

Electronic Supplementary Information

Fe₄[Fe(CN)₆]₃: A Cathode Material For Sodium-Ion Batteries

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Table S1. The lattice parameters, unit cell volume, total energy and formation energy of the undoped and doped Prussian blue ($\text{Fe}_8\text{C}_{24}\text{N}_{24}$ without defects).

Sample	a(Å)	b(Å)	c(Å)	α	β	γ	Volume (Å ³)	Total energy (eV)	Formation Energy(eV)
$\text{Fe}_8\text{C}_{24}\text{N}_{24}$	9.90	9.90	9.90	90.00	90.00	90.00	969.00	-17128.28	0.00
$\text{Fe}_8\text{C}_{24}\text{N}_{24}\text{-Na}$	9.91	9.91	9.91	90.17	89.91	89.52	972.42	-18435.49	-4.27
$\text{Fe}_8\text{C}_{24}\text{N}_{24}\text{-Na}_2$	9.91	9.92	9.92	89.32	90.01	89.51	975.26	-19742.84	-8.68
$\text{Fe}_8\text{C}_{24}\text{N}_{24}\text{-Na}_4$	9.93	9.95	9.94	88.46	89.56	88.44	981.34	-22357.25	-17.20
$\text{Fe}_8\text{C}_{24}\text{N}_{24}\text{-Na}_8$	10.00	9.97	9.95	88.73	91.94	89.18	991.61	-27583.30	-31.47
$\text{Fe}_8\text{C}_{24}\text{N}_{24}\text{-Na}_{12}$	10.03	10.19	10.08	93.40	90.28	90.77	1027.38	-32796.31	-32.71
$\text{Fe}_8\text{C}_{24}\text{N}_{24}\text{-Na}_{16}$	12.48	9.76	9.78	95.05	78.01	86.88	1157.95	-38014.47	-39.10
$\text{Fe}_7\text{C}_{24}\text{N}_{24}\text{-Na(Fe}^{2+}\text{)}$	10.12	10.12	10.12	90.00	90.00	90.00	1037.81	-17555.53	10.81
$\text{Fe}_7\text{C}_{24}\text{N}_{24}\text{-Na(Fe}^{3+}\text{)}$	10.09	10.09	10.09	90.00	90.00	90.00	1027.20	-17559.55	6.79
$\text{Fe}_8\text{C}_{24}\text{N}_{24}\text{-Fe}$	9.84	9.84	9.84	89.94	90.01	90.03	953.17	-17989.27	3.89

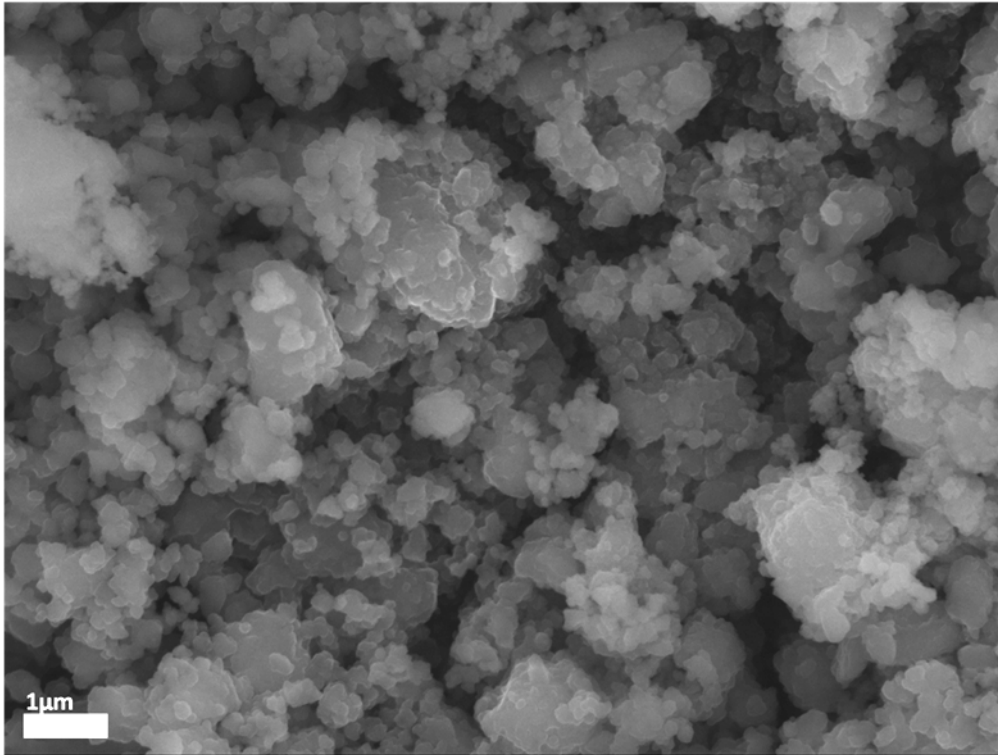


Figure S1. SEM of the as-synthesized $\text{Fe}_4[\text{Fe}(\text{CN})_6]_3$.

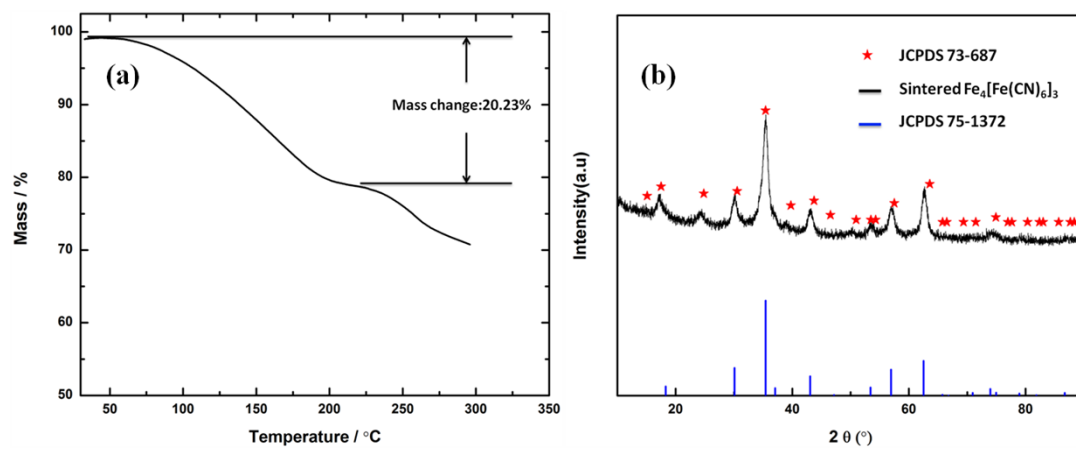


Figure S2. (a) TGA of as-synthesized $\text{Fe}_4[\text{Fe}(\text{CN})_6]_3$ (b) XRD of the sintered $\text{Fe}_4[\text{Fe}(\text{CN})_6]_3$.

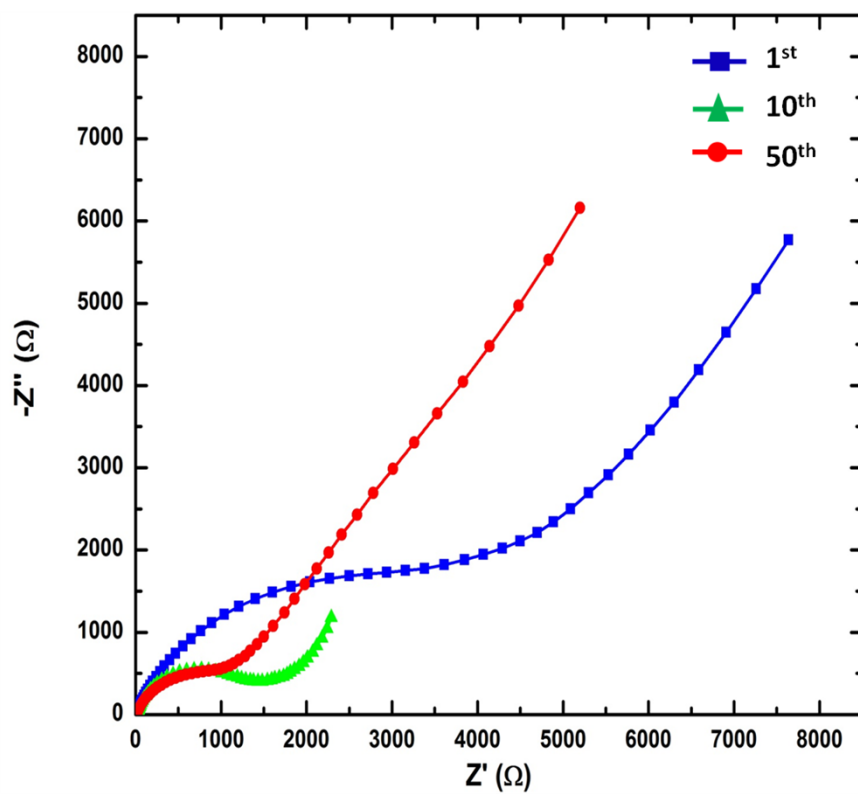


Figure S3. Impedance spectra for different cycles.