Supporting Information

Operando Synchrotron-Based X-Ray Study of Prussian Blue and Its Analogue as Cathode Materials for Sodium-Ion Batteries

Jeesoo Seok[†], Seung-Ho Yu^{*,‡}, and Héctor D, Abruña^{*,†}

[†]Baker Laboratory, Department of Chemistry and Chemical Biology, Cornell University, Ithaca, New York, 14853, United States

‡Department of Chemical and Biological Engineering, Korea University, 145 Anam-ro, Seongbuk-gu, Seoul 02841, Republic of Korea

Corresponding Authors

S.-H. Yu (E-mail: seunghoyu@korea.ac.kr), H. D. Abruña (E-mail: hda1@cornell.edu)

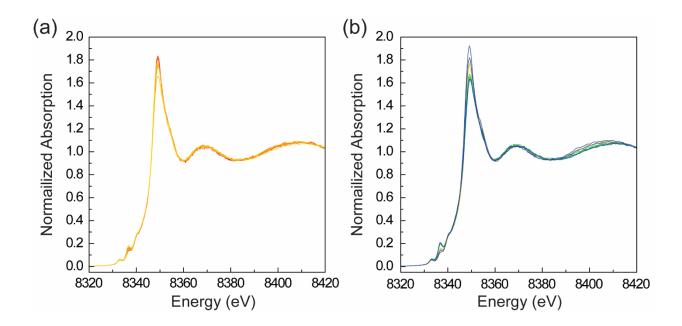


Figure S1. *Operando* X-ray absorption near edge structure (XANES) spectra at Ni K-edge of the Prussian blue (PB) analogue with iron replaced with nickel (PBN) during (a) discharging and (b) charging.

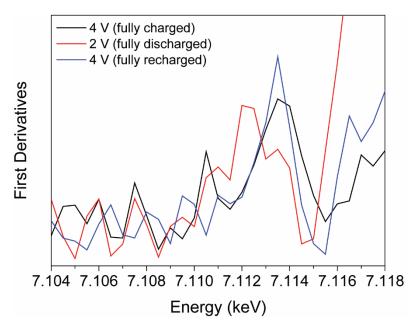


Figure S2. The first derivatives of the XANES spectrum of PB in a coin cell after charging, discharging and recharging.

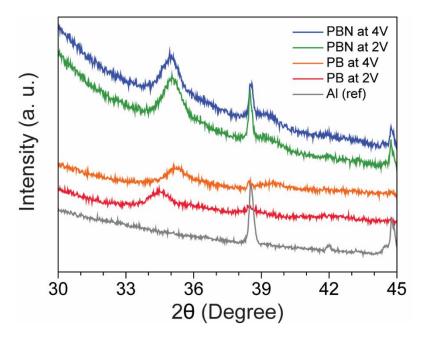


Figure S3. Ex situ X-ray diffraction (XRD) patterns of PB and PBN electrodes.

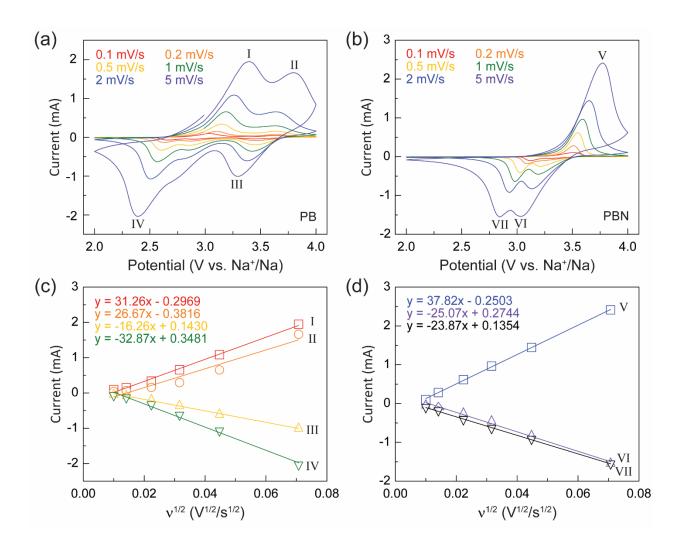


Figure S4. (a, b) Cyclic voltammetric profiles (CV) of the PB and PBN electrodes at various sweep rates and (c, d) the corresponding linear relationship between the anodic/cathodic peak currents and the square root of the sweep rate.

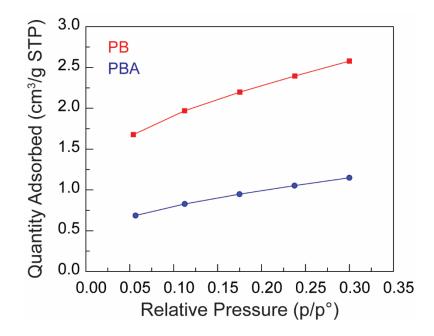


Figure S5. Brunauer-Emmett-Teller (BET) surface analysis of PB and PBN nanoparticles from nitrogen adsorption.

	PB		PBN	
	4 V	2 V	4 V	2 V
a	10.207 Å	10.396 Å	10.264 Å	10.235 Å
b	10.096 Å	10.838 Å	10.274 Å	10.383 Å

Table S1. The Calculated Lengths of the Cell Edges from *Ex Situ* XRD Patterns in Figure S3.

		$D ({\rm cm}^2{\rm s}^{-1})$	
РВ	Ι	$1.6 imes 10^{-12}$	
	Π	4.7×10^{-12}	
	III	$1.8 imes 10^{-12}$	
	IV	$1.8 imes 10^{-12}$	
PBN	V	$1.0 imes 10^{-11}$	
	VI	3.7×10^{-11}	
	VII	3.2×10^{-11}	

Table S2. Calculated Diffusion Coefficients from the Randles–Sevcik Equation.