

Electronic Supplementary Information

**4,4'-biphenyldicarboxylate sodium coordination compounds as an anode
for Na-ion batteries**

Aram Choi,^{‡a} Yun Kyeong Kim^{‡b}, Tae Kyung Kim^b, Mi-Sook Kwon^a, Kyu Tae Lee^{*a} and Hoi Ri Moon^{*b}

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^a School of Energy & Chemical Engineering, Ulsan National Institute of Science and Technology (UNIST)
100 Banyeon-ri, Eonyang-eup, Ulju-gun, Ulsan, 689-798, South Korea
E-mail: ktle@unist.ac.kr

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^b School of Chemistry, Ulsan National Institute of Science and Technology (UNIST) 100 Banyeon-ri, Eonyang-
eup, Ulju-gun, Ulsan, 689-798, South Korea
E-mail: hoirimoon@unist.ac.kr

Table S1 X-ray crystallographic data of [(Na₂bpdc)·H₂O]_n (*hyd*-Na₂bpdc) and [NaHbpdc]_n (NaHbpdc).

Compound	[(Na ₂ bpdc)·H ₂ O] _n	[NaHbpdc] _n
formula	Na ₂ C ₁₄ H ₁₀ O ₅	Na ₁ C ₁₄ H ₉ O ₄
crystal system	<i>Monoclinic</i>	<i>Triclinic</i>
space group	<i>P 21/c</i>	<i>P-1</i>
fw	304.21	264.21
<i>a</i> , Å	27.720(6)	3.6550(7)
<i>b</i> , Å	5.8060(12)	11.214(2)
<i>c</i> , Å	7.5530(15)	12.985(3)
<i>α</i> , deg	-	89.55(3)
<i>β</i> , deg	92.70(3)	84.39(3)
<i>γ</i> , deg	-	88.78(3)
<i>V</i> , Å ³	1214.2(4)	529.54(18)
<i>Z</i>	4	2
<i>ρ</i> _{calcd} , g cm ⁻³	1.665	1.657
temp, K	95(2)	100(2)
<i>λ</i> , Å	0.64999	0.69999
<i>μ</i> , mm ⁻¹	0.185	0.156
goodness-of-fit (<i>F</i> ²)	1.037	1.003
<i>F</i> (000)	616	272
reflections collected	16907	5662
independent reflections	5223 [<i>R</i> (int) = 0.0448]	2827 [<i>R</i> (int) = 0.0307]
completeness to <i>θ</i> _{max} , %	98.6	93.2
data/parameters/restraints	5223/190/0	2827/179/0
<i>θ</i> range for data collection, deg	3.28-33.36	1.55-29.55
diffraction limits (<i>h</i> , <i>k</i> , <i>l</i>)	-42 ≤ <i>h</i> ≤ 41, -8 ≤ <i>k</i> ≤ 8, -12 ≤ <i>l</i> ≤ 12	-5 ≤ <i>h</i> ≤ 5, -15 ≤ <i>k</i> ≤ 15, -18 ≤ <i>l</i> ≤ 18
refinement method	Full-matrix least squares on <i>F</i> ²	Full-matrix least squares on <i>F</i> ²
<i>R</i> ₁ , <i>wR</i> ₂ [<i>I</i> > 2σ(<i>I</i>)]	0.0351 ^a , 0.0996 ^b	0.0623 ^a , 0.1720 ^c
<i>R</i> ₁ , <i>wR</i> ₂ (all data)	0.0375 ^a , 0.1011 ^b	0.0748 ^a , 0.1859 ^c
largest peak, hole, eÅ ⁻³	0.870, -0.363	0.533, -0.887

^a*R* = Σ||*F*_o| - |*F*_c||/Σ|*F*_o|. ^b*wR*(*F*²) = [Σ*w*(*F*_o² - *F*_c²)/Σ*w*(*F*_o²)²]^{1/2} where *w* = 1/[σ²(*F*_o²) + (0.0518*P*)² + (0.7461)*P*], *P* = (*F*_o² + 2*F*_c²)/3. ^c*wR*(*F*²) = [Σ*w*(*F*_o² - *F*_c²)/Σ*w*(*F*_o²)²]^{1/2} where *w* = 1/[σ²(*F*_o²) + (0.1536*P*)² + (0.0000)*P*], *P* = (*F*_o² + 2*F*_c²)/3.

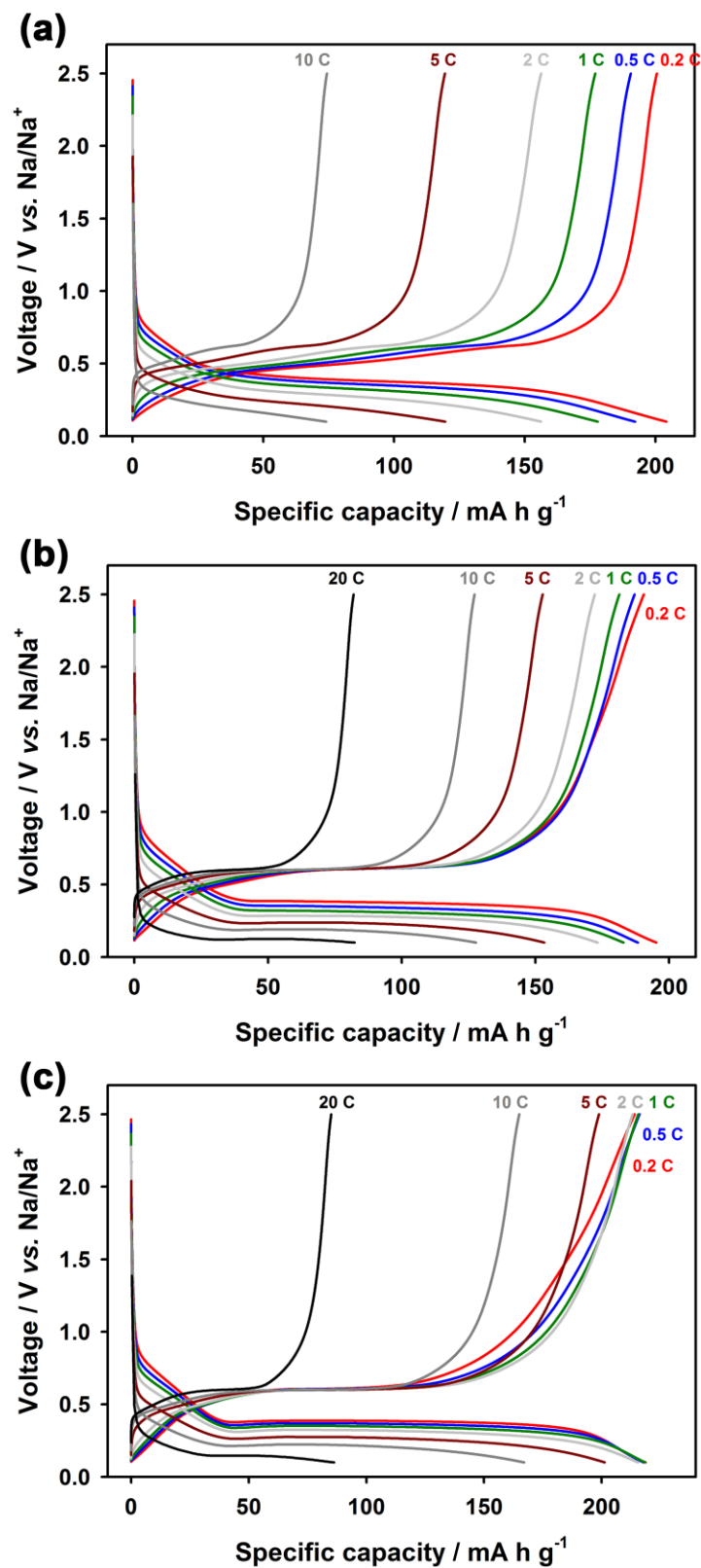


Fig. S1 Rate performance of NaHbpdC, *hyd*-Na₂bpdC, and Na₂bpdC: voltage profiles of (a) NaHbpdC, (b) *hyd*-Na₂bpdC, and (c) Na₂bpdC.

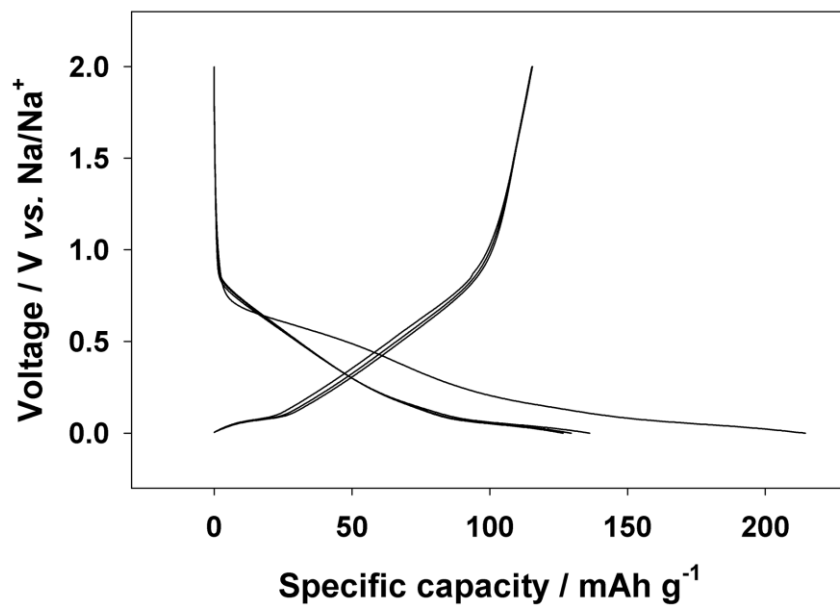


Figure S2. Voltage profiles of super P carbon.

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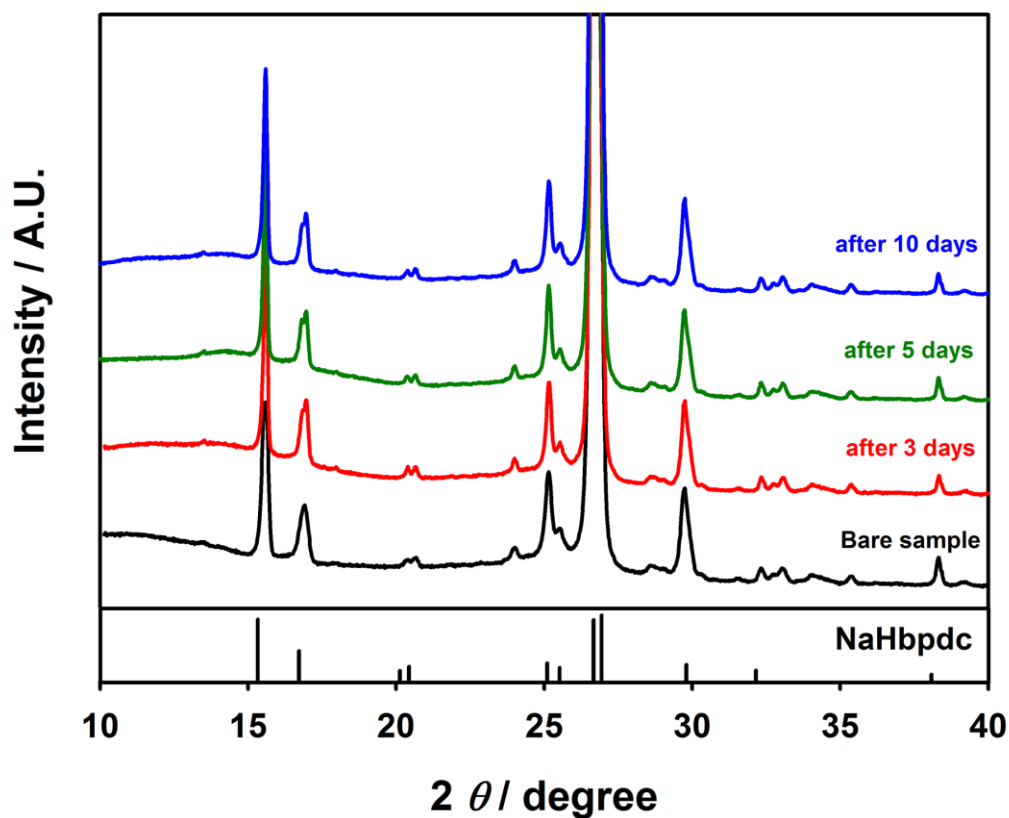


Figure S3. XRD patterns of NaHbpdc powders after storage in electrolytes for 3, 5, and 10 days.