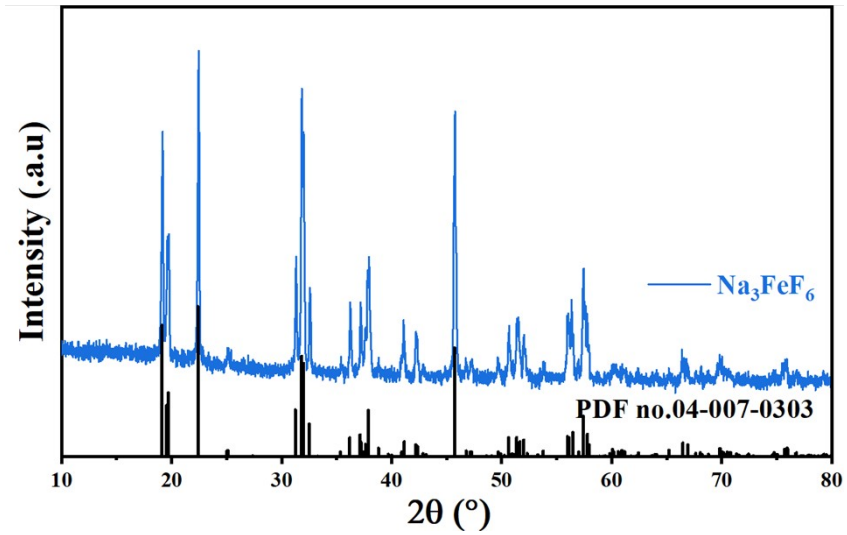

Figure S1. The XRD diffraction peaks of the precipitate, which was produced by the addition of saturated sodium chloride solution.

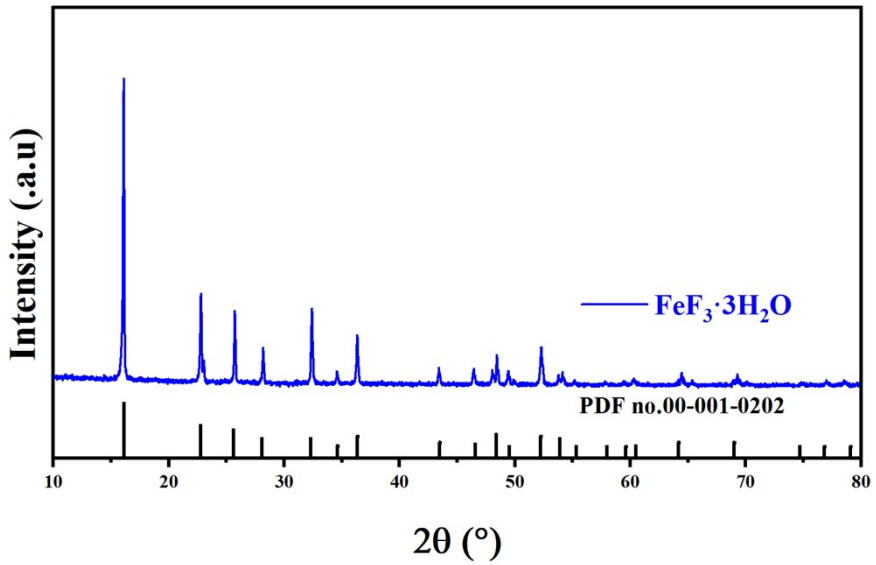

Figure S2. The XRD diffraction peaks of sample after cryodesiccation.

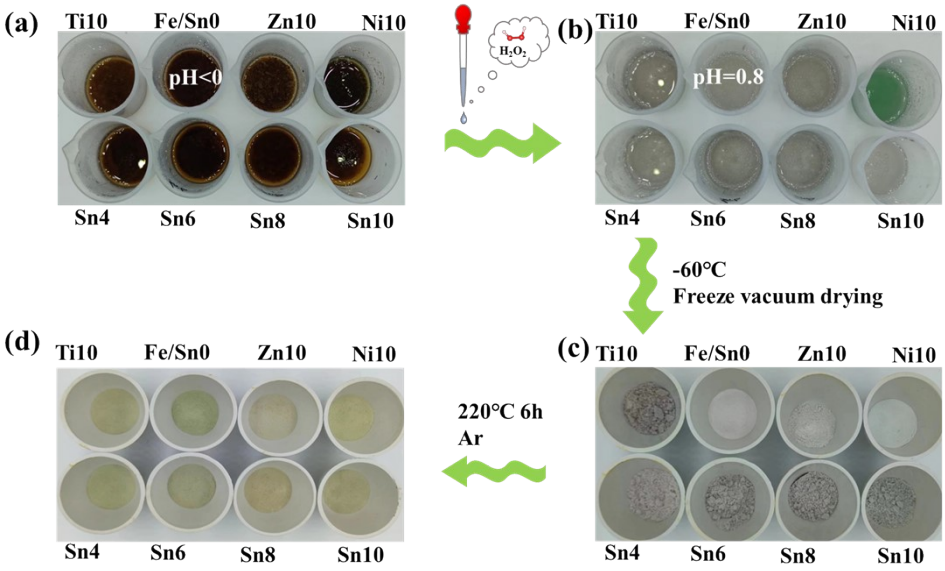

Figure S3. The color change of each step during the synthesis process of $Me_xFe_{1-x}F_3 \cdot 0.33H_2O$ without GO.

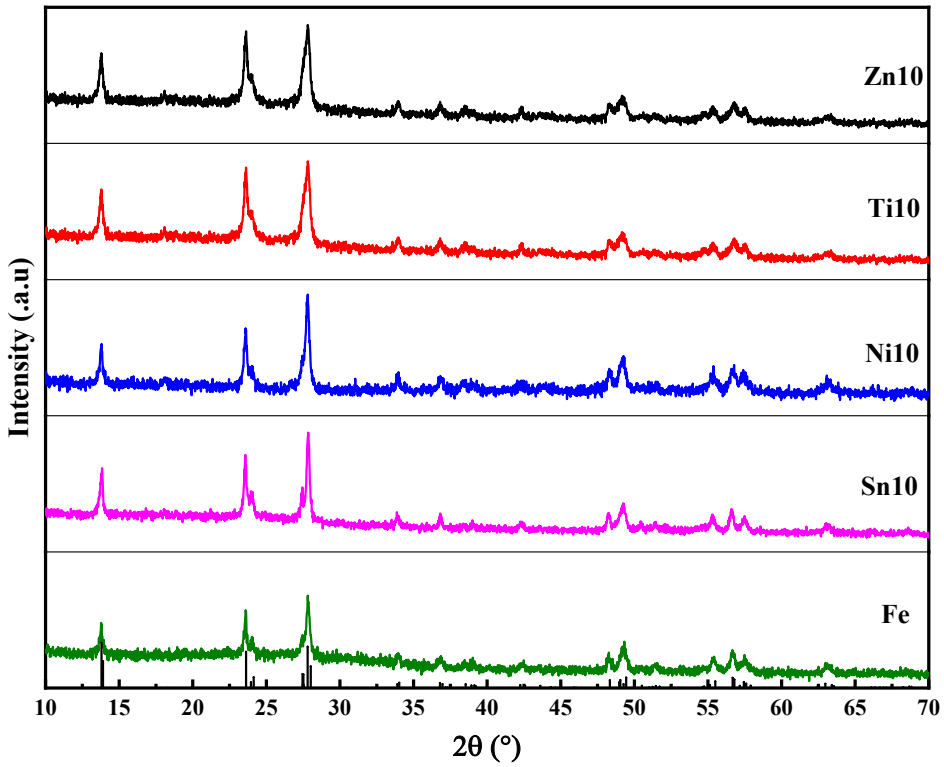

Figure S4. XRD pattern of Zn10, Ti10, Ni10, Sn10, Fe without GO.

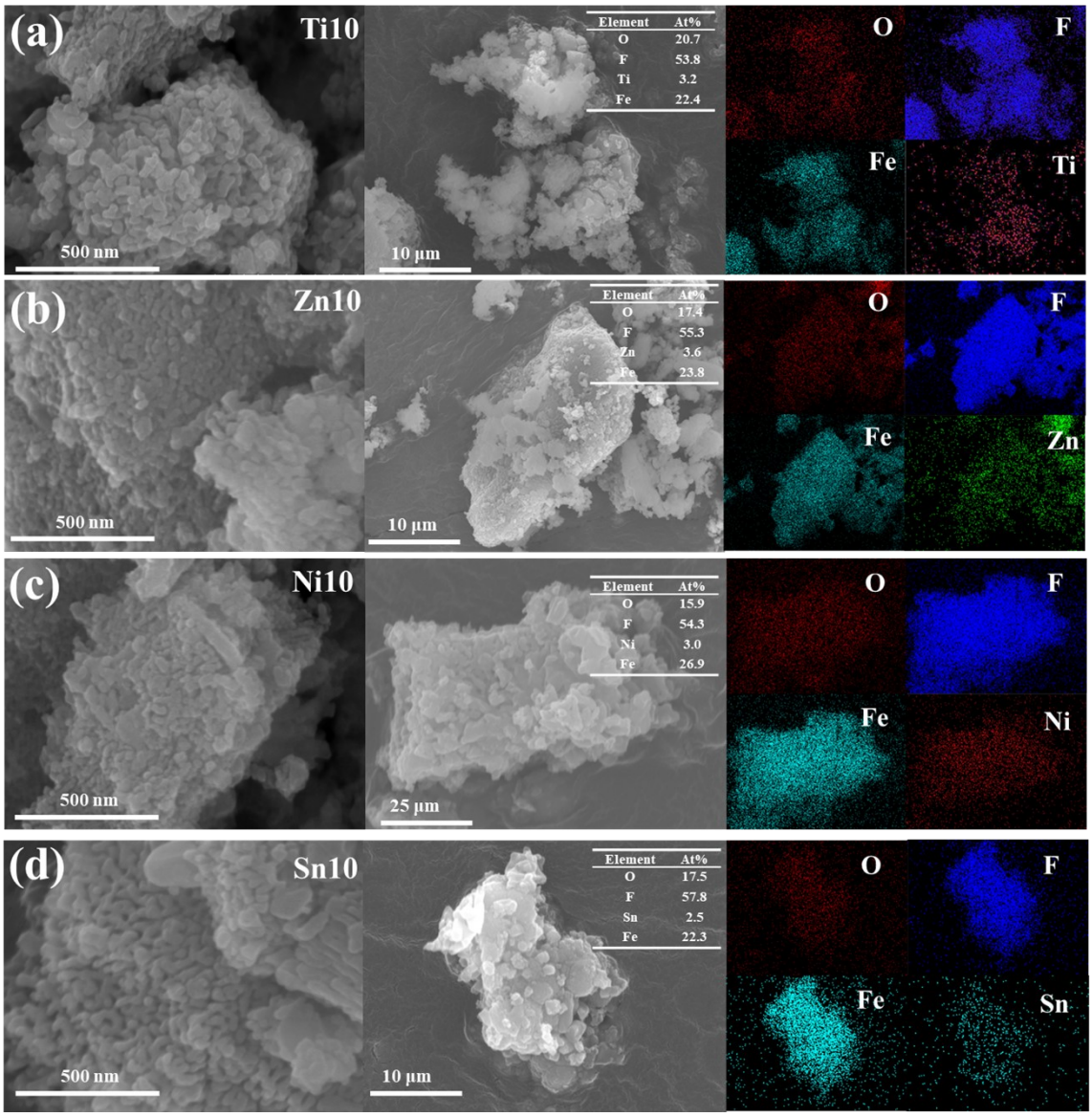

Figure S5. EDS mapping of SEM for (a)Ti10, (b)Zn10, (c)Ni10 and (d)Sn10 without GO.

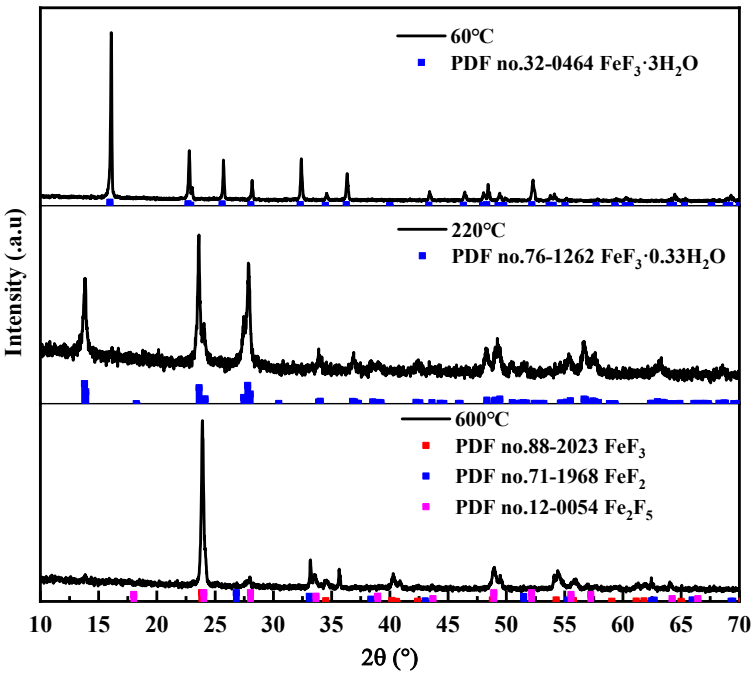

Figure S6. XRD pattern of S60, S220 and S600.

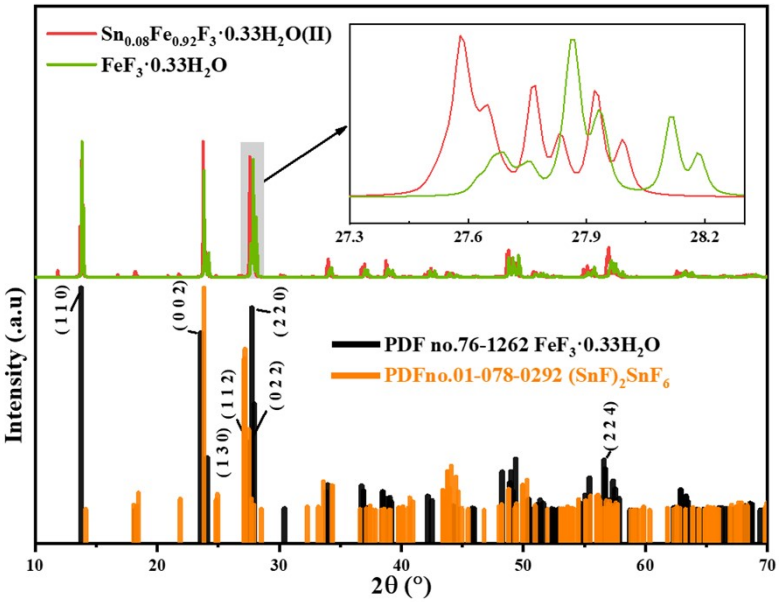

Figure S7. Simulated XRD diffraction patterns fitted with DFT computational models of $FeF_3·0.33H_2O$ and $Sn_{0.08}Fe_{0.92}F_3·0.33H_2O$-mid, along with the standard $FeF_3·0.33H_2O$ and tin fluoride PDF card.

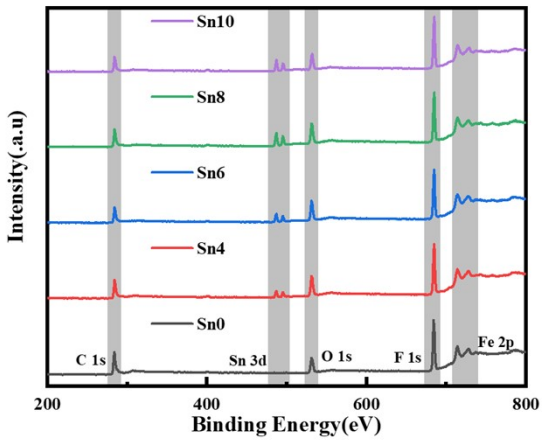

Figure S8. Total XPS spectra of Sn0, Sn4, Sn6, Sn8, and Sn10.

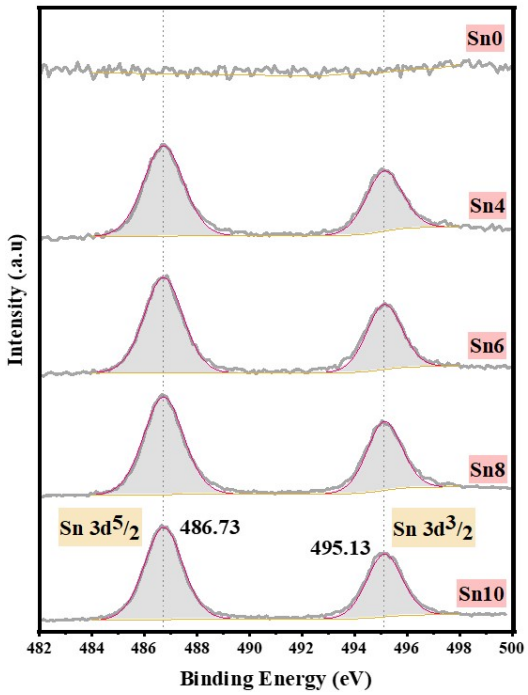

Figure S9. XPS spectra in the region of the Sn 3d peak of Sn0, Sn4, Sn6, Sn8 and Sn10, respectively.

Table S1. Summary of cell parameters used for GITT calculation

			Sn0	Sn8
τ	the applied current time interval	min	3	3
M	atomic weight of active material	g mol^{-1}	119	124
V_m	the molar volume of active material	cm^3 mol^{-1}	30.75	32.04
m	mass of active material	mg	2.01	2.12
S	the electrode surface area	cm^2	16.01	16.02

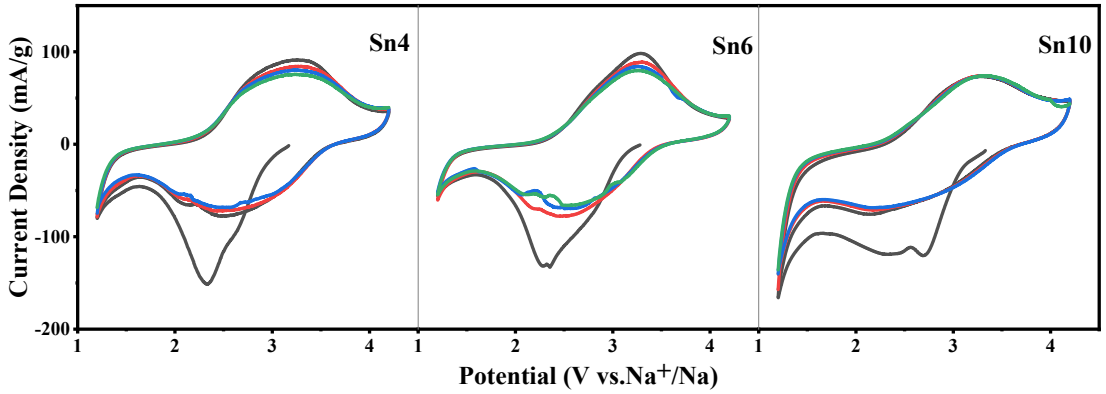

Figure S10. The cyclic voltammetry curves of Sn4, Sn6 and Sn10 for the initial four cycles at a scan rate of 0.2 mV s^{-1}.

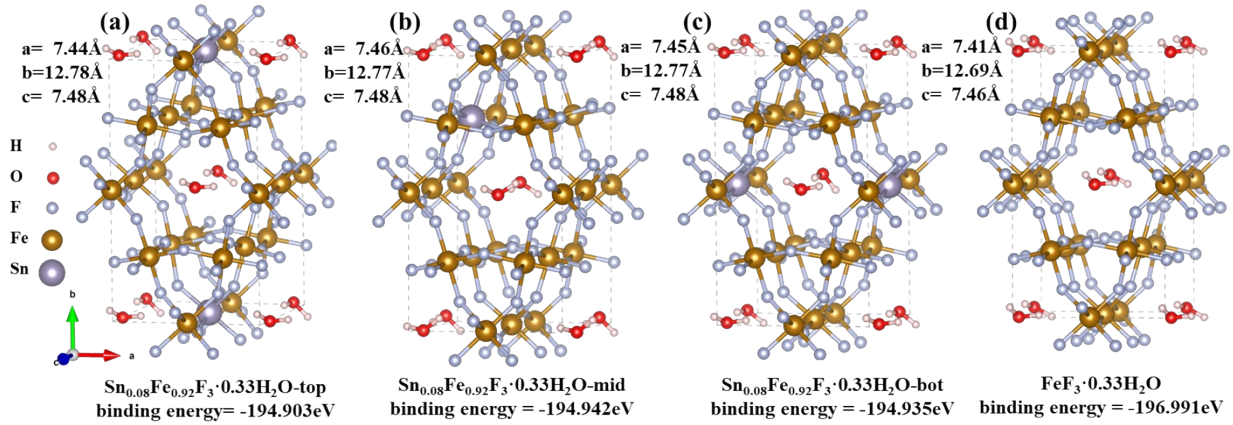

Figure S11. Models of the cell structures of (a) $Sn_{0.08}Fe_{0.92}F_3 \cdot 0.33H_2O$-top, (b) $Sn_{0.08}Fe_{0.92}F_3 \cdot 0.33H_2O$-mid, (c) $Sn_{0.08}Fe_{0.92}F_3 \cdot 0.33H_2O$-bot and (d) $FeF_3 \cdot 0.33H_2O$ obtained from DFT calculations and the binding energies of their corresponding cells.