The supporting information

Enhanced Charge Storage of Li_3FeF_6 with Carbon Nanotubes for Lithium-Ion Batteries

Yueli Shi[a,b], Shubin Sun[a], Jingjing Liu[a], Yongli Cui[a], Quanchao Zhuang[a]*, Xiaobo Chen[b]*

[a] *Lithium-ion Batteries Laboratory, School of Materials Science and Engineering, China University of Mi*

[b] *Department of Chemistry, University of Missouri – Kansas City (UMKC) Kansas City, MO 64110, USA*

Fig. S1-S8

Table. S1-S3

To whom correspondence should be addressed.

[a.] *Lithium-ion Batteries Laboratory, School of Materials Science and Engineering, China University of Mining and technology, Xuzhou 221116, China.Quanchao Zhuang,Tel: +8613605215324, E-mail: zhuangquanchao@126.com,Fax: +86 516 83591870*

[b.] *Department of Chemistry, University of Missouri – Kansas City (UMKC) Kansas City, MO 64110, USA.Xiaobo Chen, Tel: 816-235-6420, E-mail: Email: chenxiaobo@umkc.edu.*

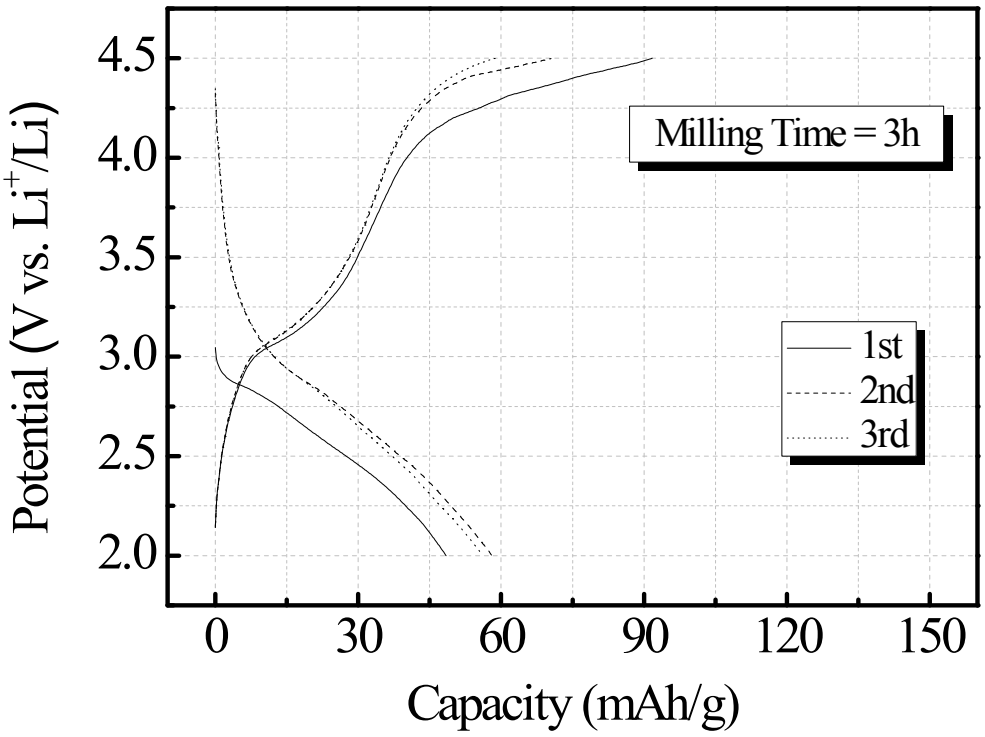

Fig. S1. Charge-discharge profiles of Li_3FeF_6/C cathode obtained by milling for 3 h at the current density of 14 mA g^{-1} under the potential range of 4.5~2.0 V

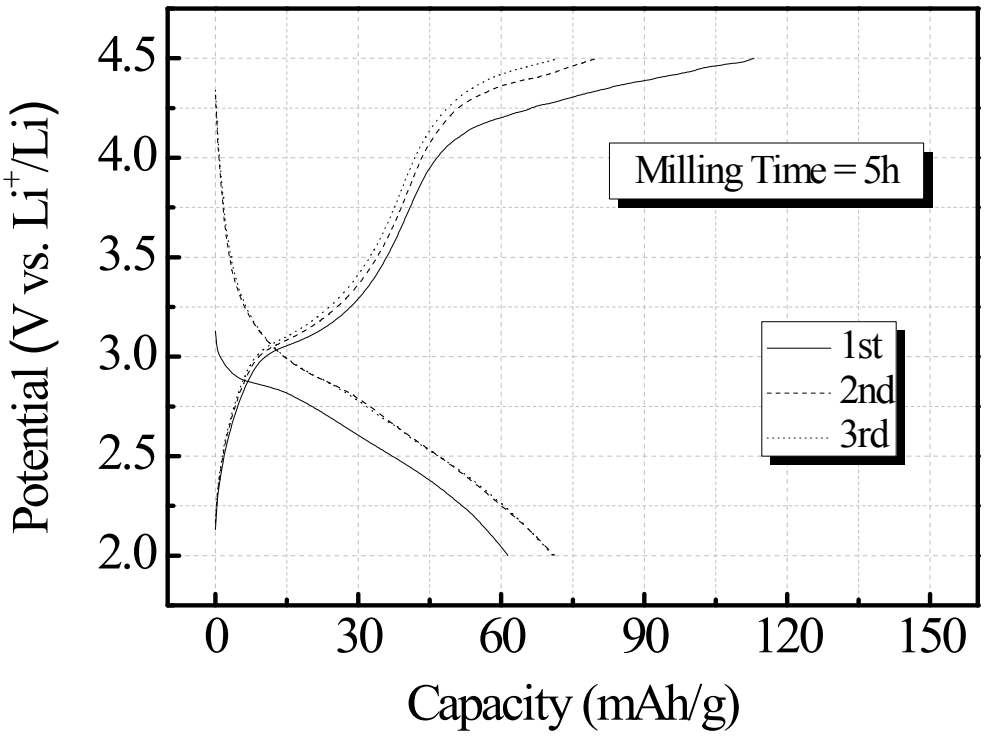

Fig. S2. Charge-discharge profiles of Li_3FeF_6/C cathode obtained by milling for 5 h at the current density of 14 mA g^{-1} under the potential range of 4.5~2.0 V

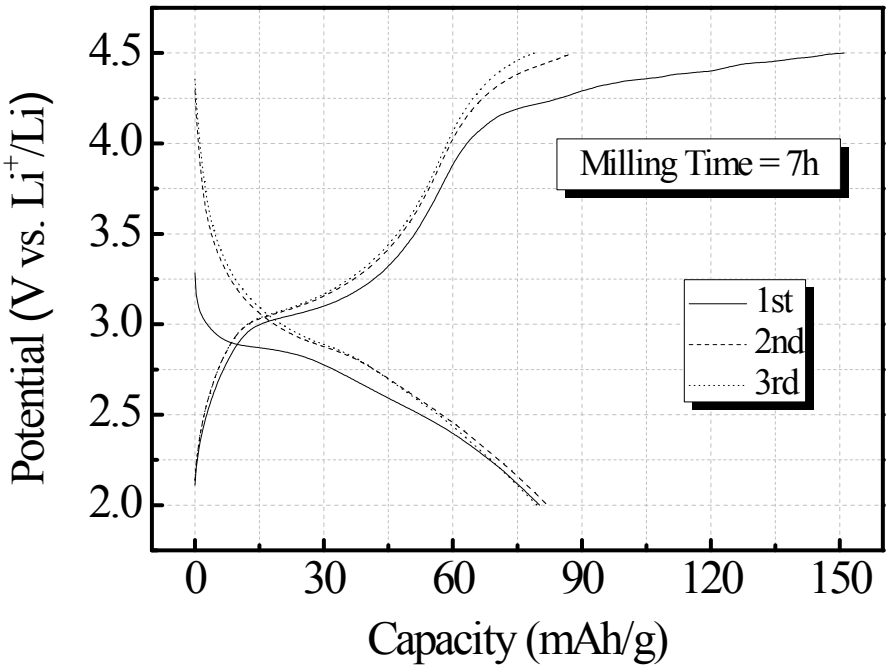

Fig. S3. Charge-discharge profiles of Li_3FeF_6/C cathode obtained by milling for 7 h at the current density of 14 mA g^{-1} under the potential range of 4.5~2.0 V

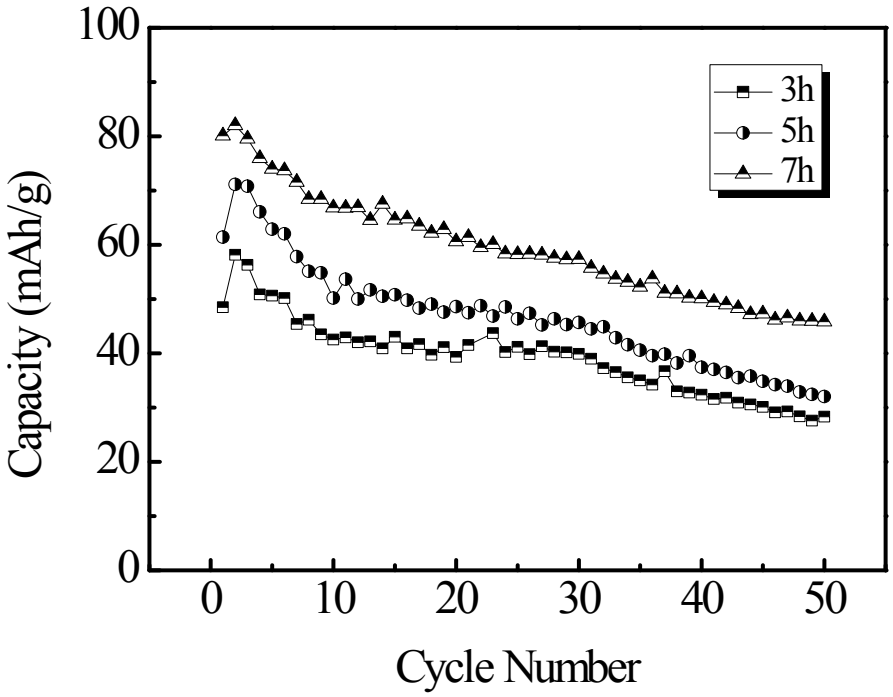

Fig. S4. The capacity-cycle profiles of Li_3FeF_6/C cathode obtained by milling at different times for 3 h, 5 h and 7 h, at the current density of 14 mA g^{-1} under the potential range of 4.5~2.0 V

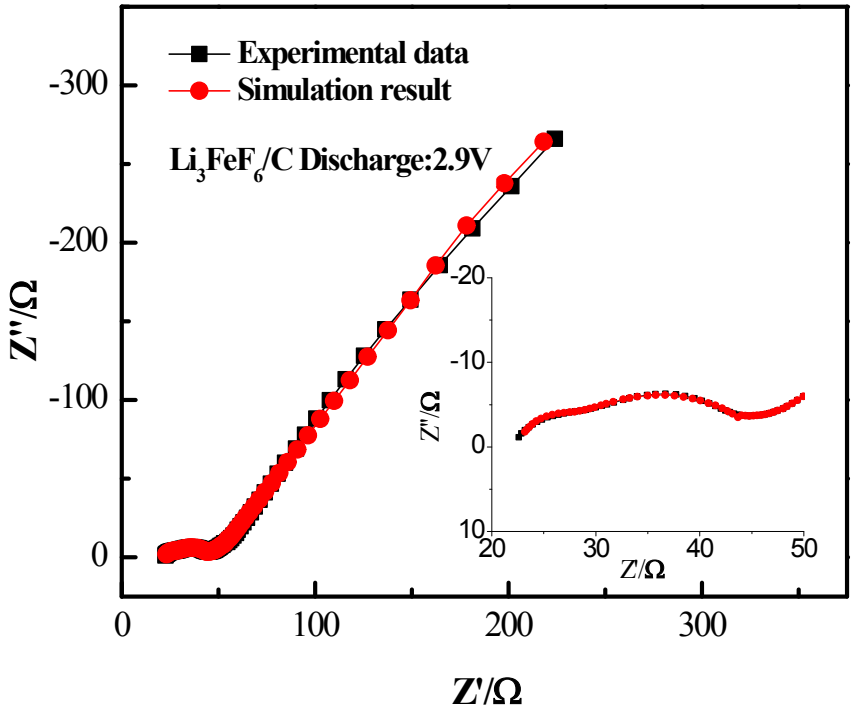

Fig. S5. Comparisons of EIS of Li_3FeF_6/C cathode experimental data recorded at 2.9 V during discharge process with the simulation result obtained from the proposed equivalent circuit

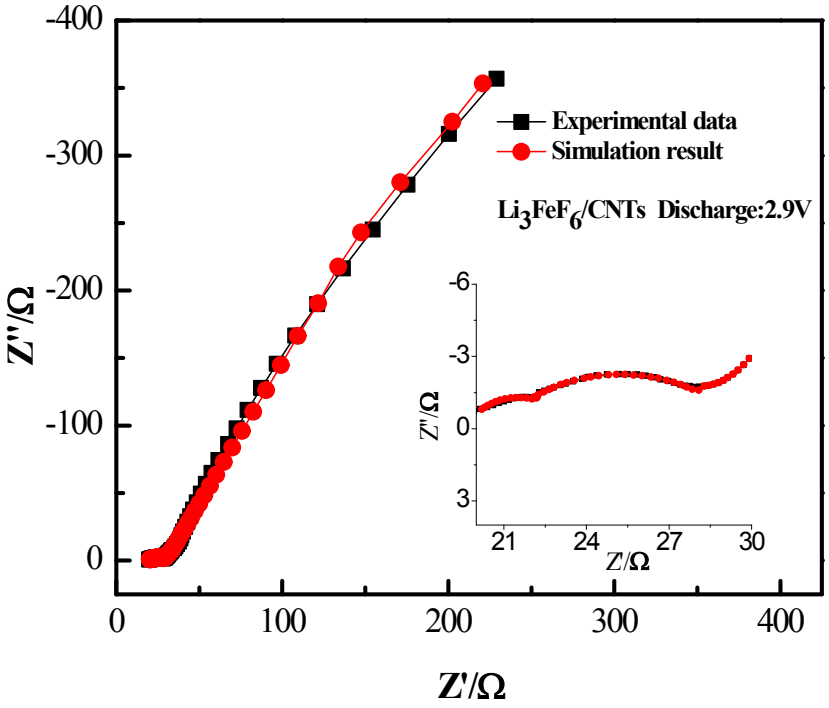

Fig. S6. Comparisons of EIS of Li_3FeF_6/CNTs cathode experimental data recorded at 2.9 V during discharge process with the simulation result obtained from the proposed equivalent circuit

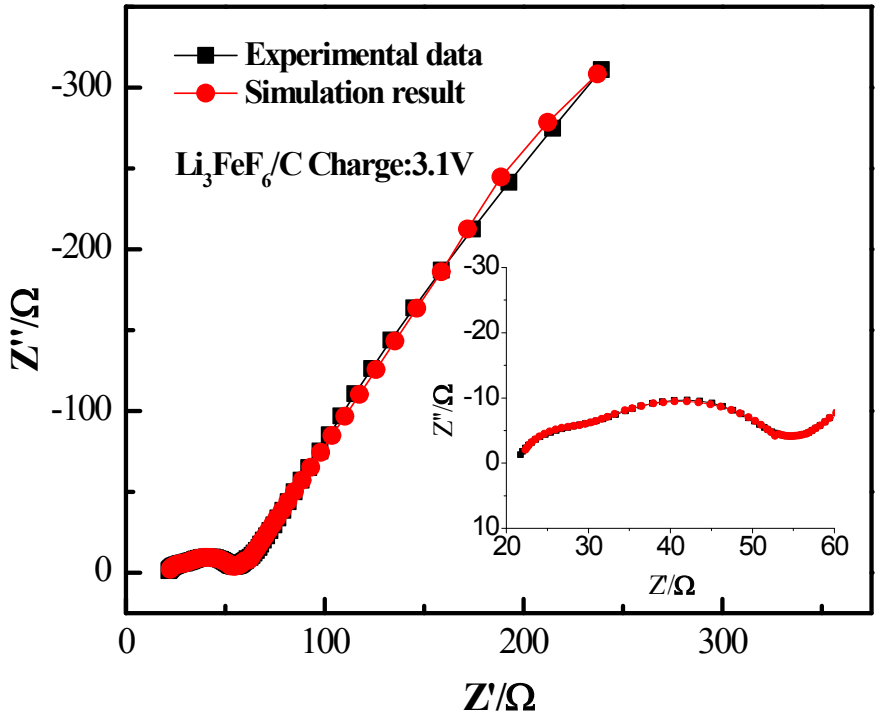

Fig. S7. Comparisons of EIS of Li_3FeF_6/C cathode experimental data recorded at 3.1 V during charge process with the simulation result obtained from the proposed equivalent circuit

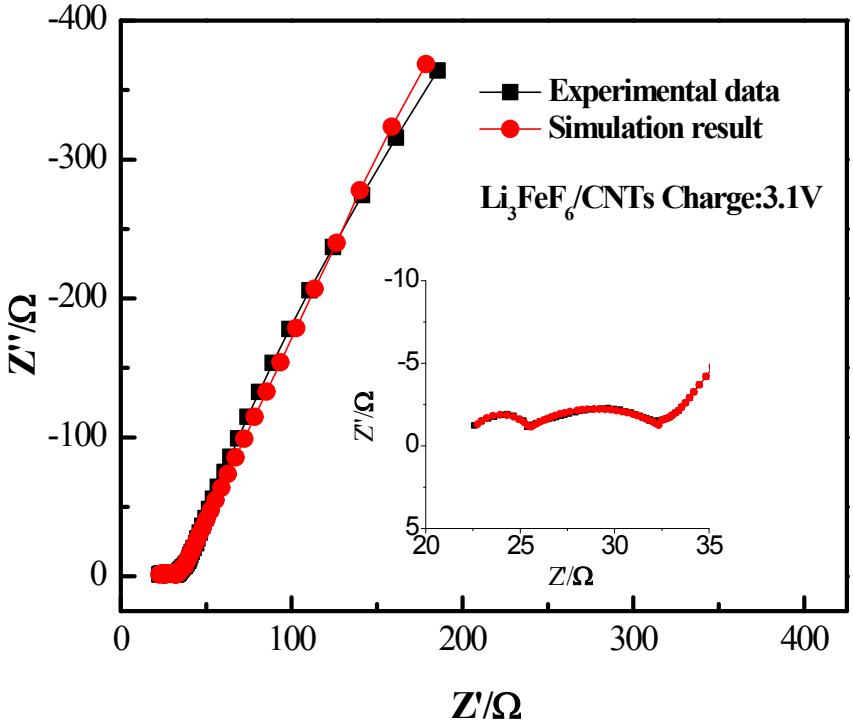

Fig. S8. Comparisons of EIS of Li_3FeF_6/CNTs cathode experimental data recorded at 3.1 V during charge process with the simulation result obtained from the proposed equivalent circuit

Table S1

The comparison of the LIBs performance in the manuscript with related research.

Reporter	Electrode composition (wt%)	Current (mA g^{-1})	Maximum capacity (mA h g^{-1})	Cycles	Capacity retention (%)
The manuscript	Li_3FeF_6: 84 CNTs: 1 Binder: 15	14(C/10)	120	50	83
G. Lieser *et al.*	Li_3FeF_6: 72 C: 25 binder: 3	7(C/20)	128	100	47
A. Basa *et al*.	Li_3FeF_6: 72 C: 25 binder: 3	7.8(C/18)	140	30	85

Table S2

Equivalent circuit parameters of Li_3FeF_6/C and Li_3FeF_6/CNTs cathode at 2.9 V in the discharge process .

parameters	Li_3FeF_6/C		Li_3FeF_6/CNTs	
	value	Uncertainty (%)	value	Uncertainty (%)
R_s (Ω)	22.54	0.32164	19.61	0.76145
R_{SEI} (Ω)	3.939	10.318	3.9	10.099
Q_{SEI} – n	1.4478×10^{-6}	14.629	4.8253×10^{-5}	14.315
Q_{SEI} – Y_0	1.032	3.5135	0.059305	7.9561
R_{ct}(Ω)	20.12	2.9232	9.205	2.2128
Q_{ct} – n	1.6137×10^{-4}	9.1194	8.1569×10^{-4}	9.1795
Q_{ct} – Y_0	0.68284	2.2607	0.57871	2.1588
R_D（Ω）	1398	5.5611	1657	2.8228
Q_D-n	158	9.0924	108.2	4.5205
Q_D-Y_0	0.64799	0.32931	0.71588	0.45348

Table S3

Equivalent circuit parameters of Li_3FeF_6/C and Li_3FeF_6/CNTs cathode at 3.1 V in the charge process .

parameters	Li_3FeF_6/C		Li_3FeF_6/CNTs	
	value	Uncertainty (%)	value	Uncertainty (%)
R_s (Ω)	21.7	0.39569	22.33	0.34665
R_{SEI} (Ω)	6.574	6.9597	3.434	3.6034
Q_{SEI} – n	2.2386×10^{-6}	14.922	6.2463×10^{-7}	14.669
Q_{SEI} – Y_0	0.97191	2.6469	1.058	2.3672
R_{ct}(Ω)	27.05	2.1553	9.324	2.3292
Q_{ct} – n	7.2796×10^{-5}	6.8645	7.5269×10^{-4}	10.282
Q_{ct} – Y_0	0.75932	1.5485	0.57374	2.3307
R_D（Ω）	1572	2.6303	2844	7.9058
Q_D-n	138.4	4.1897	204.9	10.603
Q_D-Y_0	0.6839	0.25071	0.7681	0.35093

References

1 G. Lieser, M. Schroeder, H. Geßwein, V. Winkler, S. Glatthaar, M. Yavuz, R. Binder, *J. Sol-Gel Sci Technol*, 2014, **71**, 50–59.

2 A. Basa, E. Gonzalo, A. Kuhn, F. Alvarado,*J.Power Sources*, 2012, **197**, 260–266.