Electronic Supplementary Material (ESI) for Nanoscale.

Elucidating the Capacitive Desalination Behavior of Na_xCoO_2: the Significance of Electrochemical Pre-activation

Zhenzhen Liu, Wei Ma, Haibo Li*

Ningxia Key Laboratory of Photovoltaic Materials, Ningxia University, Yinchuan, Ningxia, 750021, P. R. China

*Corresponding author. Fax/Tel.: +86 0951 2062414; E-mail: lihaibo@nxu.edu.cn

(Haibo Li)

Experimental

The crystallite size was calculated as the following equation:

$$D = \frac{K\lambda}{\beta \cos\theta} \quad \text{(S1)}$$

Where D is the crystallite size, K is a constant (0.943), λ is the x-ray wavelength (0.154056 nm), β is the full width at half maximum of the diffraction peak, and θ is the diffraction angle. In the calculation, the full width at half maximum (β) needs to be converted into radians and substituted into the formula.

Table S1 The average crystallite size of Na_xCoO_2.

Sample	D (nm)
$Na_{0.2}CO_2$	42.8705
$Na_{0.5}CO_2$	45.0451
$Na_{0.7}CO_2$	45.1625
$Na_{1.0}CO_2$	45.0527
$Na_{1.6}CO_2$	44.8798

Table S2 Pore texture of Na_xCoO_2.

Sample	S_{BET} (m^2/g)	V (cm^3/g)	D_{avg} (nm)
$Na_{0.2}CO_2$	3.832	0.048	50.3
$Na_{0.5}CO_2$	2.827	0.031	43.571
$Na_{0.7}CO_2$	3.260	0.049	59.934
$Na_{1.0}CO_2$	1.552	0.013	33.202
$Na_{1.6}CO_2$	1.720	0.013	30.261

Table S3 R_s and R_{ct} fitted from the equivalent circuit.

Sample	R_s	R_{ct}
$Na_{0.2}CO_2$	5.87	0.47
$Na_{0.5}CO_2$	7.39	1.35
$Na_{0.7}CO_2$	0.83	0.12
$Na_{1.0}CO_2$	3.55	1.31
$Na_{1.6}CO_2$	5.48	3.09

Figure caption

Fig. S1 The elemental mapping image of (a) $Na_{0.2}CoO_2$, (b) $Na_{0.5}CoO_2$, (c) $Na_{0.7}CoO_2$, (d) $Na_{1.0}CoO_2$ and (e) $Na_{1.6}CoO_2$.

Fig. S2 Current (a) and energy (b) profiles of $Na_{0.7}CoO_2$ || AC system in NaCl solution with an initial conductivity of 1000 μS/cm.

Fig. S3 (a) The conductivity transient of $Na_{0.7}CoO_2$ in NaCl solution with an initial conductivity of 1000 μS/cm at 0.3 and 0.6 V, (b) XRD patterns of $Na_{0.7}CoO_2$ after applying different potential

Fig. S4 The current transient of $Na_{0.7}CoO_2$ at 1.2 V and 0.6 V in NaCl solution with an initial conductivity of 1000 μS/cm.

Fig. S5 XRD patterns of the initial Na_xCoO_2 and Na_xCoO_2 after sodium insertion (red line), the insert are corresponding SEM images of Na_xCoO_2 electrodes after sodium insertion.

Fig. S6(a) salt removal capacity (mg/g) in terms of potential (V) for Na_xCoO_2 with an initial conductivity of 1000 μS/cm. (b) the effect of voltage on the CDI Ragone Kim-Yoon-Plot in NaCl solution.

Fig. S1

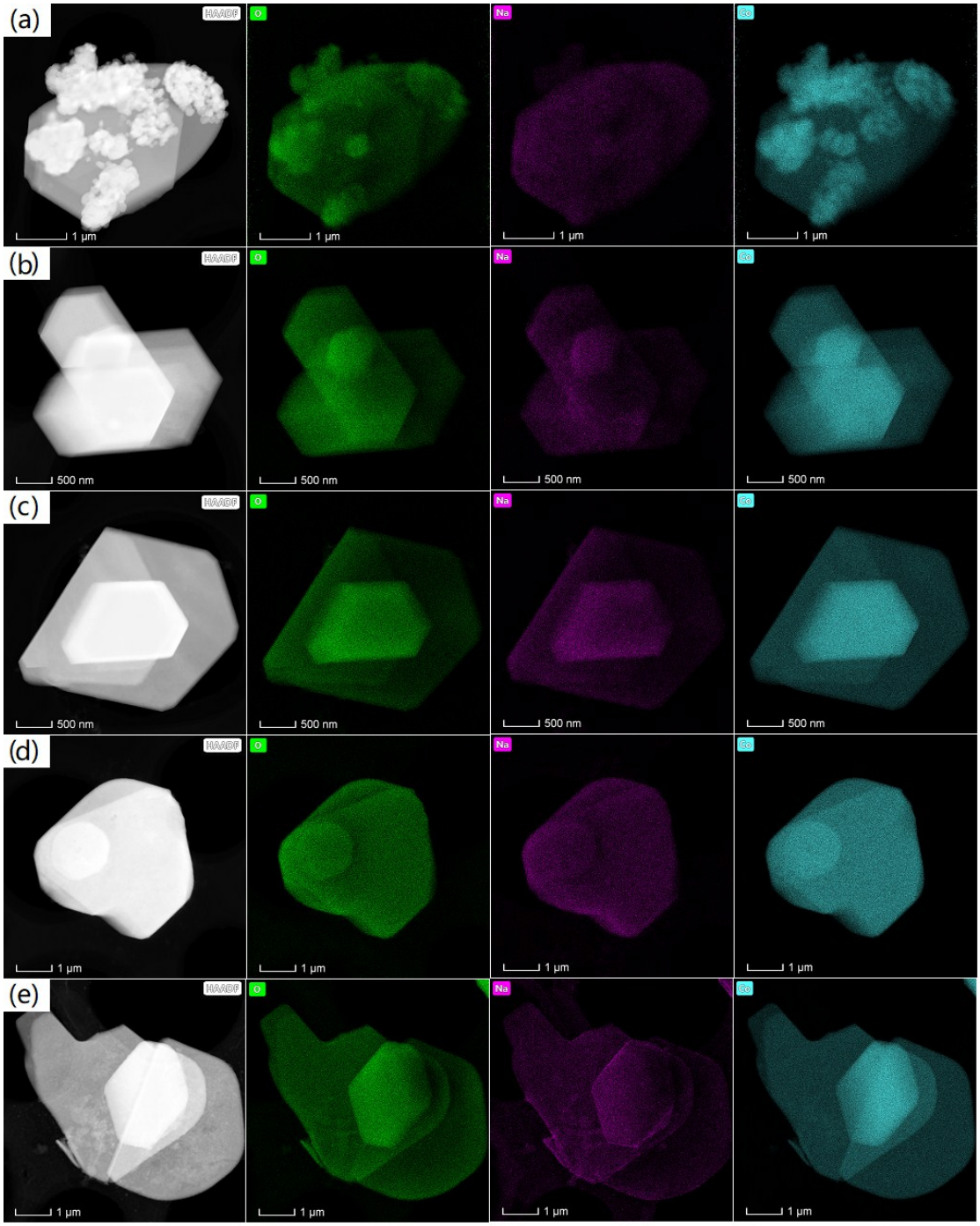


Fig. S2

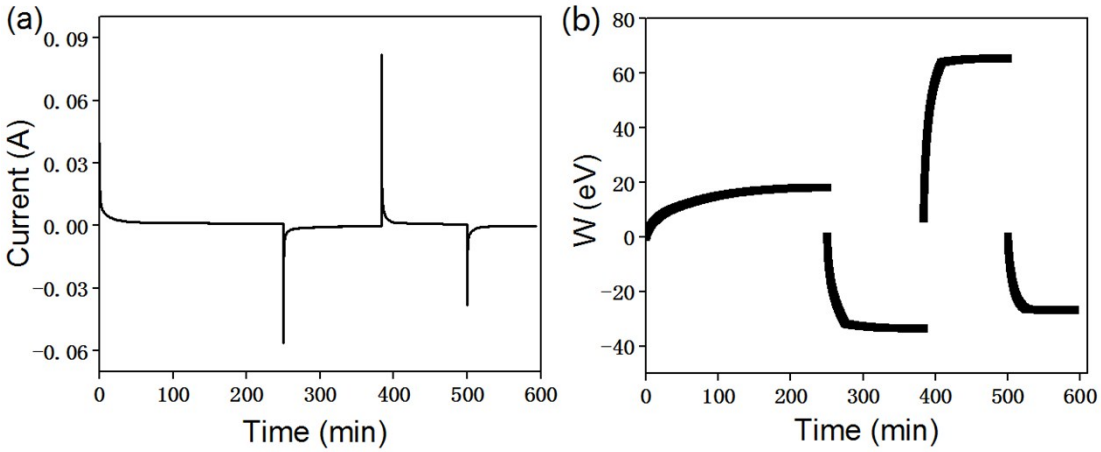

(a)
Current (A)
0. 09
0. 06
0. 03
0. 00
−0. 03
−0. 06
0
100
200
300
400
500
600
Time (min)
(b)
W (eV)
80
60
40
20
0
−20
−40
0
100
200
300
400
500
600
Time (min)

Fig. S3

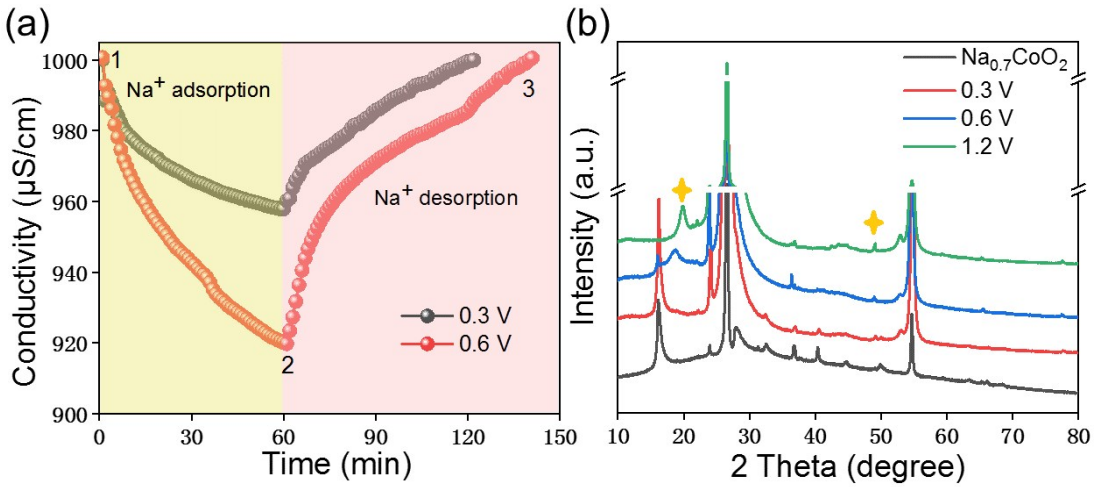

(a)
Conductivity (μS/cm)
1000
980
960
940
920
900
1
Na+ adsorption
2
3
Na+ desorption
0.3 V
0.6 V
0
30
60
90
120
150
Time (min)
(b)
Intensity (a.u.)
Na0.7CoO2
0.3 V
0.6 V
1.2 V
10
20
30
40
50
60
70
80
2 Theta (degree)

Fig. S4

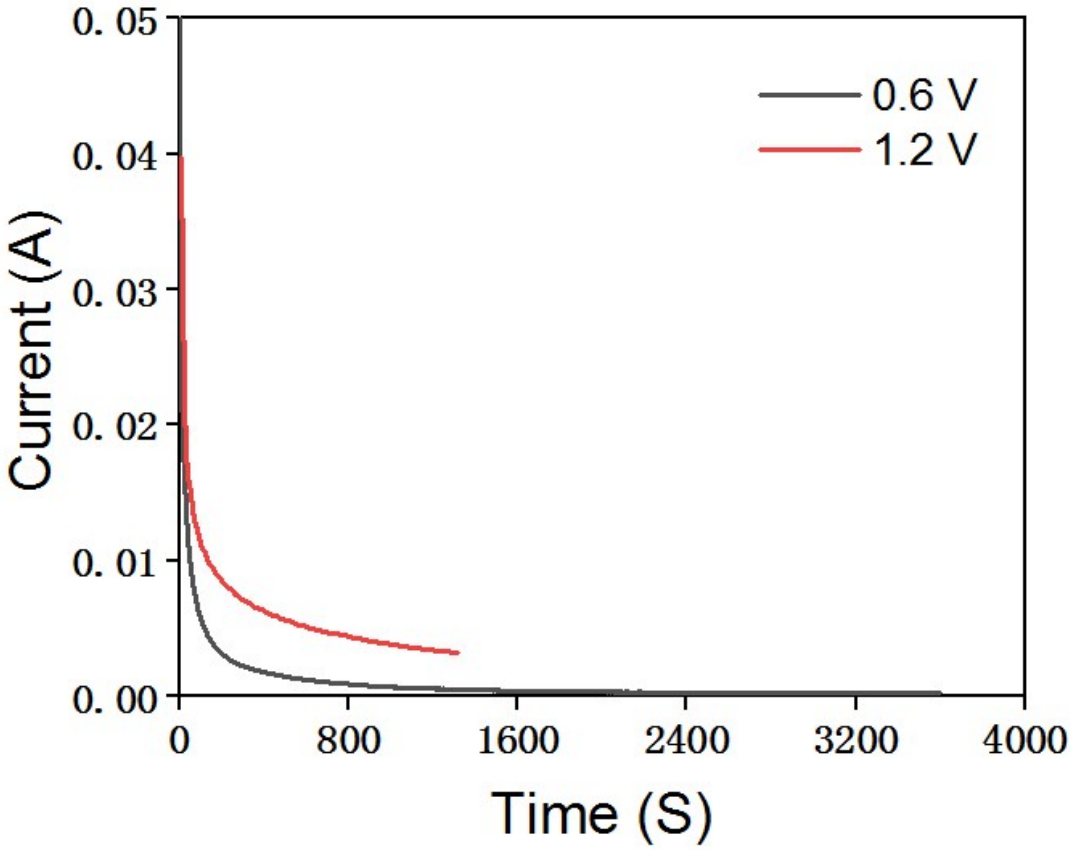

0. 05
0. 04
0. 03
0. 02
0. 01
0. 00
Current (A)
0
800
1600
2400
3200
4000
Time (S)
0.6 V
1.2 V

Fig. S5

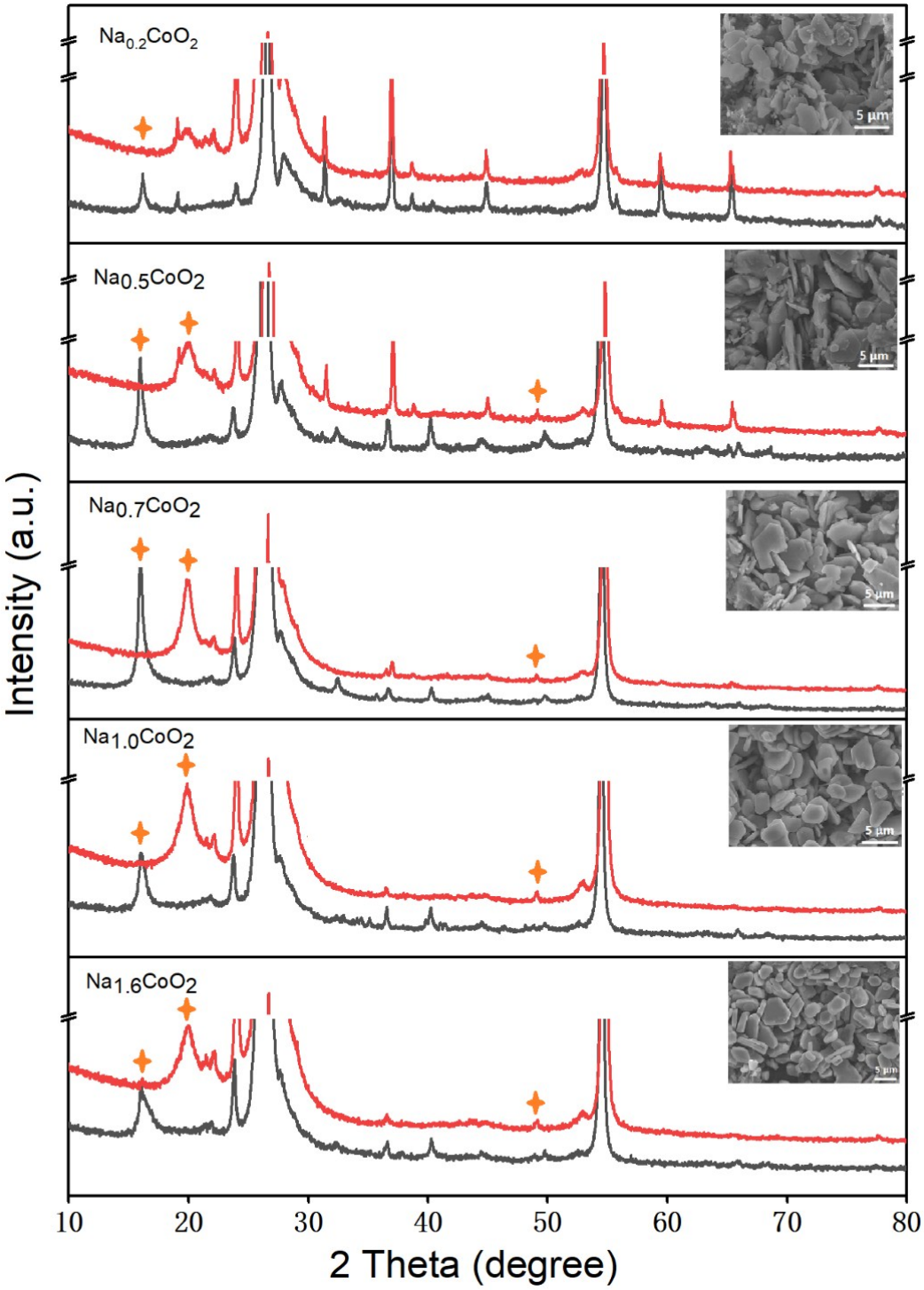
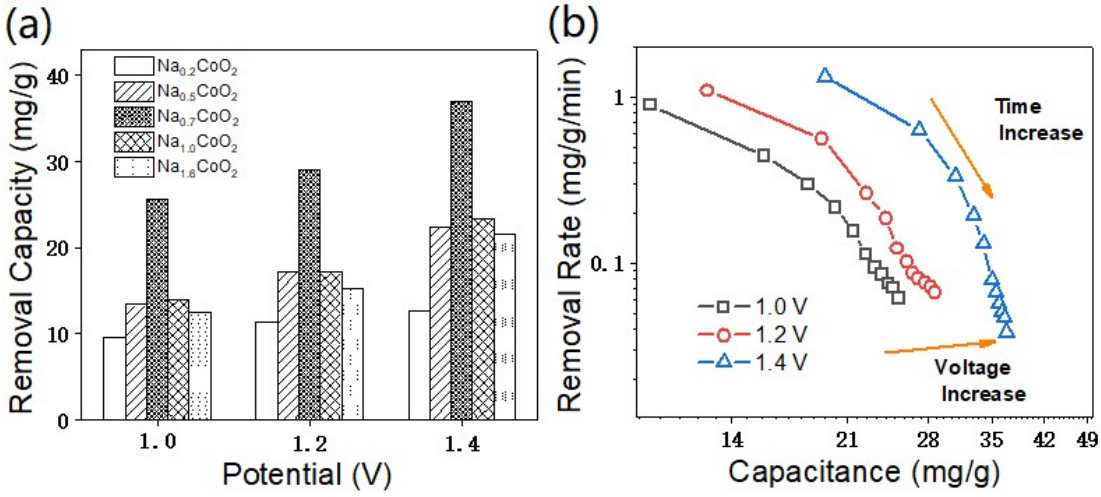

Na0.2CoO2
Na0.5CoO2
Na0.7CoO2
Na1.0CoO2
Na1.6CoO2
5 μm
Intensity (a.u.)
10
20
30
40
50
60
70
80
2 Theta (degree)

Fig. S6


(a)
Removal Capacity (mg/g)
40
30
20
10
0
$Na_{0.2}CoO_2$
$Na_{0.5}CoO_2$
$Na_{0.7}CoO_2$
$Na_{1.0}CoO_2$
$Na_{1.6}CoO_2$
1.0
1.2
1.4
Potential (V)
(b)
Removal Rate (mg/g/min)
1
0.1
Time
Increase
1.0 V
1.2 V
1.4 V
Voltage
Increase
14
21
28
35
42
49
Capacitance (mg/g)