# Supporting information

## Spray-Drying Synthesis of High-Performance $Na_4MnCr(PO_4)_3$ for Sodium-Ion Batteries via CNT-Induced Conductive Network and Optimized Interface Kinetics

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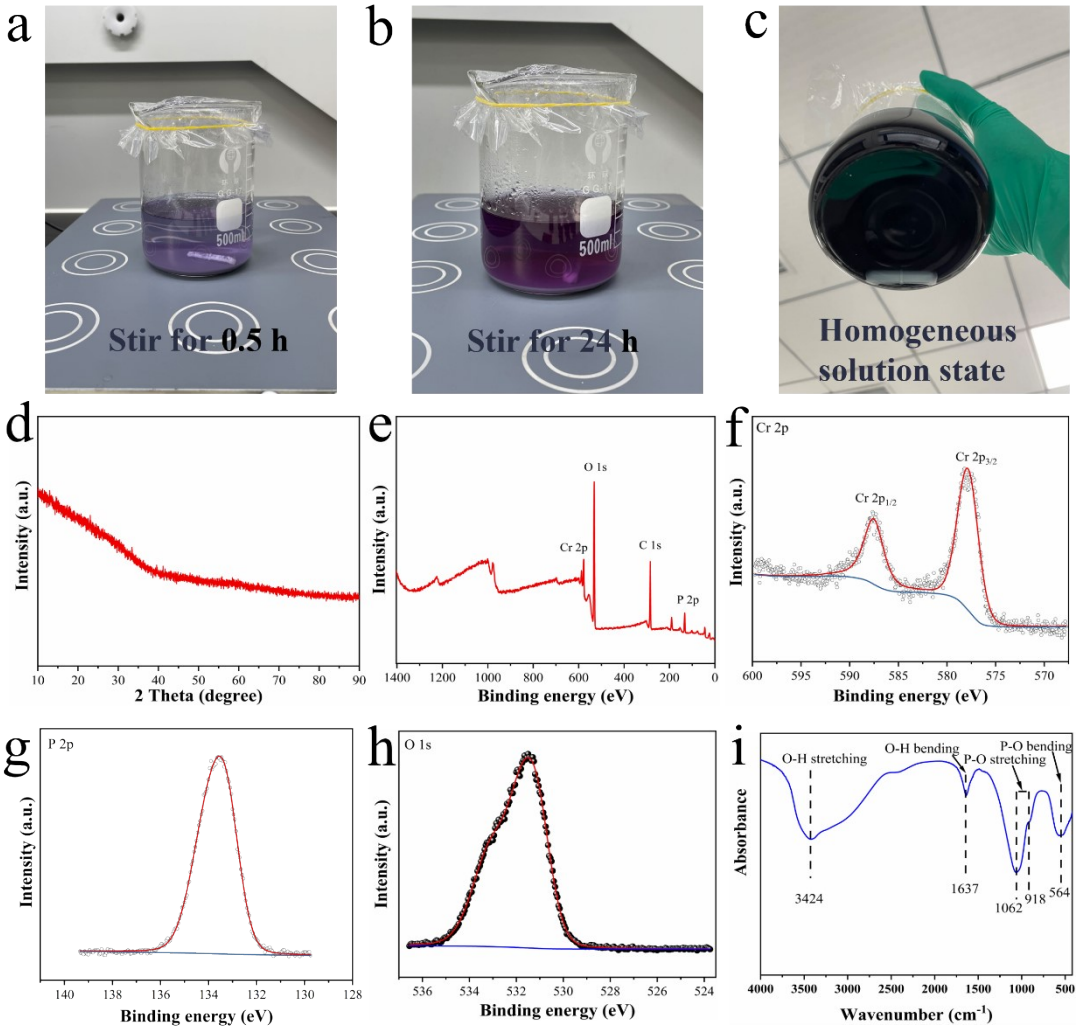
## Experimental section

Synthesis procedure of $Na_4MnCr(PO_4)_3$/C/xCNTs (x = 0, 5, 10, 15) composites: At room temperature, the following reagents were sequentially weighed and added into

200 mL of deionized water: 20 mmol of anhydrous citric acid ($C_6H_8O_7$, Aladdin, AR), 40 mmol of anhydrous sodium acetate ($CH_3COONa$, Aladdin, AR), 10 mmol of manganese acetate tetrahydrate ($Mn(CH_3COO)_2 \cdot 4H_2O$, Aladdin, AR), 10 mmol of chromium nitrate nonahydrate ($Cr(NO_3)_3 \cdot 9H_2O$, Aladdin, AR), 30 mmol of ammonium dihydrogen phosphate ($NH_4H_2PO_4$, Aladdin, AR), and 1 g of ascorbic acid ($C_6H_8O_6$, Sinopharm, AR). The mixture was then transferred to a 80 ℃ hot plate and stirred for approximately 4 hours (Why we do this: We observed that after adding all precursor components, a precipitate identified as $CrPO_4 \cdot xH_2O$ would form, which could not be completely dissolved even after 24 hours of stirring at room temperature. Further investigation revealed that under heated and stirred conditions, this precipitate could be fully dissolved, resulting in a transparent solution state of the entire precursor liquid. Notably, this transparent state remained stable even when cooled back to room temperature. Here, we elucidate this process in detail, aiming to facilitate the solution-based preparation of $Na_4MnCr(PO_4)_3$). After cooling to room temperature, specified quantities (5 g, 10 g, and 15 g) of 10 wt% carbon nanotube aqueous solution (XFNANO, product code: 100320) were added for spray drying (Shanghai Pilotech, YC-015) with an inlet air temperature of 220 °C. The collected precursor was sintered at 650 °C for 4 hours in an Ar atmosphere with a heating rate of 5 °C/min to obtain the final product. For convenience, samples with different CNT addition amount are labeled as NMCP/C/5CNTs, NMCP/C/10CNTs, and NMCP/C/15CNTs, respectively, while the CNT-free sample is designated as NMCP/C.

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| Element | Cr | Mn | P |
|---|---|---|---|
| Proportion | 1 | 0.024 | 1.06 |

**Figure only for Experimental section**. The states of the precursor solution after being stirred at room temperature for (a) 0.5 h and (b) 24 h, respectively. (c) Solution state at room temperature after preheating treatment. (d) XRD patterns and (e) XPS whole spectra of the precipitate, respectively. (f-h) Fitted high-resolution core-level spectra of Cr 2p, P 2p and O 1s, respectively, and no significant Mn signal was detected. (i) FTIR spectra of the precipitate. (j) ICP-OES analysis results of the precipitate: The presence of a certain amount of Mn is due to the fact that the Cr on the surface of the generated precipitate chelates with citric acid, which in turn also

chelates the Mn in the solution, resulting in their co-precipitation.

Materials characterization: The quantitative analysis of the precipitation was carried out by inductively coupled plasma optical emission spectrometry (ICP-OES, Prodigy Plus). Fourier transform infrared spectroscopy (FT-IR, Nicolet iS50R) was used to characterize types of functional groups present in the precipitation in the frequency range of 400–4000 $cm^{-1}$. The carbon content of $Na_4MnCr(PO_4)_3$/C/xCNTs (x = 0, 5, 10, 15) composites was measured from room temperature to 800 °C by a thermogravimetric analysis (TG, NETZSCH STA449F3) meter under a flowing air atmosphere with a heating rate of 10 °C $min^{-1}$. The crystal structure of the samples was evaluated by X-ray diffraction (XRD, PANalytical, X'Pert3 powder) using Cu Kα radiation in the 2θ range of 10-90°. SEM (Nova NanoSEM 450) and TEM（FEI Talos F200x G2）were used to characterize the morphology and detailed microstructure of the final products. The properties of the amorphous carbon of the prepared cathode materials were analyzed by Raman spectrometer (LabRAM HR800). The specific surface area and pore size distribution of the composites were determined using N2 gas adsorption/desorption techniques on a TriStar II 3020 system. Photoelectron Spectroscopy (XPS, AXIS-DLD-660 W) was adopted to probe the chemical state of elements on the surface of precipitates and $Na_4MnCr(PO_4)_3$/C composites.

Electrochemical measurements: The electrochemical performance of the

$Na_4MnCr(PO_4)_3$/C/xCNTs (x = 0, 5, 10, 15) cathodes was measured using CR2025 coin half cells assembled in an argon-filled glove box. The cathode was fabricated by mixing the active material powder, Super P and polyvinylidene fluoride (PVDF) binder (70:20:10 by weight) in N-methyl-2-pyrrolidone (NMP) to form a homogeneous slurry. The slurry was then coated onto an Al foil and dried at 120 °C for 12 hours. 1 M $NaClO_4$ in propylene carbonate (PC) with 5% fluoroethylene carbonate (FEC) additive was used as electrolyte. Whatman Glass Microfiber (Grade GF/C) was employed as the separator in the half cells. Galvanostatic charge/discharge tests were carried out on a LAND battery test system in the voltage range of 1.5–4.3 V (vs. $Na^+$/Na). The cyclic voltammetry tests were implemented by an electrochemical workstation (AUTOLAB) in the potential range of 1.5-4.3 V (vs. $Na^+$/Na) at various scanning rates. Electrochemical impedance spectroscopy (EIS) measurements were tested on CHI 660E electrochemical workstation within a frequency range from 100 kHz to 0.01 Hz.

Computational Details: Structural optimization, energy barriers, and other DFT-related calculations were performed using the Vienna Ab-initio Simulation Package (VASP) version 6.4.1, employing the Perdew-Burke-Ernzerhof (PBE) functional and the projector augmented wave (PAW) method.[1] [2] For slab structures, a 15 Å vacuum layer along the z direction was introduced to prevent periodic interactions. The Na+ diffusion barrier was determined using the climbing-image nudged elastic band (Cl-NEB) method.[3] The convergence tolerances for energy and force were set to $1\times10^{-6}$

eV and 0.02 eV $Å^{-1}$, respectively (detailed configuration parameters of the material structure in VASP format are provided in the final section of the Supporting Information).

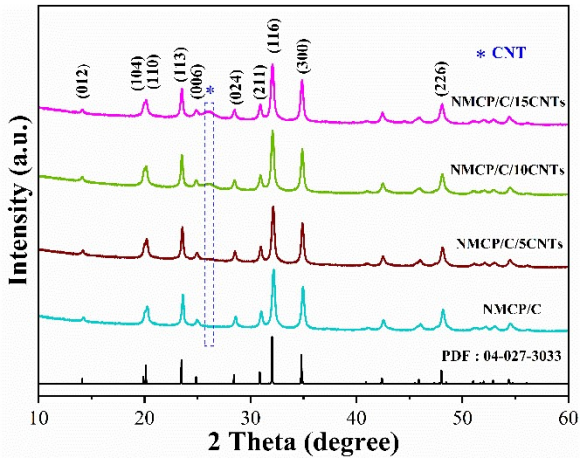


**Figure S1**. XRD patterns of $Na_4MnCr(PO_4)_3$/C/xCNTs (x = 0, 5, 10 ,15).

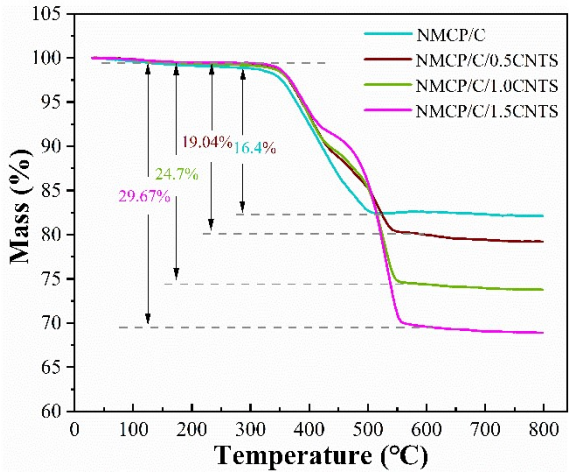


**Figure S2**. TG curves of $Na_4MnCr(PO_4)_3$/C/xCNTs (x = 0, 5, 10 ,15).

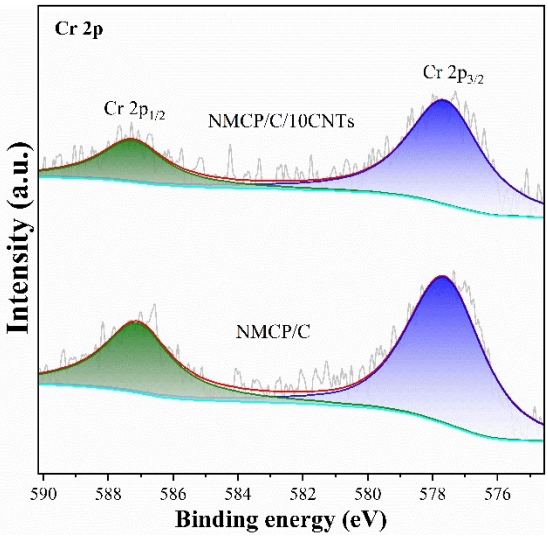


**Figure S3.** High-resolution XPS spectra of Cr 2p for NMCP/C and NMCP/C/10CNTs.

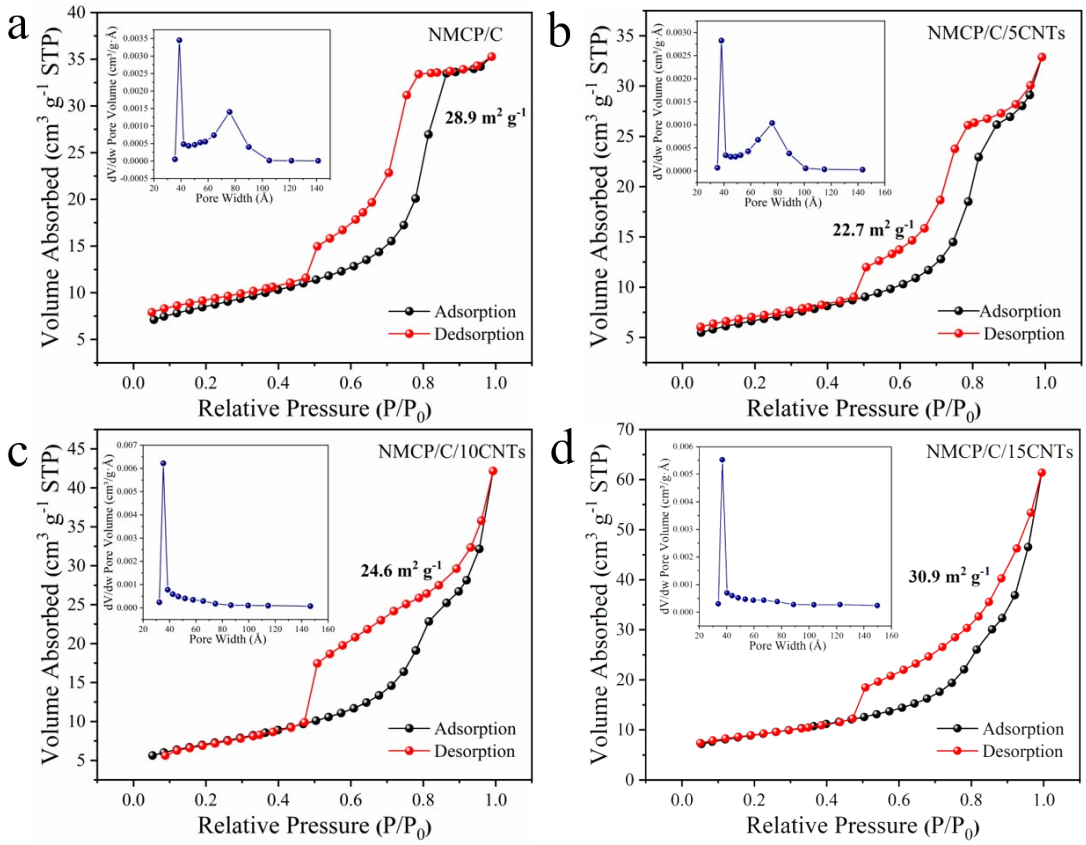


**Figure S4.** Nitrogen adsorption–desorption curves and Barrett-Joyner-Halenda (BJH) pore distribution of (a) NMCP/C, (b) NMCP/C/5CNTs, (c) NMCP/C/10CNTs and (d) NMCP/C/15CNTs, respectively.

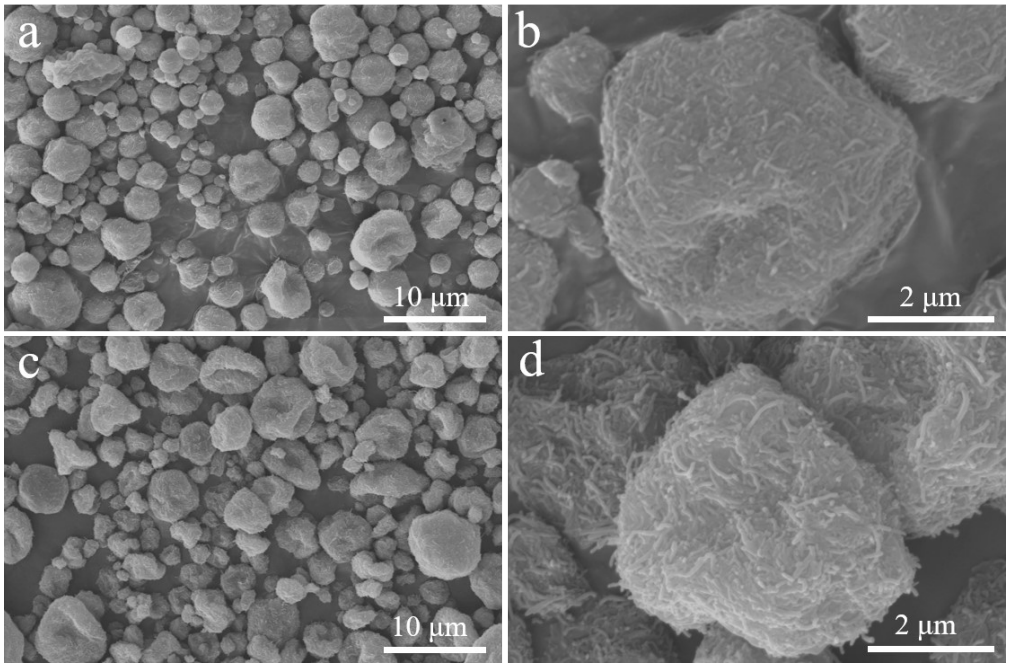


**Figure S5.** SEM images with different resolution: (a and b) NMCP/C/5CNTs and (c and d) NMCP/C/15CNTs, respectively.

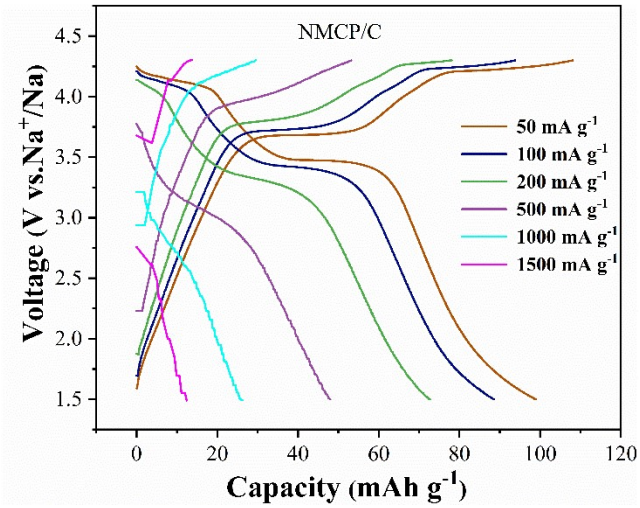


**Figure S6.** GCD curves of NMCP/C cathode at different current densities.

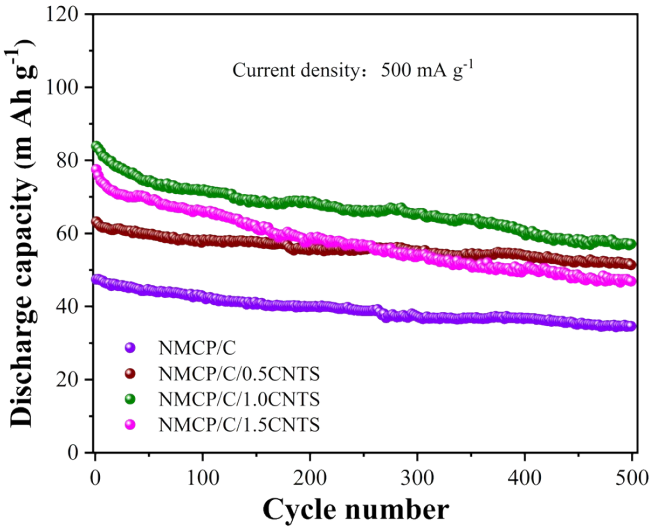


**Figure S7.** Cycling capability of the four cathodes at 500 mA $g^{-1}$.

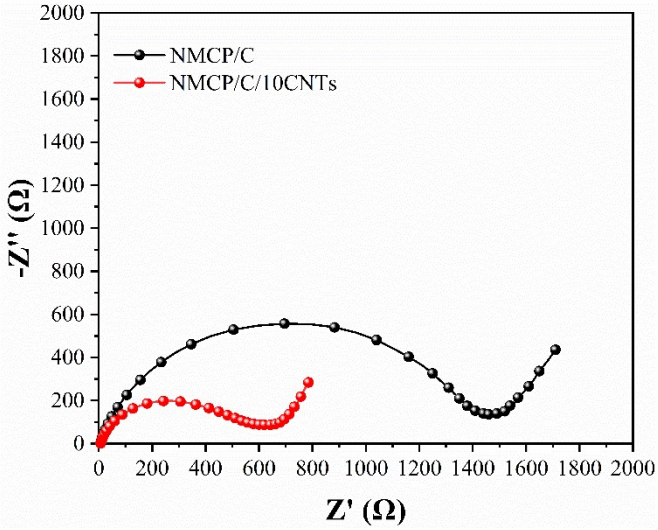


**Figure S8.** EIS of the uncycled NMCP/C and NMCP/C/10CNTs electrodes indicates that the $R_{ct}$ is significantly lower after CNTs incorporation.

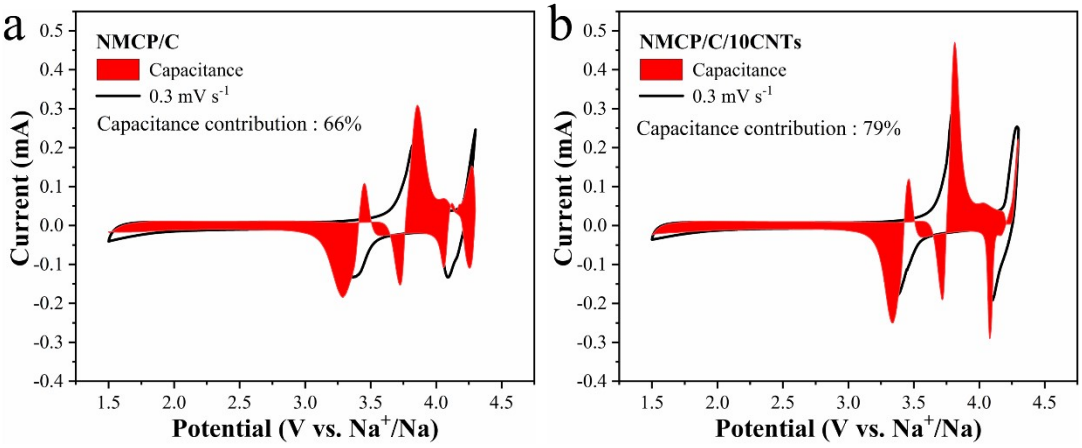


**Figure S9.** Capacitive contribution ratio at a scan rate of 0.3 mV $s^{-1}$ of (a) NMCP/C and (b) NMCP/C/10CNTs, respectively.

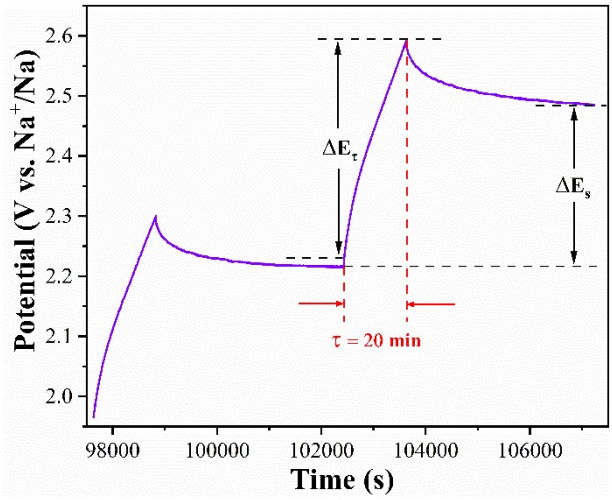


**Figure S10.** Schematic diagram of a single GITT titration step during the charging process.

The sodium ion diffusion coefficient （$D_{Na}$） measured based on the GITT technique can be deduced from equation :

$$D_{Na} = \frac{4}{\pi\tau}\left(\frac{m_B V_M}{M_B A}\right)^2 \left(\frac{\Delta E_s}{\Delta E_\tau}\right)^2 \quad \left(\tau \ll \frac{L^2}{D_{Na}}\right)$$

where $m_B$ is the mass of the active material, $V_M$ is the molar volume, $M_B$ is the molecular weight, $A$ is the total contact area between electrode and electrolyte, $\Delta E_s$ is the difference between two consecutive stable voltages after relaxation, $\Delta E_\tau$ is the

difference between the equilibrium potential and the potential maximum at the end of the current pulse, and $L$ is the thickness of the electrode.

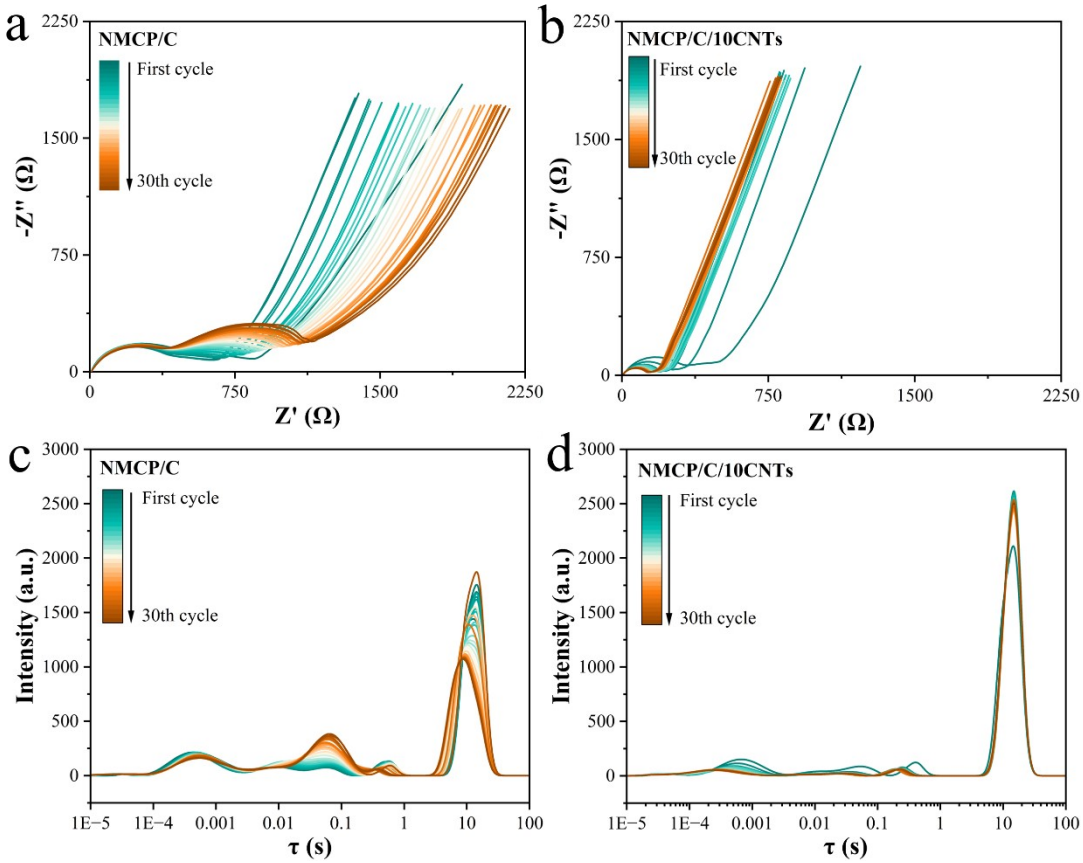


**Figure S11.** The Nyquist plots of the EIS for the initial thirty cycles and the DRT curves of (a,c) NMCP/C and (b,d) NMCP/C/10CNTs, respectively.

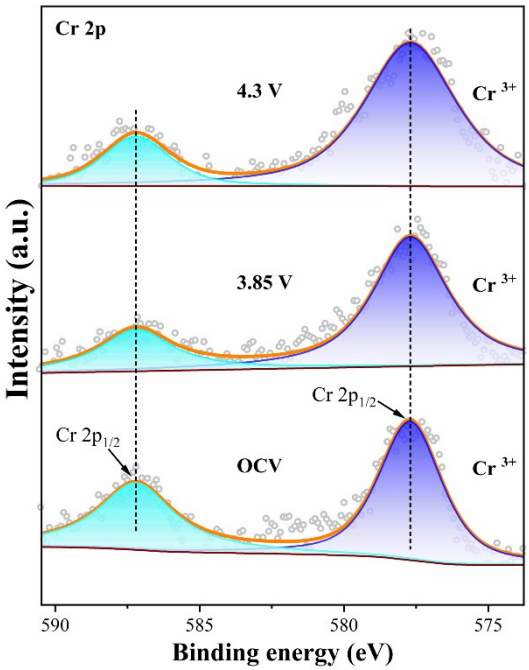


**Figure S12.** Ex situ XPS of high-resolution Cr 2p spectra at selected charged states of NMCP/C/10CNTs cathode..

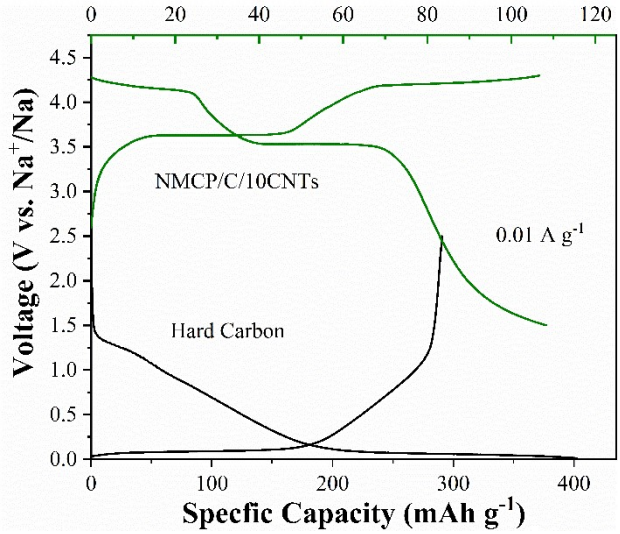


**Figure S13.** galvanostatic charge/discharge curves of NMCP/C/10CNTs and hard carbon at 0.01 A $g^{-1}$ in the half battery, respectively.

**Table S1.** Detailed structural information of NMCP/C/10CNTs derived from Rietveld Refinement.

| space group = R-3c | | $R_p$ = 1.84% | | $R_{wp}$ = 2.44% | |
|---|---|---|---|---|---|
| a (Å) = 8.92476 | | c (Å) = 21.4913 | | α(º) = 90 | |
| β(º) = 90 | | γ(º) = 120 | | V (Å$^3$) = 1482.47 | |
| Atom | Wyckoff site | x | y | z | Occupancy |
| Na1 | 6b | 0.0000 | 0.0000 | 0.0000 | 1 |
| Na2 | 18e | 0.64892 | 0.0000 | 0.2500 | 1 |
| Mn | 12c | 0.0000 | 0.0000 | 0.15047 | 0.5 |
| Cr | 12c | 0.0000 | 0.0000 | 0.15047 | 0.5 |
| P1 | 18e | 0.29505 | 0.0000 | 0.2500 | 1 |
| O1 | 36f | 0.18141 | 0.17802 | 0.08057 | 1 |
| O2 | 36f | 0.01593 | 0.21199 | 0.19277 | 1 |

**Table S2.** Detailed structural information of NMCP/C/10CNTs derived from Rietveld Refinement.

| **Peak** | **O1** | **O2** | **R1** | **R2** |
|---|---|---|---|---|
| **$D_{Na+}$** | **$6.17\times10^{-10}$** | **$1.01\times10^{-10}$** | **$4.87\times10^{-11}$** | **$1.00\times10^{-11}$** |

**Detailed configuration parameters of the material structure used in the DFT calculation**

Na1-Na1 initial

Na24 Mg6 Al6 P18 O72
1.00000000000000
9.0766804151787568 0.0000000000000000 0.0000000000000000
-4.5383402075893784 7.8606358215880077 0.0000000000000000
0.0000000000000000 0.0000000000000000 21.4551710187697786
Na Mn Cr P O
23 6 6 18 72
Direct
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0.6652969421735487 0.7030979014929342 0.0824734697428434
0.2968918927851563 0.9622663265254089 0.0824703029234966
0.6452330498000097 0.9470445185809421 0.5963489524990693

0.3020293409583053 0.3548489405220957 0.5963447011796852
0.0530866427071256 0.6980919135534734 0.5963388578099882
0.7069245545232272 0.6706413077059044 0.4162364289867445
0.3293070806539872 0.0362763025452469 0.4162180981662261
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