

Supporting Information

Facile Synthesis of C-FeF₂ Nanocomposites from CF_x: Influence of Carbon Precursor on Reversible Lithium Storage

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Table S1 Physical and chemical properties of various CF_x samples studied

Product Grade	ARC1000	ARC2065	ARC3000	ARC4000
Carbon source	Petro-coke	Carbon-black	Graphite	Carbon-fiber
Precursor code	FPC	FCB	FG	FCF
Composition	CF _{1.05}	CF _{1.12}	CF _{0.95}	CF _{1.1}
Particle size range, μm	1-45	N/A	<1 to 10	1-30
Median particle size, μm	~ 8	<1	~ 2	~ 6
Surface Area, m ² /g	130	340	N/A	344
Decomposition Temperature, °C	~ 630	~ 500	>550	N/A
Sources: Advanced Research Chemicals				

Table S2. Rietveld refinement parameters of C-FeF₂ nanocomposites

Sample	Composition	a (Å)	b (Å)	c (Å)	□ (°)	Crystallite Size (nm)	Strain (%)	R _w (%)
PC-FeF ₂	93.2 wt% FeF ₂	4.697	4.697	3.293	90	11	0.07	5.6
	6.8 wt% Fe ₅ C ₂	11.895	4.552	5.052	97.15	93	1.43	
CB- FeF ₂	100 wt% FeF ₂	4.696	4.696	3.303	90	17	0	5.4
G- FeF ₂	89.8 wt% FeF ₂	4.701	4.701	3.297	90	12	0.24	5.6
	10.2 wt% Fe ₅ C ₂	11.821	4.564	5.039	98.28	73	1.33	
*CF- FeF ₂	77.5 wt% FeF ₂	4.699	4.699	3.299	90	16	0.13	6.6
	22.5 wt% Fe ₅ C ₂	11.839	4.594	5.036	98.65	16	0.04	

Table S3 Summary of hyperfine parameters obtained from fitting the ^{57}Fe Mössbauer spectra.

	FeF_2			Fe^{3+} Content			Fe Carbide						
							FeI		FeII		FeIII		
	<i>IS</i>	<i>QS</i>	%	<i>IS</i>	<i>QS</i>	%	<i>IS</i>	B_{HF}	<i>IS</i>	B_{HF}	<i>IS</i>	B_{HF}	% Carbide
PC- FeF_2	1.33(1)	2.76(1)	72	0.47*	0.65(1)	15	0.25(1)	22.1(1)	0.31(1)**	19.2(1)	0.31(1)**	11.3(1)	13
CB- FeF_2	1.33(1)	2.77(1)	79	0.47*	0.77(1)	21	-	-	-	-	-	-	
G- FeF_2	1.33(1)	2.77(1)	60	0.47*	0.70(1)	10	0.26(1)	22.0(1)	0.25(1)**	18.7(1)	0.25(1)**	10.7(1)	30
CF- FeF_2	1.33(1)	2.78(1)	47	0.47(1)	0.68(1)	15	0.27(1)	22.2(1)	0.21**	18.0(1)	0.21**	10.1(1)	38

IS and *QS* are given in [mm/s]. B_{HF} in [T]
 “% Carbide” is the sum of the spectral fractions of the FeI, II, III sub-spectra.
 * Parameter is fixed to the value obtained from sample CF- FeF_2 .
 ** *IS* of FeI and FeII site are constrained to be identical, as the *IS* of these Fe sites are known to be very similar.

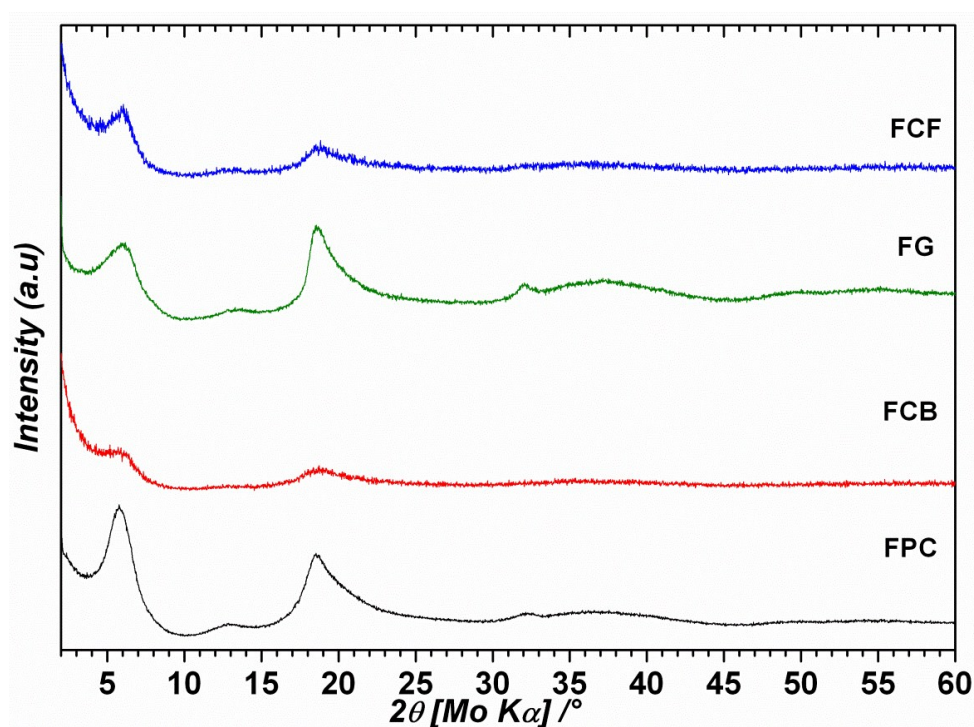


Figure S1 XRD patterns of various CF_x samples

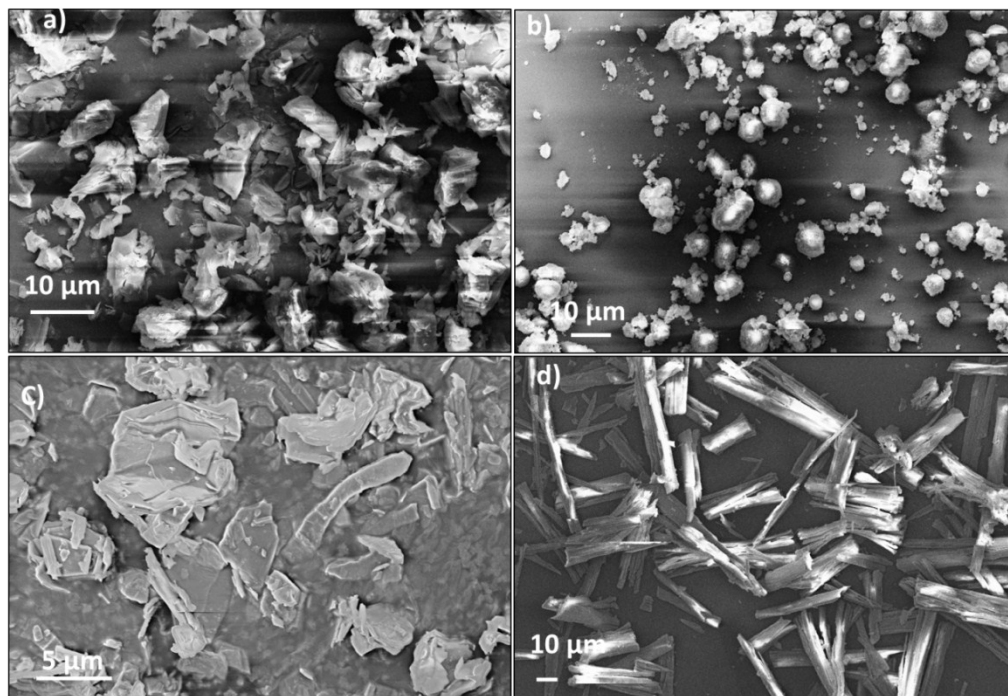


Figure S2 SEM Images of (a) FPC (ARC 1000) (b) FCB (ARC 2065) (c) FG (ARC 3000) and (d) FCF (ARC 4000).

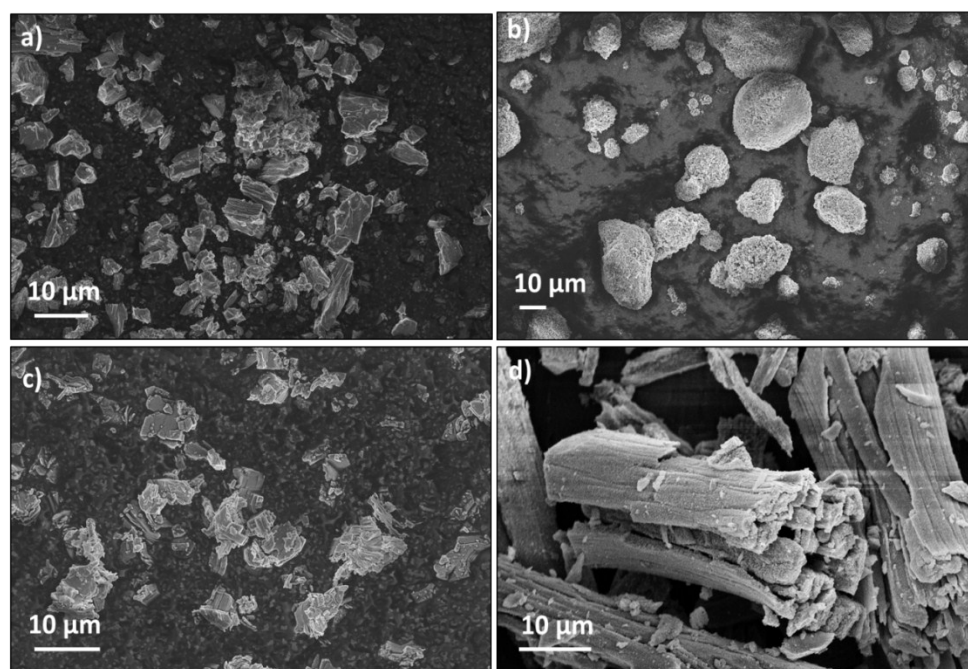
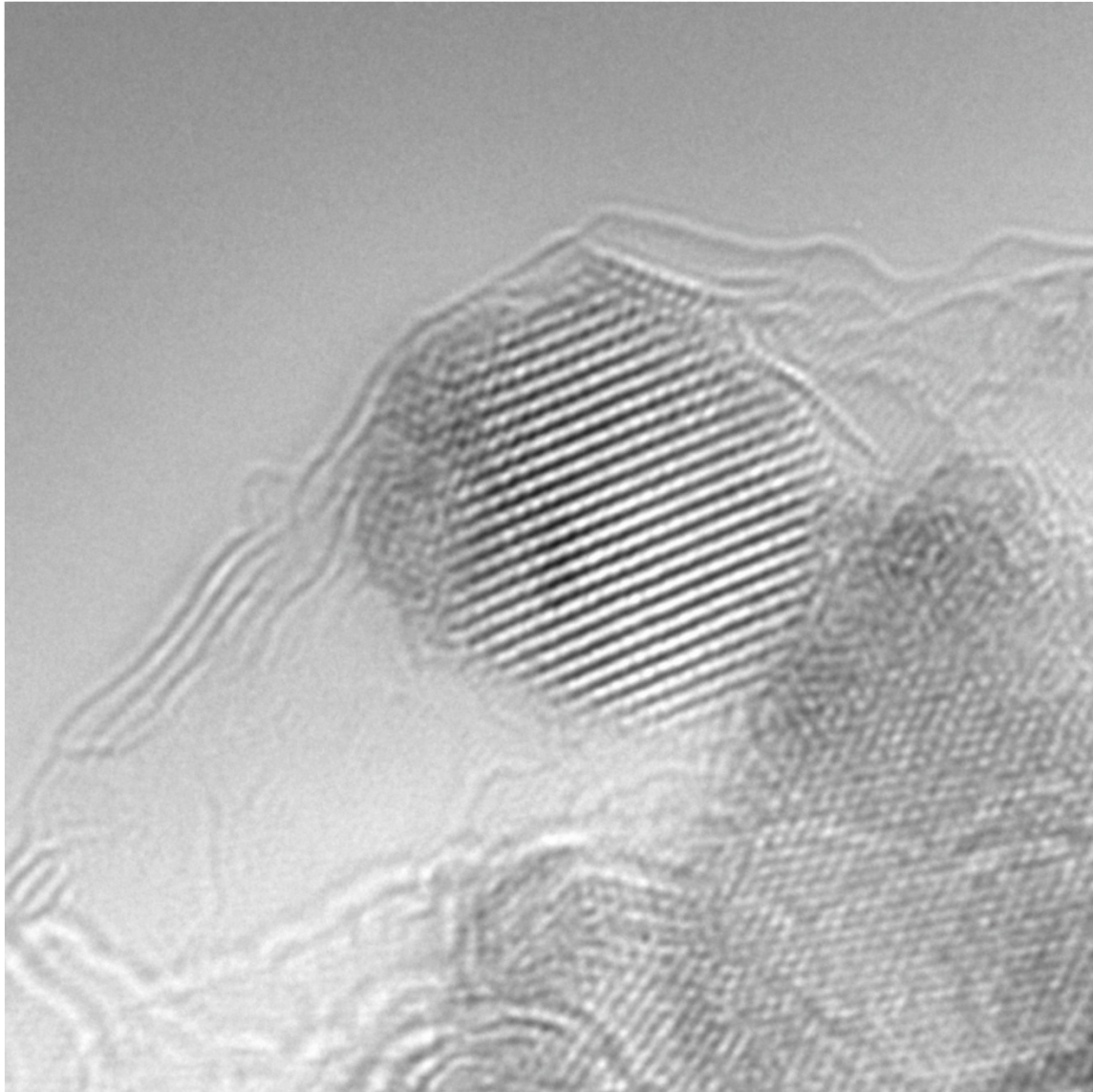


Figure S3 SEM images of (a) PC-FeF₂ (b) CB-FeF₂ (c) G-FeF₂ and (d) CF-FeF₂



— 5 nm

Figure S4 High resolution TEM image of G-FeF₂ nanocomposites

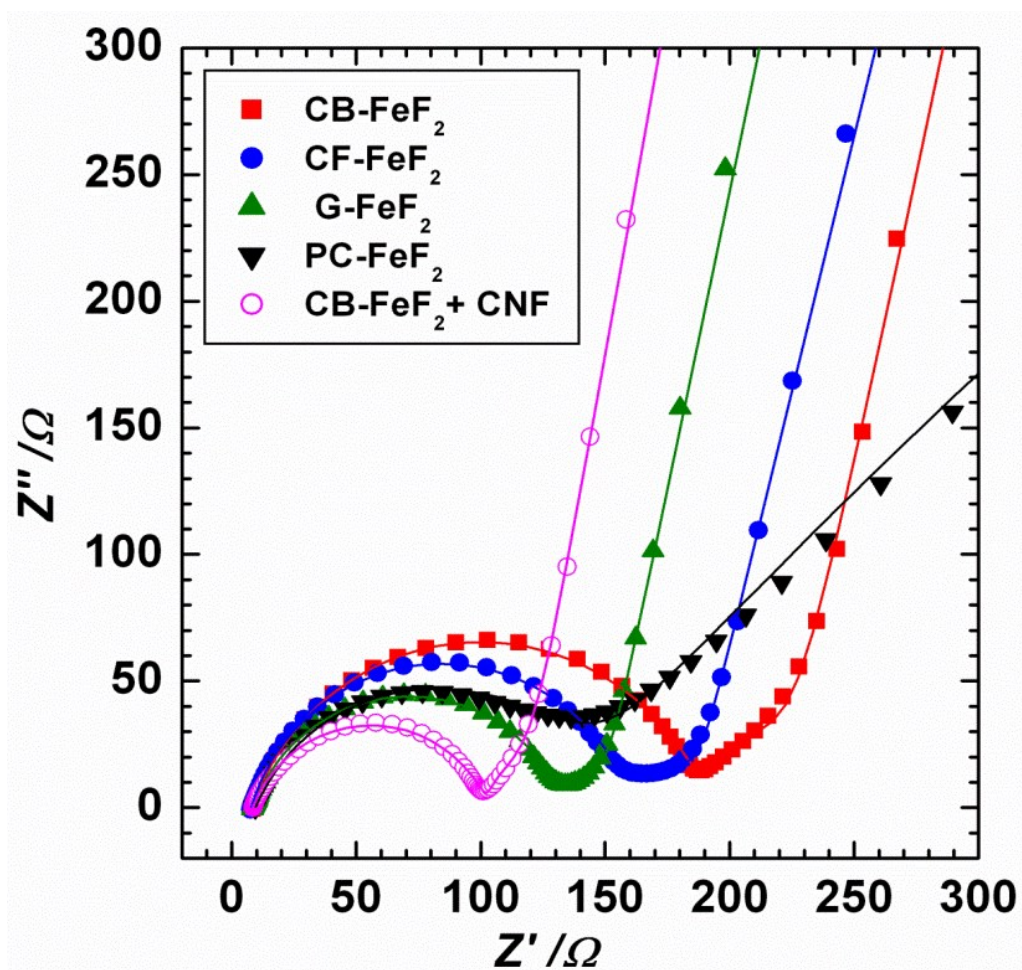


Figure S5 Electrochemical impedance spectra of C-FeF₂ nanocomposites obtained at OCV.