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Mesoporous NaTi₂(PO₄)₃/CMK-3 Nanohybrid as Promising Anode for Long-life Na-ion Batteries

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Synthesis of the mesoporous CMK-3

Following the method reported by Zhao *et al.*,¹ SBA-15 templates were synthesized using Pluronic P123 (EO₂₀PO₇₀EO₂₀, M_w ~5800) as surfactant and tetraethylorthosilicate (TEOS) as silica source. A nanocasting method was used to prepare the CMK-3 from SBA-15 template. Typically, 1.25 g of sucrose was dissolved in a solution containing 11 mL of deionization (DI) water and 7.2 mL of 0.2 M H₂SO₄. 1.0 g of the prepared SBA-15 was then dispersed in the above solution and the mixture was ultrasonicated for 1 h. The mixture was then heated at 100 °C for 6 h and subsequently at 160 °C for another 6 h. The impregnation and baking process was repeated once with another aqueous solution containing 11 mL of DI water, 0.75 g of sucrose and 7.2 mL of 0.2 M H₂SO₄. The composite was completely carbonized at 900 °C for 5 h in an inert nitrogen atmosphere. To remove the SBA-15 silica template, the composite was stirred in 2 M hot NaOH solution twice. After that, the obtained CMK-3 carbon templates were functionalized by 6 M HNO₃.

- 1 D. Y. Zhao, J. L. Feng, Q. S. Huo, N. Melosh, G. H. Fredrickson, B. F. Chmelka and G. D. Stucky, *Science*, 1998, **279**, 548.

Table S1 Atomic coordinates, isotropic thermal parameters and occupation numbers for the NTP phase refined from X-ray powder diffraction data. NASICON-type structure in space group R-3c (No. 167); cell parameters: $a = 8.4884 (5) \text{ \AA}$, $c = 21.8123 (3) \text{ \AA}$, $V = 1361.07 (2) \text{ \AA}^3$ and $Z = 6$; $R_{wp} = 10.32 \%$, $R_p = 7.03 \%$, $R_I = 4.47 \%$, $S = 2.97$.

Atom	Site	g	x	y	Z	B (\AA^2)
Na	6b	1.0	0.0	0.0	0.0	2.8(2)
Ti	12c	1.0	0.0	0.0	0.1447(1)	0.5(1)
P	18e	1.0	0.2868(3)	0.0	1/4	0.6(1)
O1	36f	1.0	0.1751(6)	0.9781(6)	0.1934(2)	0.7(1)
O2	36f	1.0	0.1941(4)	0.1635(4)	0.0903(2)	0.6(1)

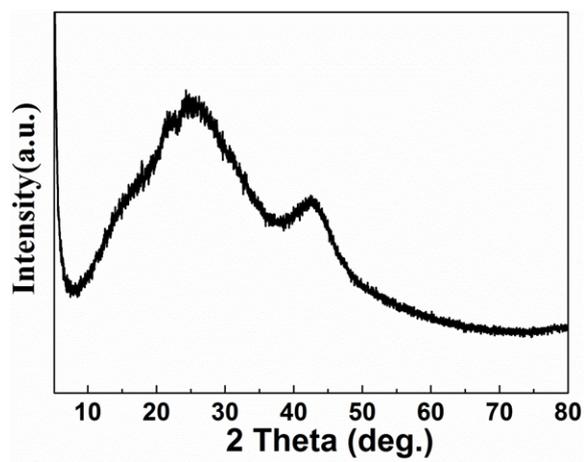


Fig. S1 Wide angle X-ray diffraction pattern of the CMK-3.

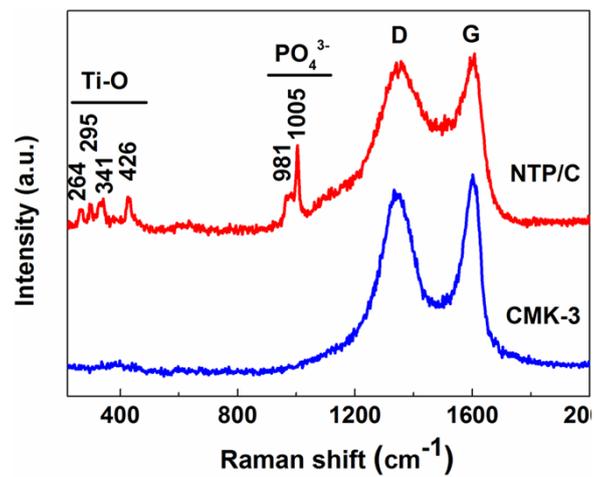


Fig. S2 Raman spectrums of mesoporous NTP/C nanohybrid and CMK-3, showing the Raman band of Ti-O, PO_4^{3-} and C.

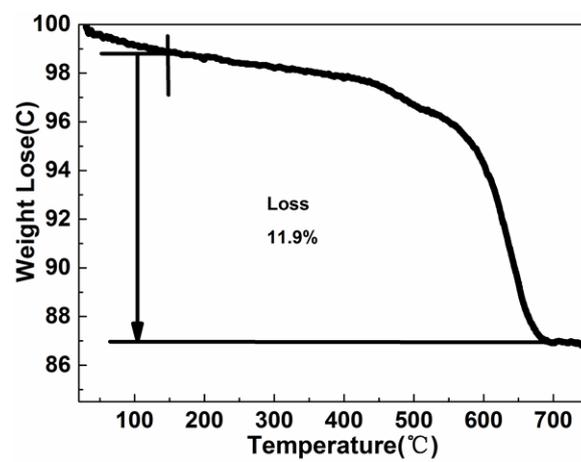


Fig. S3 TG curve of the mesoporous NTP/C sample in air atmosphere.

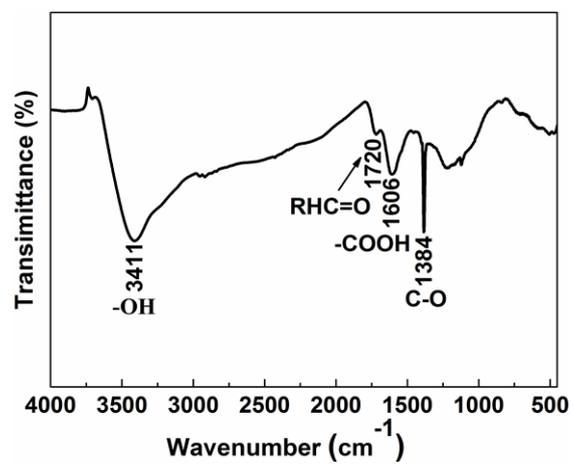


Fig. S4 FT-IR spectrum of the acid-treated CMK-3 recorded in the range of 450-4000 cm⁻¹.

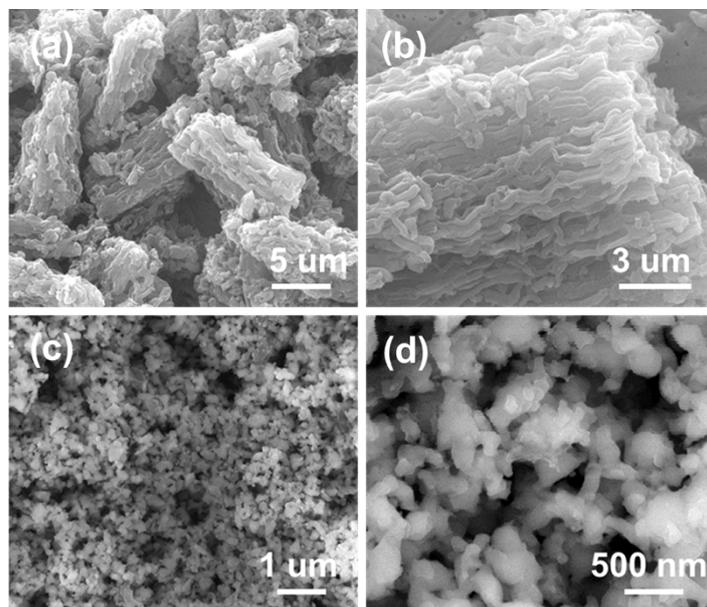


Fig. S5 FESEM images of the CMK-3 (a, b) and mesoporous NTP/C nanohybrid (c, d).

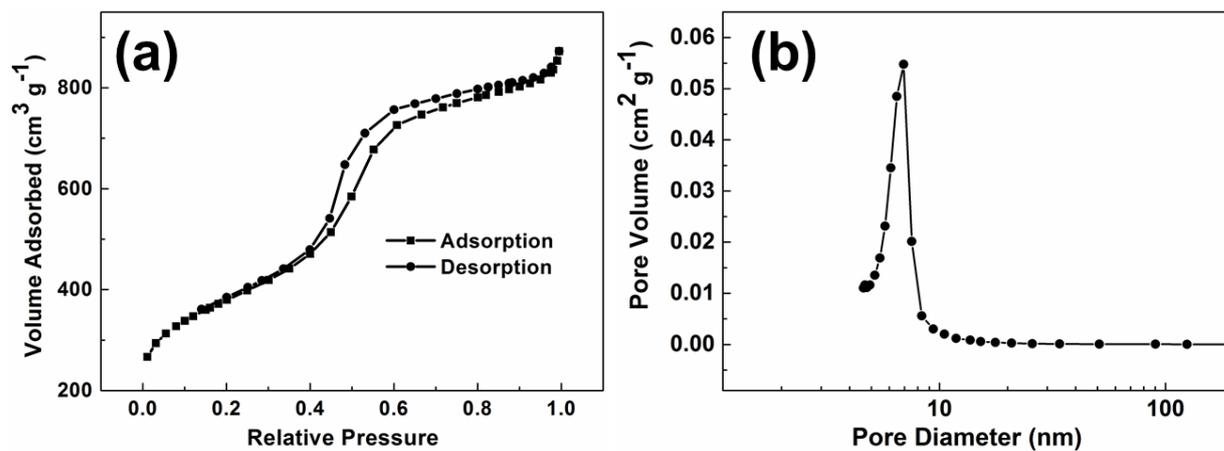


Fig. S6 Nitrogen sorption isotherms (a) and PSD data (b) of the mesoporous CMK-3.

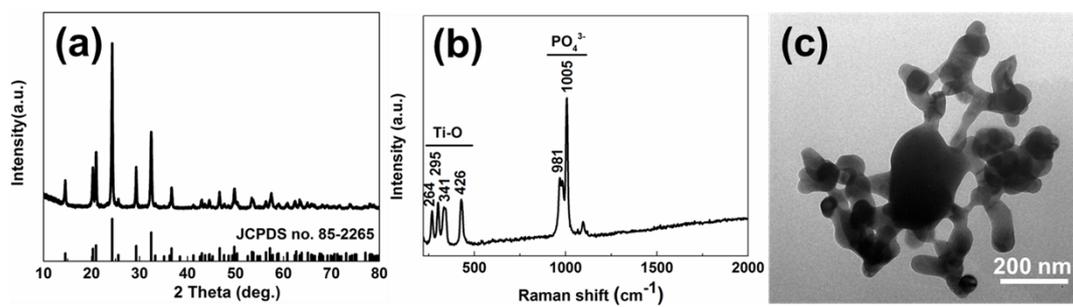


Fig. S7 XRD pattern (a), Raman spectrum (b) and TEM image (c) of pure NTP. The black vertical lines in (a) for the standard spectrum of JCPDS no. 85-2265.