Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Investigating the role of interstitial water molecules in copper hexacyanoferrates for sodium-ion battery cathodes

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Table S1 | The Results of ICP Analysis of CuHCFe-1.4H_2O, CuHCFe-1.6H_2O, and CuHCFe-1.8H_2O.

mg/kg	Cu	Fe
CuHCFe-1.4H_2O	245660	141986
CuHCFe-1.6H_2O	231223	134597
CuHCFe-1.8H_2O	232902	137121

Table S2 | The Results of EA of CuHCFe-1.4H_2O, CuHCFe-1.6H_2O, and CuHCFe-1.8H_2O for C and N.

wt%	C	N
CuHCFe-1.4H_2O	22.68	23.42
CuHCFe-1.6H_2O	23.33	24.73
CuHCFe-1.8H_2O	23.55	24.71

Table S3 | The Chemical Formula of CuHCFe-1.8H_2O and CuHCFe-1.4H_2O at Pristine State, SOC 0 and SOC 100.

	Pristine	SOC 0	SOC 100
CuHCFe-1.8H_2O	$Cu[Fe(CN)_6]_{0.658}\cdot 1.75H_2O$	$Na_{\mathbf{0.488}}Cu[Fe(CN)_6]_{0.657}\cdot 2.88H_2O$	$Na_{\mathbf{0.279}}Cu[Fe(CN)_6]_{0.673}\cdot 2.12H_2O$
CuHCFe-1.4H_2O	$Cu[Fe(CN)_6]_{0.670}\cdot 1.41H_2O$	$Na_{\mathbf{0.611}}Cu[Fe(CN)_6]_{0.667}\cdot 3.87H_2O$	$Na_{\mathbf{0.291}}Cu[Fe(CN)_6]_{0.674}\cdot 2.07H_2O$

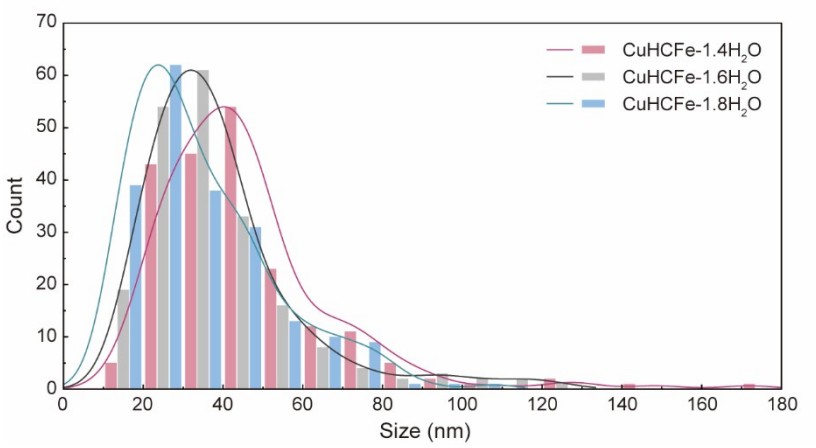

Figure S1 | The Particle Size Distribution of CuHCFe Samples.

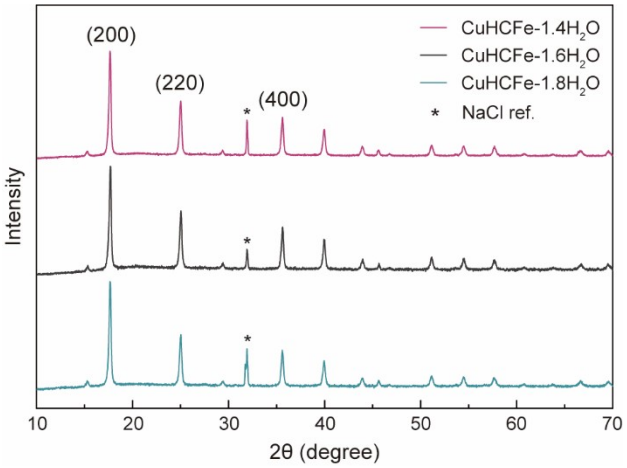

Figure S2 | The XRD Spectra of CuHCFe Samples. The structures of CuHCFe-1.4H_2O, CuHCFe-1.6H_2O, and CuHCFe-1.8H_2O are cubic.

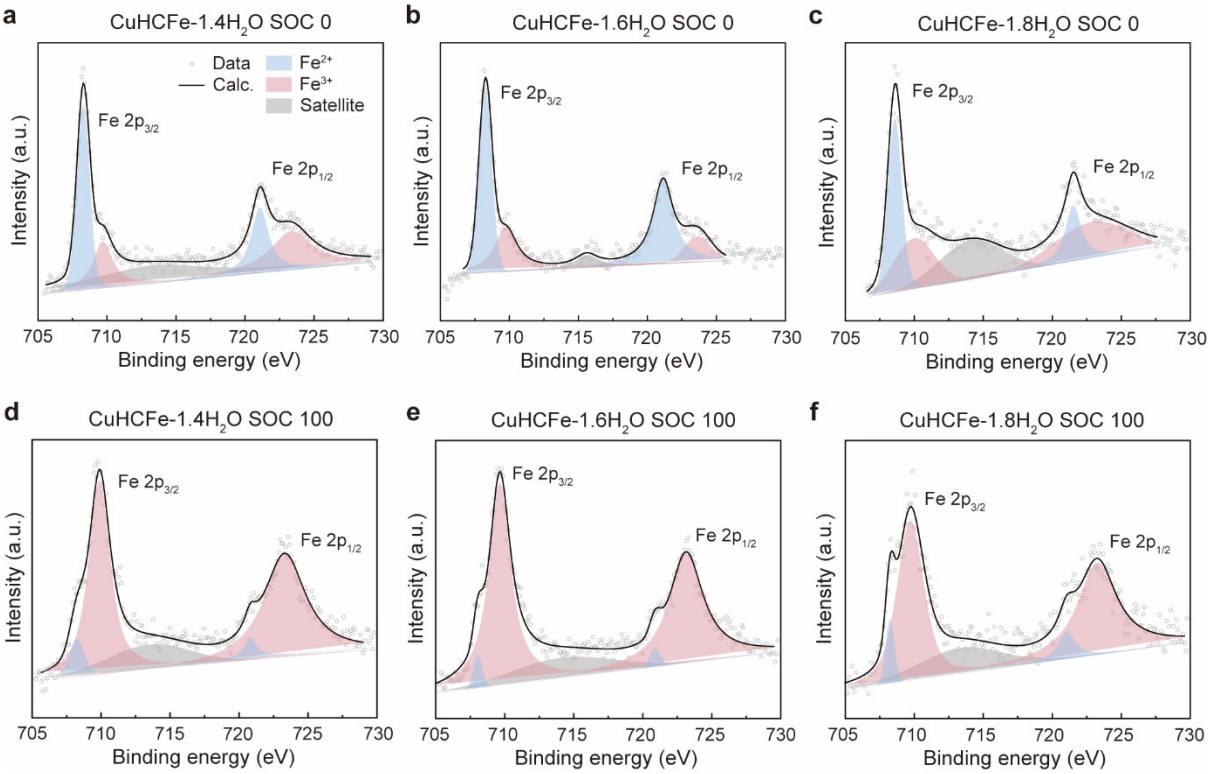

Figure S3 | The X-ray Photoelectron Spectroscopy (XPS) Spectra of Fe 2p. CuHCFe Electrode in Aqueous Electrolyte. a-c) The XPS Spectra of a) CuHCFe-1.4H_2O, b) CuHCFe-1.6H_2O, and c) CuHCFe-1.8H_2O at SOC 0. d-f) The XPS Spectra of d) CuHCFe-1.4H_2O, e) CuHCFe-1.6H_2O, and f) CuHCFe-1.8H_2O at SOC 100.

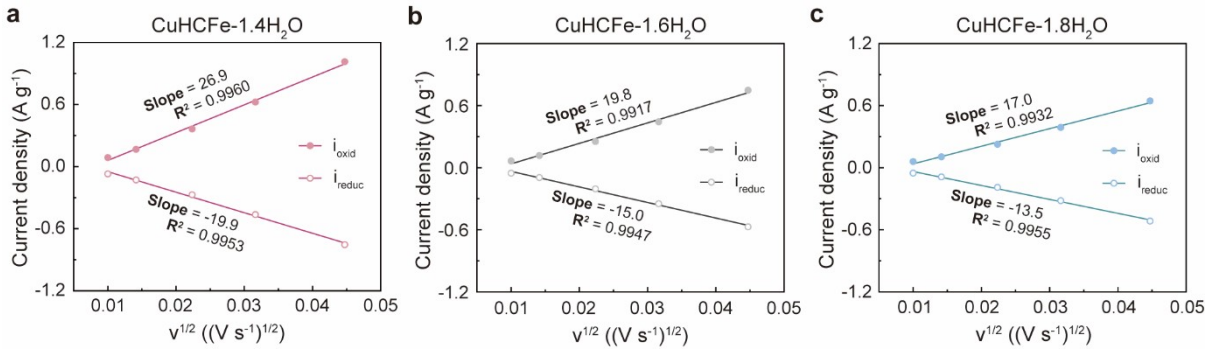

Figure S4 | Scan Rate-current Density Graph of a) CuHCFe-1.4H_2O, b) CuHCFe-1.6H_2O, and c) CuHCFe-1.8H_2O.

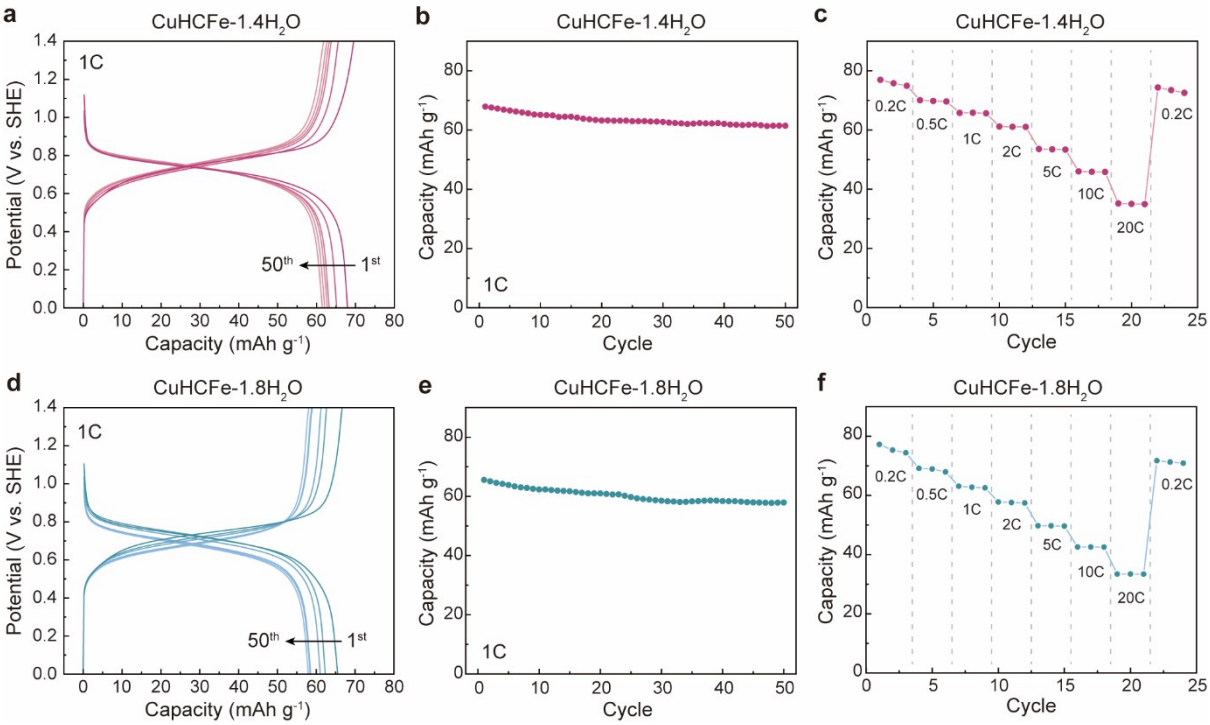

Figure S5 | The Electrochemical Properties of CuHCFe Samples in 1M $NaClO_4$ in DEGDME. The charge-discharge curves of a) CuHCFe-1.4H_2O and d) CuHCFe-1.8H_2O. The specific capacity of b) CuHCFe-1.4H_2O and e) CuHCFe-1.8H_2O for 50 cycles at 1C. The rate capability of c) CuHCFe-1.4H_2O and f) CuHCFe-1.8H_2O from 0.2C (12 mA g^{-1}) to 20C (1200 mA g^{-1}).

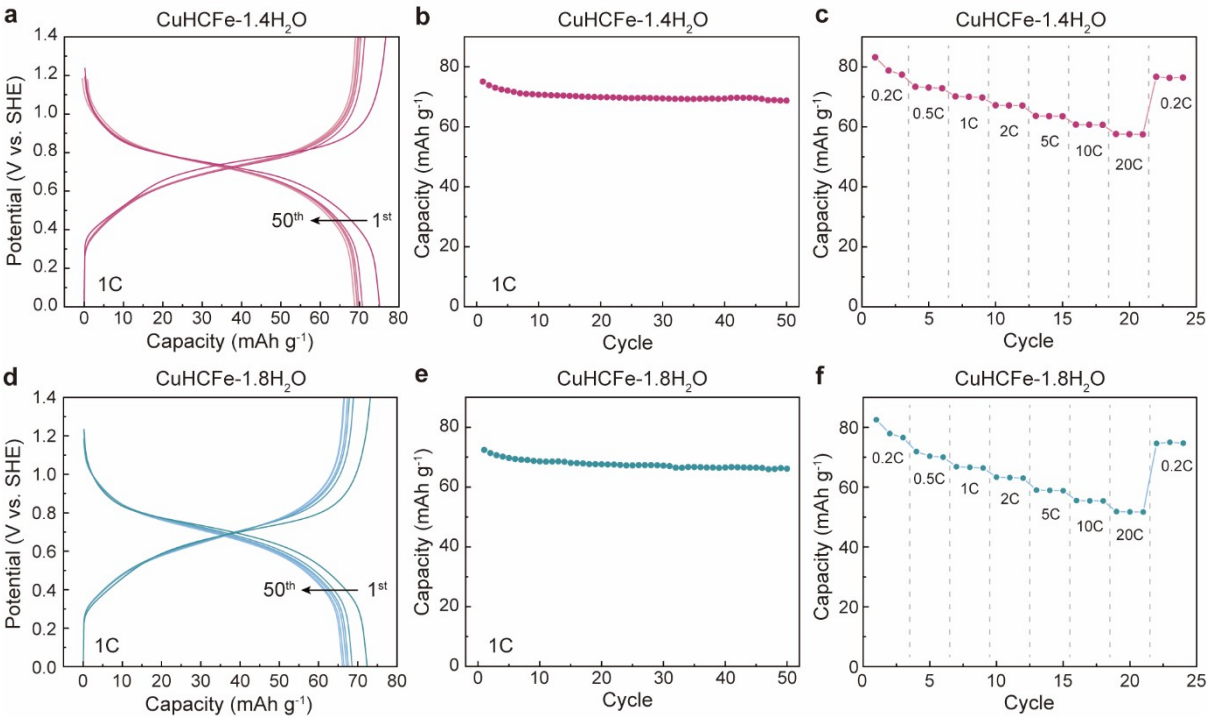

Figure S6 | The electrochemical properties of CuHCFe samples in 1M $NaClO_4$ in acetonitrile. The charge-discharge curves of a) CuHCFe-1.4H_2O and d) CuHCFe-1.8H_2O. The specific capacity of b) CuHCFe-1.4H_2O and e) CuHCFe-1.8H_2O for 50 cycles at 1C. The rate capability of c) CuHCFe-1.4H_2O and f) CuHCFe-1.8H_2O from 0.2C (12 mA g^{-1}) to 20C (1200 mA g^{-1}).

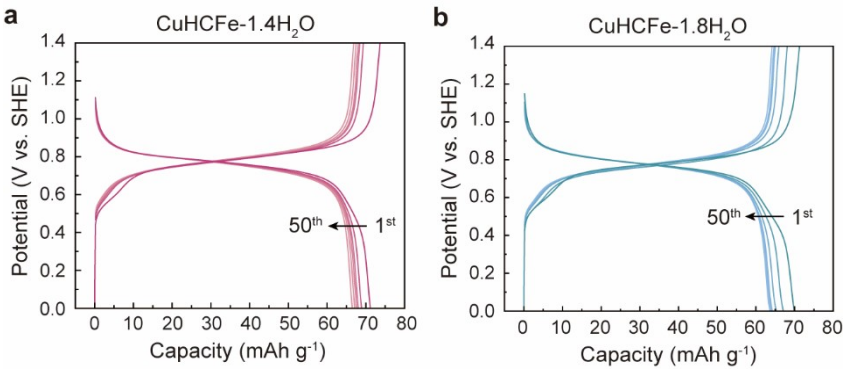

Figure S7 | The Charge-discharge Curves of a) CuHCFe-1.4H_2O and b) CuHCFe-1.8H_2O in 1M $NaClO_4$ in EC:DEC (1:1) at 1C (60 mA g^{-1})