SUPPORTING INFORMATION

Guest water hinders sodium diffusion in low-defect Berlin green cathode material

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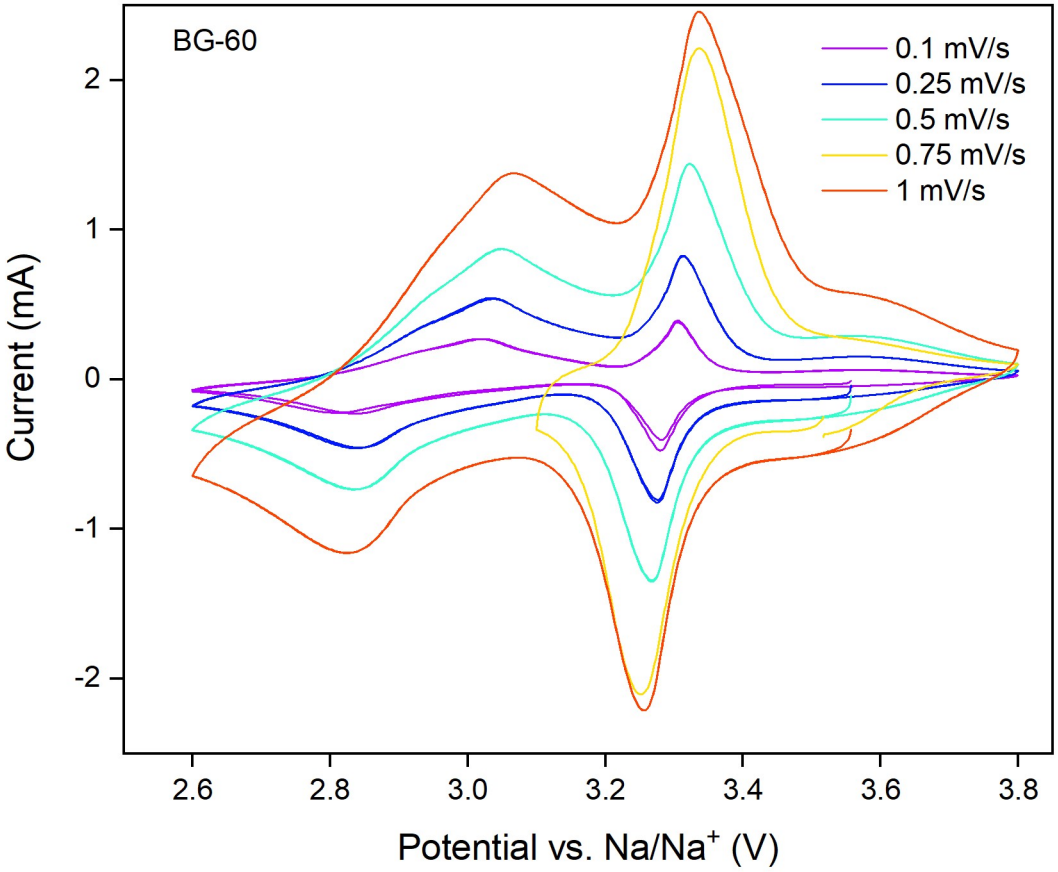

Figure S1. Cyclic voltammograms of BG-60 at different scan rates: 0.1, 0.25, 0.5, 0.75, and 1 mV/s in the voltage range of 2.6 – 3.8 V vs. Na/Na^+. The peaks at higher and lower potentials are assigned to the redox reactions of low-spin Fe_C^{3+}/Fe_C^{2+} and high-spin Fe_N^{3+}/Fe_N^{2+} couples, respectively. As demonstrated by the 0.75 mV/s scan rate, the cut-off potential of 3.1 – 3.8 V vs. Na/Na^+ was implemented to only focus on the low-spin Fe_C^{3+}/Fe_C^{2+} and avoid the characteristic cubic–rhombohedral phase conversion which introduces strain and particle cracking due to the associated volume change.[1,2]

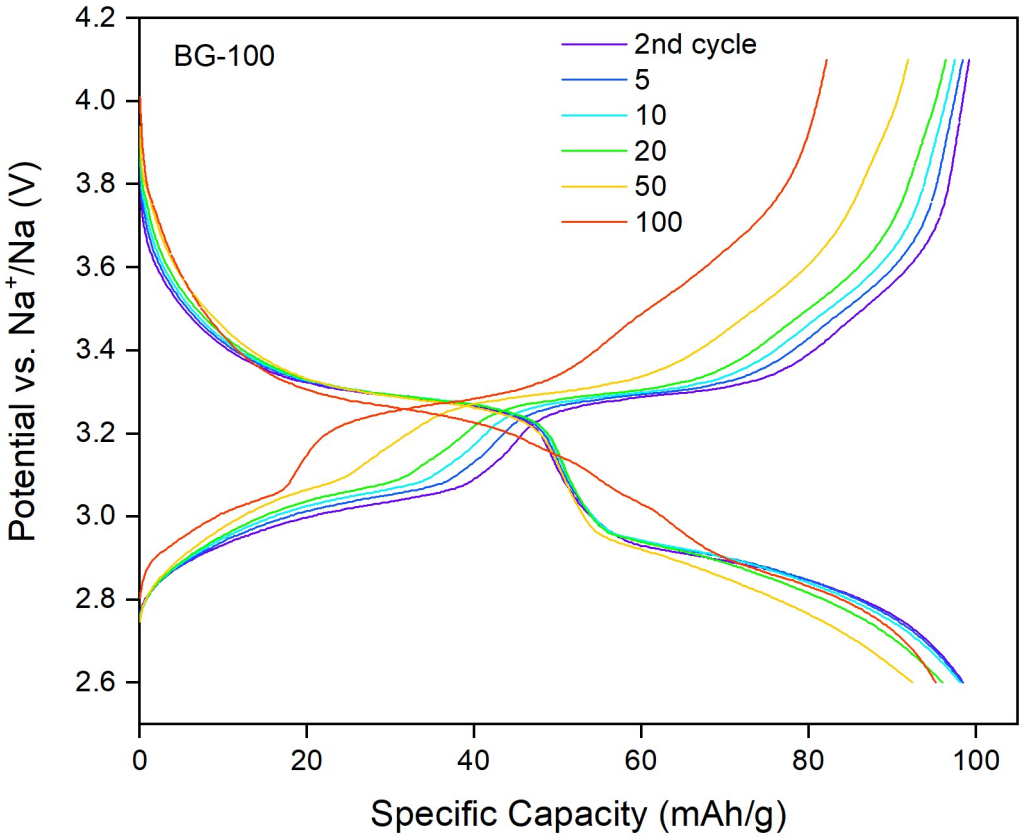

Figure S2. Selected charge/discharge profiles of BG-100 electrode/PB full cell at the current rate of 15 mA/g (1C = 150 mA/g) in potential range of 2.6 – 3.8 V.

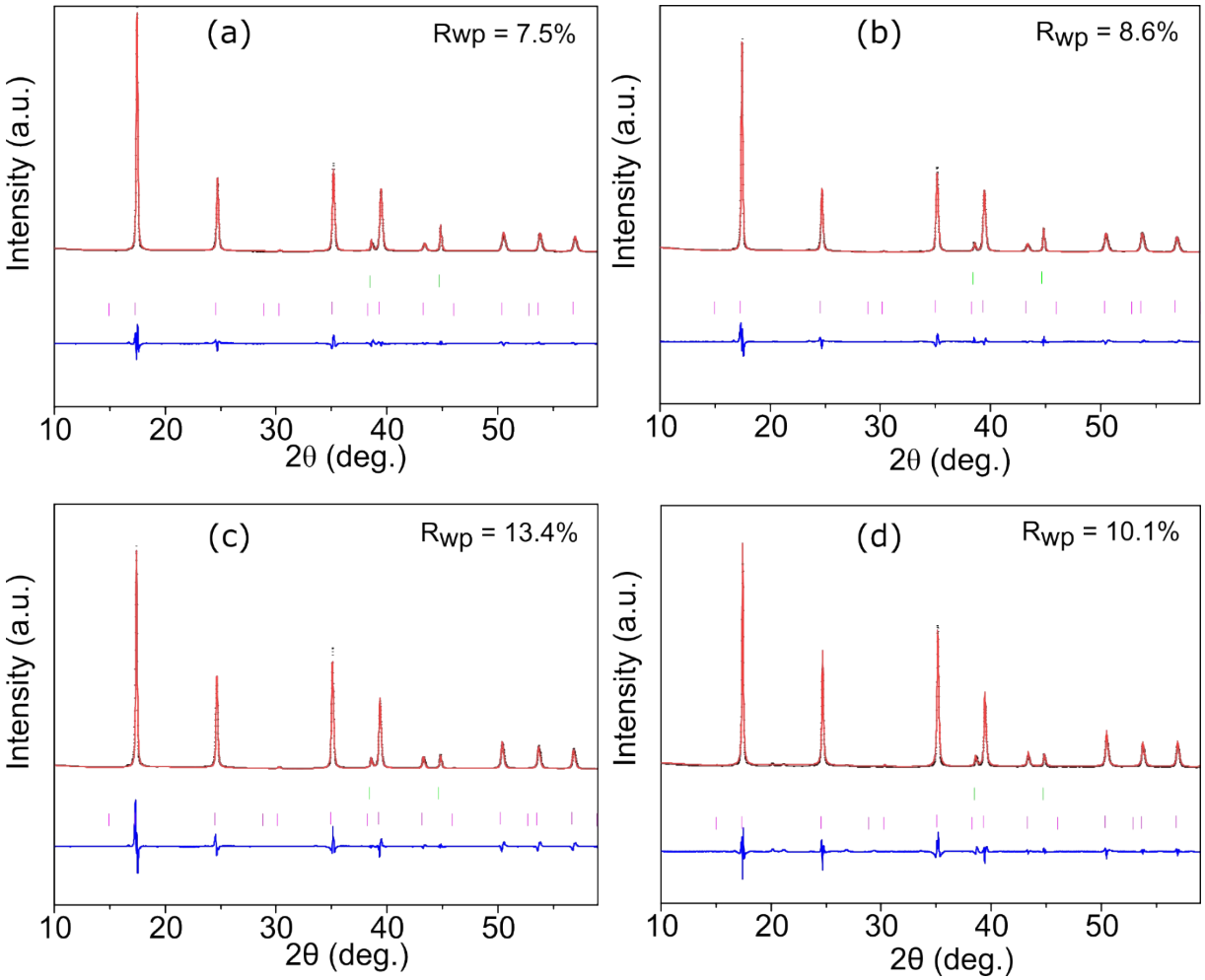

Figure S3. Pawley fits[3] of XRD patterns (λ = 1.5406 Å) of (a) uncycled, (b) mid-charge, (c) charged, and (d) discharged BG-150 electrode. The observed data is plotted in black, simulated pattern for the $Fm\bar{3}m$ model in red, and difference in blue. Vertical markers show the Bragg positions (BG electrode-pink, and Al-green). The observed Al phase comes from the Al foil used in cell fabrication. The lattice parameters are given in Table S1.

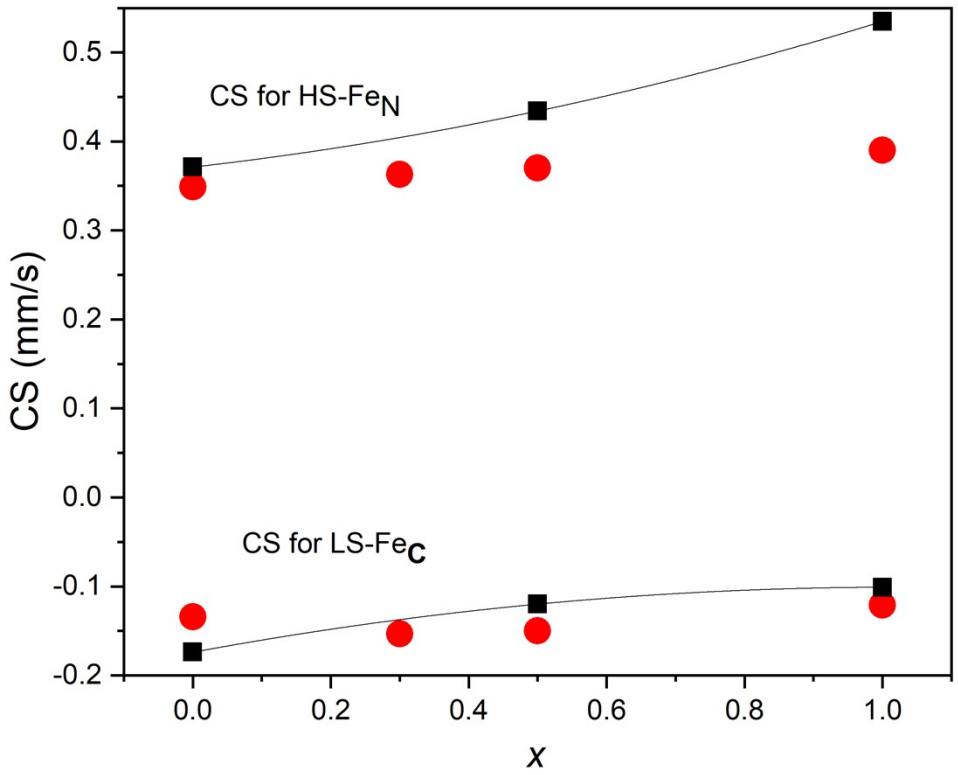

Figure S4. Center shift values for BG-150 electrode (n = 0.30(5)) as a function of nominal Na content x (red dots) and from earlier studies of $Na_xFe[Fe(CN)_6]\cdot nH_2O$. n = 0.54(5) for $x \approx 0$, and 1.79(2) for $x \approx$ 0.5 and 1.0 (black dots).[4] The lines are used as eye guides.

Table S1. Pawley fit results for BG-150 electrode (S.G. $Fm\bar{3}m$)

Electrode	Lattice parameters (Å)	Volume (Å^3)
Uncycled	$a = b = c$ = 10.240(1)	1073.6(1)
Mid-charge	$a = b = c$ = 10.248(1)	1076.4(1)
Charged	$a = b = c$ = 10.266(1)	1081.9(1)
Discharged	$a = b = c$ = 10.237(1)	1072.9(1)

References

1 D. O. Ojwang, M. Svensson, C. Njel, R. Mogensen, A. Sreekumar Menon, T. Ericsson, L. Häggström, J. Maibach and W. Brant, *ACS Appl. Mater. Interfaces*, **13**, 10054–10063.

2 W. Brant, R. Mogensen, S. Colbin, D. O. Ojwang, S. Schmid, L. Häggström, T. Ericsson, A. Jaworski, A. Pell and R. Younesi, *Chem. Mater.*, **31**, 7203–7211.

3 G. S. Pawley, *J. Appl. Cryst*, 1981, **14**, 357–361.

4 D. O. Ojwang, L. Häggström, T. Ericsson, J. Ångström and W. R. Brant, *Dalt. Trans.*, 2020, **49**, 3570–3579.