

Supplementary Information:

Ordered mesoporous TiC-C composites as cathode material for Li-O₂ batteries

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Experimental details:

Preparation of ordered mesoporous TiC-C composites (OMTC)

OMTC was prepared according to procedures previously reported with some difference.^{1,2}

Synthesis of resol precursors: 8 g of phenol was melted under 70°C, then 2 g of NaOH aqueous solution (20 Wt %) and 14.5 g of formaldehyde solution (37 wt %) were added successively with continued stirring. The mixture was kept at 70°C for 2 h and then cooled to room temperature naturally. The solution was adjusted to pH=7 with HCl solution before it was dried at 40°C under vacuum for 48 h to remove water. Next, the products were diluted by ethanol and then filtrated to remove the NaCl.

Synthesis of tetrabutyl titanium-citrate compounds: 22 g of tetrabutyl titanate was dissolved in 30 ml ethanol and 13.6 g of citric acid was dissolved in 15 ml ethanol,

and these solutions were mixed subsequently. The mixture was heated to 60°C to form gel and then dissolved in the ethanol/water mixture (1:1, v/v) to obtain a 1 mol kg⁻¹ tetrabutyl titanium-citrate solution.

Synthesis of OMTC: 2.7 g of F127, 2.4 g of resol precursor (phenol 45.4 wt %), 3.4 g of tetrabutyl titanium-citrate solution and 20 ml of ethanol/water mixture (1:1, v/v) were mixed with continued stirring to form a transparent solution. The solution was transferred to petri dishes and maintained at 35°C for 24 h, and then heated to 100°C for another 24 h. The product was calcinated under Ar atmosphere at 300°C for 3 h, 600°C for 2 h and 1300°C for 2 h in a tube furnace. The heating rate was 1°C min⁻¹ and the cooling rate was 2°C min⁻¹. The obtained material was then balled into particles before they were used.

Characterization

The scanning electron microscopy (SEM) images were collected on a Hitachi SU-8000. The transmission electron microscopy (TEM) and high resolution transmission electron microscopy (HR-TEM) results were obtained on a JEOL JEM-200CX. The X-ray photoelectron spectroscopy (XPS) results were received on a PHI 5000 VersaProbe. The X-ray diffraction (XRD) and small angle X-ray diffraction (SAXRD) patterns were got on a Bruker D8-Advanced diffractometer. The nitrogen adsorption-desorption analysis was carried out on an ASAP 2020 instrument. The content of the TiC was investigated by thermogravimetry (TG) on a SDT Q600. The gas contents during the charge process were determined by gas chromatography-mass spectrometer (GC-MS) on a Perkin-Elmer (Clarus 680 and SQ 8S).

Preparation of electrodes for Li-O₂ battery measurements.

Electrode preparation and measurement: The OMTC electrode consisted of as-prepared OMTC 40 wt %, Super P 40 wt % and polyvinylidene fluoride (PVDF) binder 20 wt %. SP electrode: Super P 80 wt % and PVDF 20 wt %; n-TiC electrode: boughten TiC nanoparticle (Aladdin, 50nm) 40 wt %, Super P 40 wt % and PVDF 20 wt %. N-methyl-2-pyrrolidone (NMP) was added to the mixture, and the formed slurry was coated onto an Al current collector. The coated electrode was then dried under vacuum at 80 °C over night. The mass loading density of total for cycling tests was about 0.2 mg cm⁻². All batteries were assembled in an Ar-filled glove box, using a lithium foil anode, a glass filter separator, the prepared electrode and electrolyte (a solution of LiCF₃SO₃ in a TEDGME solvent with a molar ratio of 1:4). The electrochemical measurements were carried out under oxygen (about 1 atm) at room temperature on a LAND battery test system and the specific capacity was normalized based on the total amount of Super P and catalyst (OMTC or n-TiC).

Results:

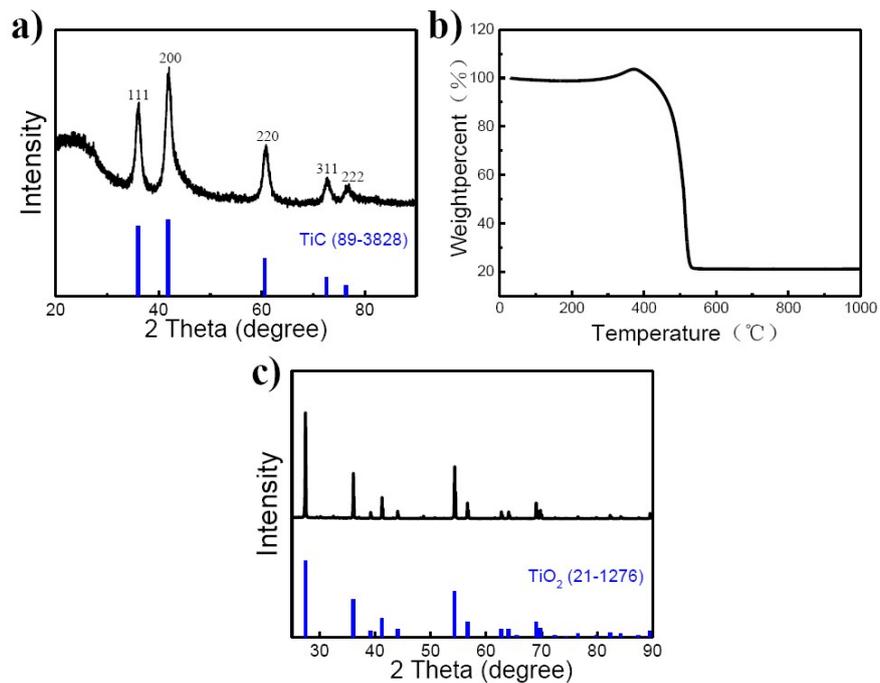


Fig. S1 a) XRD pattern of OMTc. b) TG curve of OMTc. c) XRD pattern of the calcined OMTc.

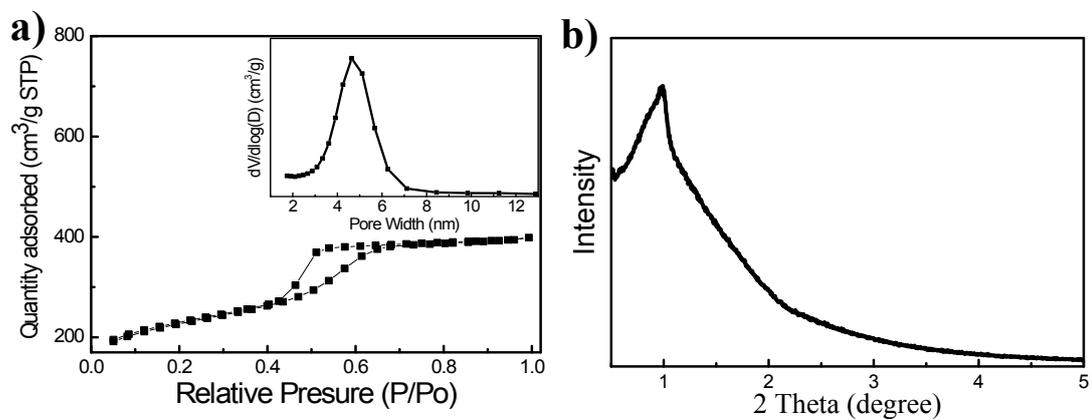


Fig. S2 a) The nitrogen adsorption–desorption and pore size distribution (inset) curves of OMTc. b) SAXRD pattern of OMTc.

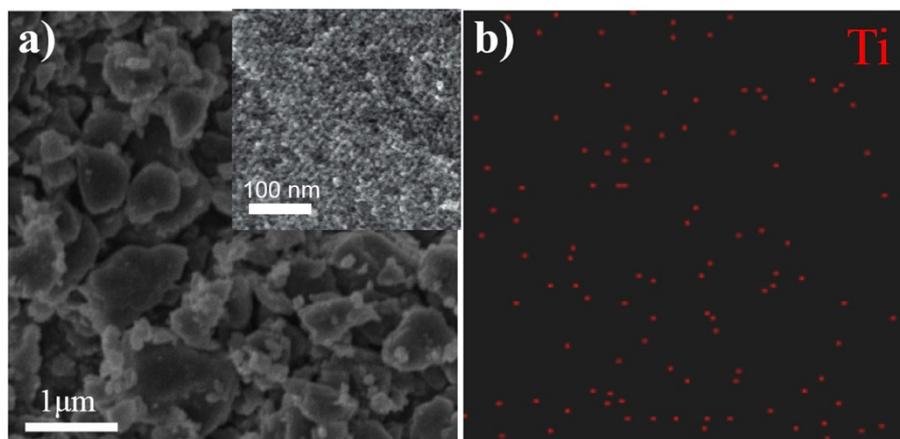


Fig. S3 a) SEM images of the OMTC particles. b) EDS mapping of the OMTC particles.

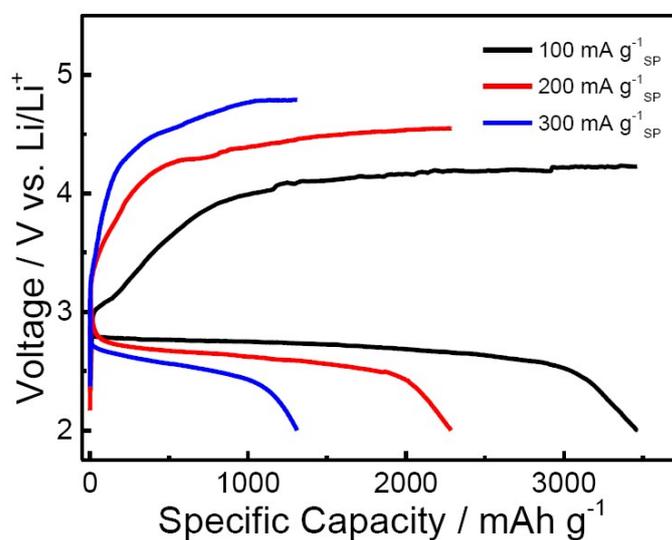


Fig. S4 Discharge and charge curves of the OMTC electrode at different rates.

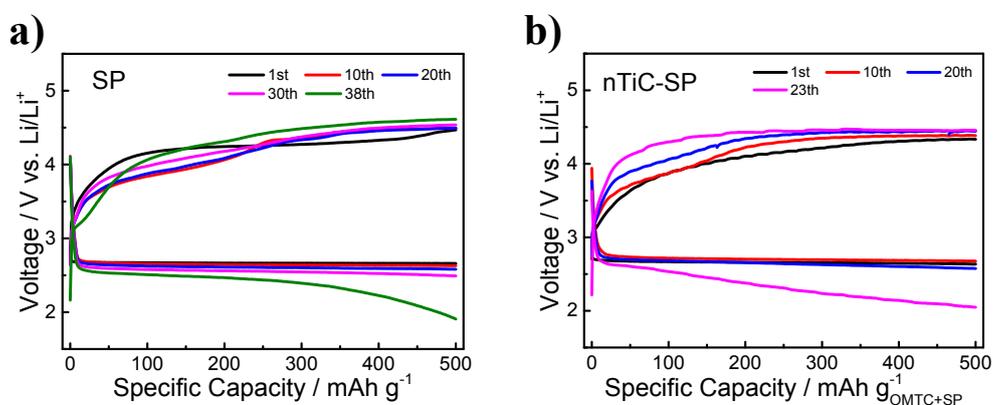


Fig. S5 a, b) Cycle curves of SP and n-TiC electrodes with a fixed capacity of 500 mAh g⁻¹, at a current density of 100 mA g⁻¹_{SP}.

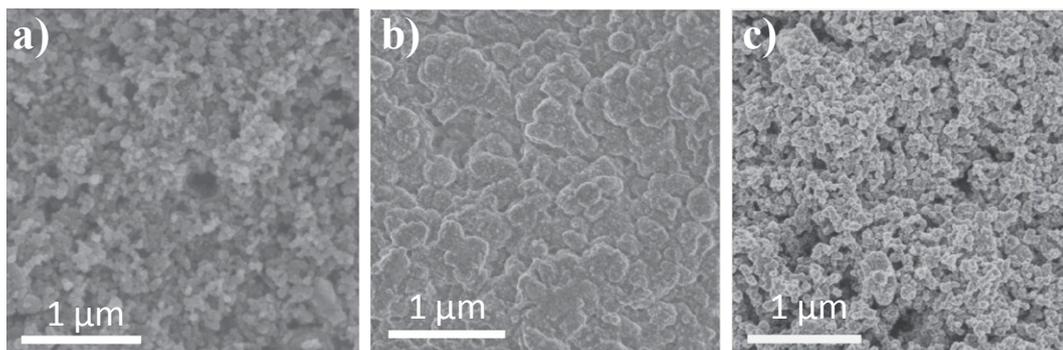


Fig. S6 SEM images of the OMTC electrodes at various states: a) Pristine. b) Discharged. c) Recharged.

Reference:

- 1 Y. Meng, D. Gu, F. Q. Zhang, Y. F. Shi, H. F. Yang, Z. Li, C. Z. Yu, B. Tu and D. Y. Zhao, *Angew Chem Int Edit*, 2005, **44**, 7053-7059.
- 2 T. Yu, Y. H. Deng, L. Wang, R. L. Liu, L. J. Zhang, B. Tu and D. Y. Zhao, *Advanced Materials*, 2007, **19**, 2301-2306.