A recrystallized organic cathode with high electrical conductivity for fast sodium-ion storage

Zixuan Shan [‡],^a Shuangqin Yang [‡],^a Xinya Zhang,^a Yuan Chen^{*a}

^aCollege of Energy Materials and Chemistry, Inner Mongolia University, Hohhot,

010070, China

‡ These authors contributed equally.

* Corresponding authors.

E-mail addresses: yuanchen@imu.edu.cn



Figure S1. Schematic of the synthesis of NDI-ONa.



Figure S2. ¹H-NMR spectrum of the NDI-OH.



Figure S3. (a) the FTIR spectra, (b) TGA curves of NDI-OH and NDI-ONa, respectively.

Table S1	LEA c	of NDI-OH	and NI	DI-ONa.

		С%	N%	Н%	O%	Na%
NDI-OH	Calculated	56.39	9.39	2.03	32.19	-
$(C_{14}H_6N_2O_6)$	Found	56.05	9.25	1.88	32.45	-
NDI-ONa	Calculated	49.14	8.19	1.18	28.05	13.44
$(C_{14}H_4N_2O_6Na_2)$	Found	48.45	8.75	1.78	28.85	14.12



Figure S4. UV spectra of NDI-OH and NDI-ONa in DME. After salinization, the NDI-ONa showed insoluble in DME solvent.



Figure S5. TEM image of NDI-ONa-r.



Figure S6. HR-TEM image of NDI-ONa-r.

Table S2. Electrical conductivity of NDI-OH and NDI-ONa

	$R(\Omega)$	<i>d</i> (mm)	σ (S m ⁻¹)
NDI-OH	2.7×10^{9}	0.29	8.1×10 ⁻¹⁰
NDI-ONa-p	3.05×10 ⁷	0.27	6.7×10 ⁻⁸
NDI-ONa-r	1.14×10^{6}	0.26	1.7×10 ⁻⁶

The electronic conductivity was calculated according to the following equation: $\sigma = \frac{d}{RS}$

where R, S, d are resistance value, area (1.33 cm^{-2}) and thickness of the pellet, respectively.



Figure S7. Calculated HOMO and LUMO energy levels of NDI-OH and NDI-ONa.



Figure S8. The CV curves of (a) NDI-ONa-r and (b) NDI-ONa-p at 0.2 mV s⁻¹, respectively.



Figure S9. The cycling performances of NDI-ONa-r and NDI-OH at 1 A g⁻¹.



Figure S10. The discharge and charge profiles of NDI-ONa-r at different current densities.



Figure S11. Comparisons of the capacity with three ratios of active materials.



Figure S12. The discharge and charge profiles of NDI-ONa-r with three ratios of active materials.

Table S3. The equivalent circuit and the values of the electrical elements of the NDI-ONa-r and NDI-ONa-p in different states.



Rs, CPE1, Rct and W1 represent the ohmic resistance, constant phase element, charge-transfer resistance and Warburg resistance, respectively.



Figure S13. (a, c) CV curves of NDI-ONa-r and NDI-ONa-p at various scan rates. (b, d) The linear fits of log(i) vs. log(v) plots.



Figure S14. The GITT curves of (a) NDI-ONa-p and (b) NDI-ONa-r cathodes at 0.1 A g⁻¹, respectively.



Figure S15. GITT potential response curve with time for one typical discharge step of (a) NDI-Oa-r and (b) NDI-ONa-p, respectively. The lower IR values also further indicated that NDI-ONa-r exhibited faster electrochemical reaction kinetics.

The Na^+ ion diffusion coefficient (D_{Na^+}) was further calculated by according to the following equation:

$$\mathbf{D}_{Na+} = (4/\pi\tau) \times ({}^{m_B V_M/M_B S})^2 \times ({}^{\Delta E_s/\Delta E_t})^2$$

where τ is the time of current pulse, and m_B, V_M, M_B, and S are the mass loading, molar volume, molar mass and electrode-electrolyte interface area of the material, respectively. ΔE_s is the voltage difference between the initial state and the steady state of each step, and ΔE_t is the voltage change resulting from the current pulse excluding the IR drop.



Figure S16. (a) The discharge and charge profiles and (b) cycling performance at 0.05 A g^{-1} of HC anode.



Figure S17. Charge-discharge curves of NDI-ONa-r//HC full cell at different densities.

 Table S4. Comparison of NDI-ONa-r cathode and the organic cathode materials

 reported in the literature for SIBs.

Materials (reference)	Electrode composition	Specific capacity (mAh g ⁻¹) (Current density, A g ⁻¹)	Cycle Stability Retention/ Cycles/ Current density	Ref.
NaO-N NDI-ONa-r	7:2:1	145 (0.1) 70 (20)	87%, 30000, 10A g ⁻¹	This work
HN O PTCDI	7:2:1	138 (0.02) 103 (0.6)	90%, 300, 0.2 A g ⁻¹	ACS Appl. Mater. Interfaces 2015, 7, 21095
NaOOC N COONA Na2BNDI	6:3:1	111 (0.1 C) 77 (50C)	57.3%, 70000, 10C	Adv. Energy Mater. 2021, 11, 2101972
NaO NaO NaO ONa Na4C ₆ O ₆	7:2:1	170 (0.5)	71.9%, 1000, 0.1 A g ⁻¹	J. Am. Chem. Soc. 2024, 146, 1619- 1626
ONa ONa ONa Na ₂ C ₆ O ₆	7:2:1	205 (0.02) 102 (1)	75%, 500, 0.05 A g ⁻¹	<i>Chem</i> 2017, <i>3</i> , 1050
TAPQ	7:2:1	257 (0.1) 236 (5)	72%, 1000, 1 A g ⁻¹	Angew. Chem. Int. Ed. 2021, 60, 26806-26812
N N N N N N N N N N N N N N N N N N N	7:2:1	80.9 (2) 64.3 (12)	97.9%, 5000, 64 A g ⁻¹	Chem. Eng. J. 2023, 451, 138652
	6:3:1	193 (0.1) 150 (10) 101 (40)	95.8%, 1000, 0.05 A g ⁻¹	ACS Nano 2022, 16, 14590
	70:15:10:5	129 (0.05) 75 (1) 11 (5)	63%, 300, 0.05 A g ⁻¹	<i>Adv. Mater.</i> 2016, 28, 9182

PT				
$\overbrace{PI2}^{\circ}$	6:3:1	137 (0.2 C) 75 (5 C)	86%, 5000, 0.8C	Adv. Energy Mater. 2014, 4, 1301651
PTCDA	6:3:1	126 (0.2) 99 (5)	94%, 400, 1 A g ⁻¹	Energy Storage Materials, 2022, 61-68
NaO, S, O O O Na ₂ AQ26DS	active materials: KB:CNTs:La133 :PVDF=70:10:1 0:7:3	87 (0.5) 30 (5)	72%, 1000, 0.5 A g ⁻¹	ChemSusChe m 2020, 13, 1991-1996
$= \underbrace{\begin{array}{c} R_{1} \\ N \\ N \\ R_{1} \\ R_{1} \\ M = 2H \text{ or } Cu \\ PTO \\ \end{array}}_{R_{1} M = 2H \text{ or } Cu \\ PTO$	85:5:10	172 (0.2) 138 (10)	93%, 600, 5 A g ⁻¹	Nano-Micro Lett. 2021, 13, 71
F HN EFID	7:2:1	135 (0.1) 28 (5)	91.2%, 2000, 0.2 A g ⁻¹	<i>Adv. Sci.</i> 2024, <i>11</i> , 2307134
ONa ONA ONA ONA NDI-ONA	6:3:1	170 (0.1) 159 (2)	93%, 20000, 3A g ⁻¹	ACS Nano 2023, 17, 21432-21442
PAQI	4:4:2	200 (0.05) 60 (1)	93%, 150, 0.05 A g ⁻¹	J. Mater. Chem. A 2016, 4, 11491-11497
PAQS	6:3:1	175 (0.05) 110 (1)	-	Adv. Energy Mater. 2020, 10, 2002780
PPTS	4:5:1	290 (0.1) 170 (10)	86%, 5000, 10 A g ⁻¹	Chem 2018, 4, 2600-2614

$ \begin{array}{c c} & X=Y \\ & X=N, Y=C \\ & x=N, Y=C \\ & or \\ & X=C, Y=N \\ \hline \\ & BPyPz \end{array} $	7:2:1	205 (0.5) 126 (20)	89%, 300, 0.5 Ag ⁻¹	J. Mater. Chem. A, 2023, 11, 2711
e e e e e e e e e e e e e e e e e e e	8:1:1	287.6 (0.1) 216.6 (5.0)	95.1%, 1300, 10 A g ⁻¹	Adv. Energy Mater. 2020, 11, 2002917