Electronic supplementary information (ESI)

Enhancement of pseudocapacitive performance of iron hexacyanoferrate through porosity engineering: fabrication of environment friendly symmetric coin-cell

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This document contains the structural details obtained from Rietveld refinement of laboratory Xray diffraction patterns of two Iron hexacyanoferrate nanoparticles prepared in this study. All structural details, atomic sites, occupancies, bond lengths etc. all are represented in tabular form. The representative XPS Survey curves are also included. Electrochemical measurement such as peak current (i_p) vs. scan rate (ν) to determine some important fitting parameters have also been presented.Finally diffusion coefficient calculated from EIS are and Coulombic efficiency of both the samples are also included.

Table S1: Atom positions and occupancies as obtained from Rietveld refinement of laboratory Xray diffraction data using MAUD software

		$FeHCF_{60}$				**$FeHCF_{80}$**			
Atom	Site	X	Y	Z	Occupancy	X	Y	Z	Occupancy
Fe (III)	1a	0	0	0	1	0	0	0	1
	3c	0	0.5	0.5	1	0	0.5	0.5	1
Fe (II)	1b	0.5	0.5	0.5	0.664	0.5	0.5	0.5	0.720
	3d	0.5	0	0	0.821	0.5	0	0	0.832
C	6e	0.30458	0	0	0.800	0.2656	0	0	0.822
	6f	0.333	0.5	0.5	0.664	0.2980	0.5	0.5	0.720
	12h	0.21383	0.5	0	0.870	0.2138	0.5	0	0.760
N	6e	0.20225	0	0	0.800	0.1884	0	0	0.760
	6f	0.19186	0.5	0.5	0.664	0.1890	0.5	0.5	0.720
	12h	0.30123	0.5	0	0.729	0.2995	0.5	0	0.760
O	6e	0.18611	0	0	0.221	0.2100	0	0	0.221
	6f	0.24019	0.5	0.5	0.336	0.1989	0.5	0.5	0.283
	12h	0.27804	0.5	0	0.221	0.3045	0.5	0	0.221
	8g	0.283	0.284	0.284	0.900	0.2830	0.284	0.284	0.825

Table S2: Bond length as obtained from Rietveld refinement of laboratory Xray diffraction data using MAUD software

Bond	Bond length of $FeHCF_{60}$	Bond length of $FeHCF_{80}$
($Fe_{4\_}Fe^{2+}$-$C_{3\_}C$)	2.17350(0) Å	2.168 Å
($Fe_{4\_}Fe^{2+}$-$C_{1\_}C$)	1.98 Å	2.38 Å
($Fe_{3\_}Fe^{2+}$-$C_{2\_}C$)	1.69 Å	2.05 Å
($Fe_{1\_}Fe^{3+}$-$N_{1\_}N$)	2.06 Å	1.91 Å
($Fe_{2\_}Fe^{3+}$-$N_{3\_}N$)	2.02 Å	2.033 Å
($Fe_{2\_}Fe^{3+}$-$N_{2\_}N$)	1.95 Å	1.916 Å
($C_{1\_}C$-$N_{1\_}N$)	1.04 Å	0.7833 Å
($C_{2\_}C$-$N_{2\_}N$)	1.44 Å	1.1055 Å
($C_{3\_}C$-$N_{3\_}N$)	0.88 Å	0.8686 Å
($Fe_{1\_}Fe^{3+}$-$O_{1\_}O^{2-}$)	1.89 Å	2.13 Å
($Fe_{2\_}Fe^{3+}$-$O_{2\_}O^{2-}$)	2.44 Å	2.017 Å
($Fe_{2\_}Fe^{3+}$-$O_{3\_}O^{2-}$)	2.25 Å	1.98 Å

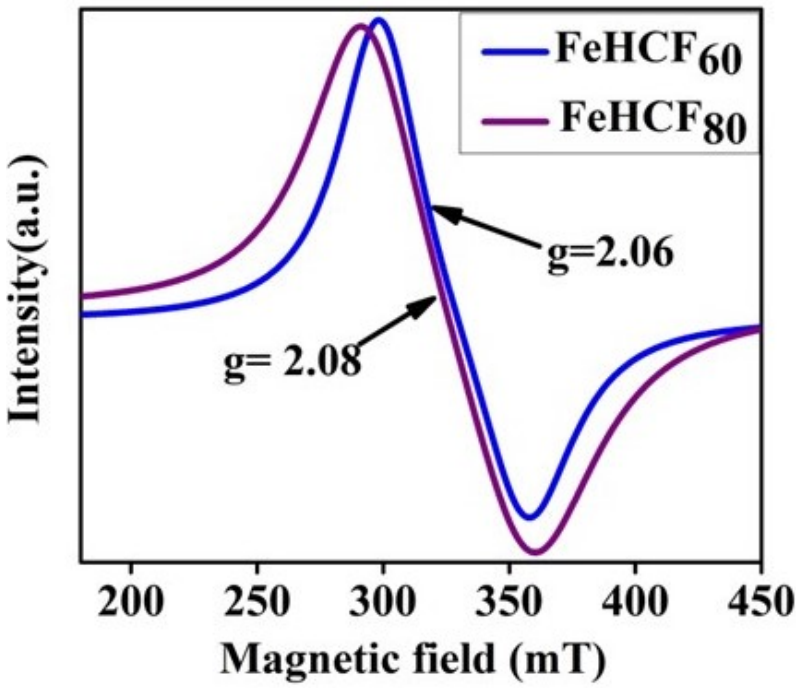

Figure S1. EPR spectra of $FeHCF_{60}$ and, (b) $FeHCF_{80}$

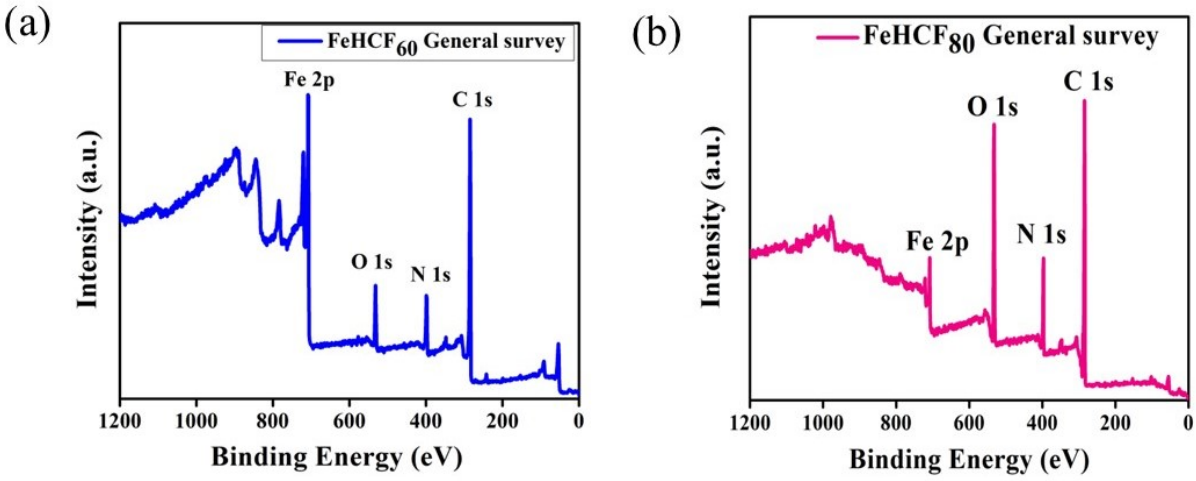

Figure S2. XPS Survey spectra for (a) $FeHCF_{60}$ and, (b) $FeHCF_{80}$

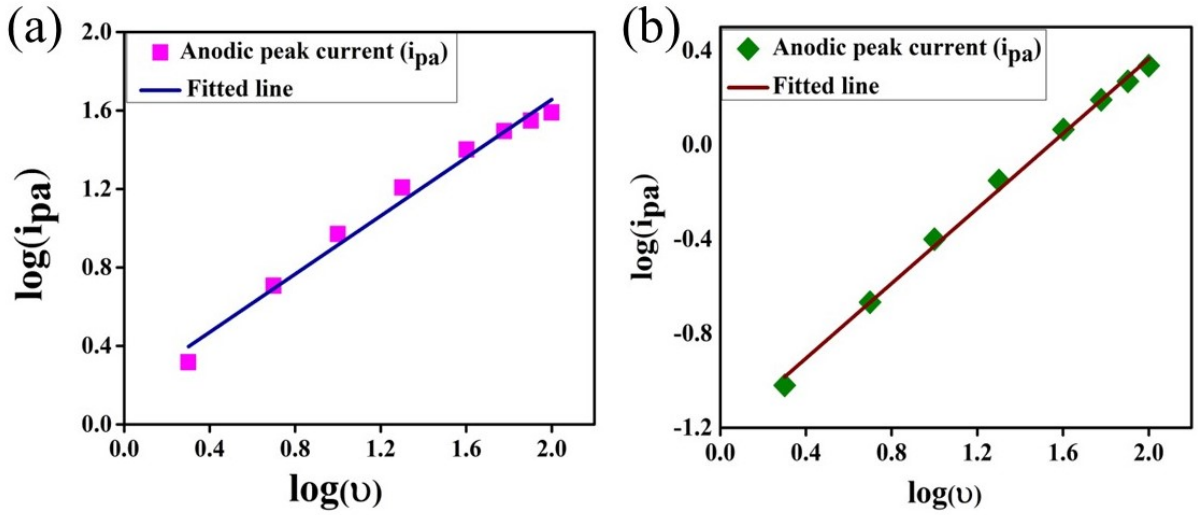

Figure S3. log i_p vs log (ν) plot of a) $FeHCF_{60}$ and b) $FeHCF_{80}$

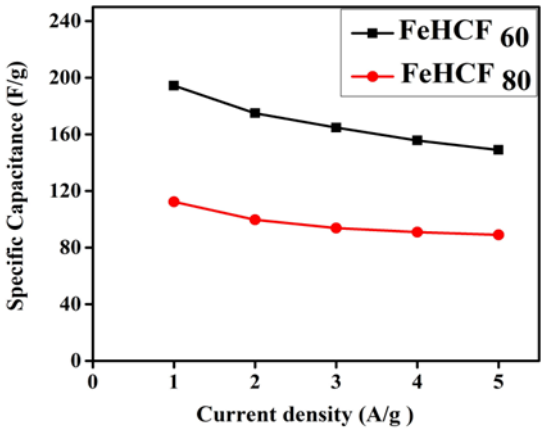

Figure S4: Current density dependence Specific capacitance obtained from GCD of $FeHCF_{60}$ and $FeHCF_{80}$

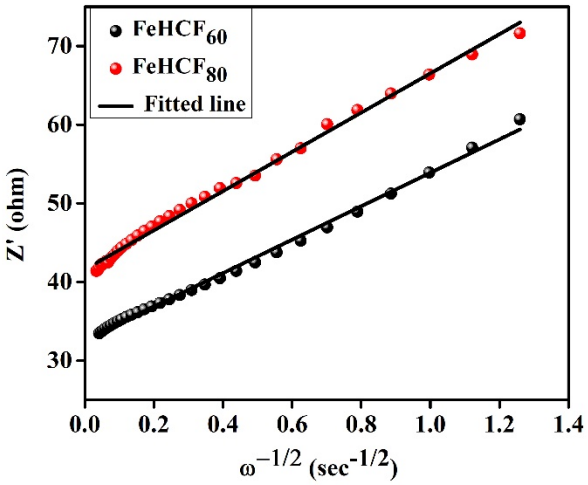

Figure S5: Ion diffusion coefficient plot for (a) $FeHCF_{60}$and (b) $FeHCF_{60}$