Supplementary Information

Peapod-like architectures with CuO microspheres encapsulated

within MXene as conversion electrode for lithium-ion batteries

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Experiments

Monodispersed CuO microspheres were synthesized by the same method reported.^{1, 2} Synthesis of single-layer Ti_3C_2 : The single-layer Ti_3C_2 was fabricated by solventassisted intercalation as stated in the literature.³⁻⁵

Synthesis of the single-layer Ti_3C_2 and CuO composite: the suspension of single-layer Ti_3C_2 was mixed with the CuO powder (the mass ratios are 3:1, 4:1, 6:1 and 8:1, respectively) in deionized water. The mixture was then ground thoroughly in a mortar by hand for 20 min, followed by freeze-drying to obtain the composite powder.

Electrode Preparation: The as-prepared CuO or CuO/Ti₃C₂ composite (70 wt%), super P (20 wt%), and carboxymethyl cellulose (10 wt%) were evenly mixed into a slurry and coated it onto a copper current collector. The coated electrodes were dried in a vacuum oven at 100 °C for 12h. The electrolyte was 1 M LiPF₆ in a mixture of ethylene carbonate (EC)/diethyl carbonate (DEC) at a ratio of 50:50 (v/v).

XRD: The material was analyzed by X-ray diffraction (XRD) on a Rigaku SmartLab

diffractometer by using Cu K α radiation at a scanning rate of 10° min⁻¹ from 5° to 90°. Ex-situ XRD sample preparation and measuring procedure: The CuO/Ti₃C₂ composite along with super P and carboxymethyl cellulose (7:2:1 in wt.%), was ground into a mixture and pressed directly into a sheet for battery assembly. After discharged or charged at the certain potential, the battery was disassembled, the electrodes were rinsed with DMC then dried under vacuum without exposure to air or water. The samples were placed in a Kapton-sealed container filled with Ar for XRD measurements.

SEM: The morphology of the materials was observed by scanning electron microscope (SEM, Hitachi S-4800).

EDX : The elemental distribution of the material was observed with Energy Dispersive X-Ray Spectroscopy. (EDX, Hitachi TM3000)

Figures



Fig. S1 XRD patterns of the Ti_3AlC_2 and the Ti_3C_2 .



Fig. S2 Ex-situ XRD patterns of the composite after charging and discharging.



Fig. S3 Electrochemical performance of MXene at 1C



Fig. S4 Rate performance of CuO and CuO/Ti $_3C_2$ composite.



Fig. S5 EDX mapping of (a) the pristine and (b) cycled electrodes.



Fig. S6 EIS results of CuO and CuO/Ti $_3C_2$ composite.

The CuO/Ti_3C_2 composite has a lower impedance than CuO, indicating that the conductivity of the composite is improved by MXene. Therefore, the composite exhibits far superior rate performance to CuO.



Fig. S7 CV curves for the CuO at various scan rates.



Fig. S8 CV curves for the CuO/ Ti₃C₂ composite at various scan rates.

Three sets of major reduction peaks were observed in CV curves for both the CuO and the CuO/Ti_3C_2 composite, which is consistent with three stages in the load curves of discharging.



Fig. S9 Cycling performance of composite electrodes with different ratio of CuO/Ti_3C_2 .

References

- 1. S. Q. Wang, J. Y. Zhang and C. H. Chen, Scr. Materi., 2007, 57, 337-340.
- 2. B. Liu and H. C. Zeng, J. Am. Chem. Soc., 2005, 127, 18262-18268.
- 3. X. Wang, T. S. Mathis, K. Li, Z. Lin, L. Vlcek, T. Torita, N. C. Osti, C. Hatter, P. Urbankowski, A. Sarycheva, M. Tyagi, E. Mamontov, P. Simon and Y. Gogotsi, *Nat. Energy*, 2019, **4**, 241-248.
- 4. L. Verger, C. Xu, V. Natu, H.-M. Cheng, W. Ren and M. W. Barsoum, *Curr. Opin. Solid St. M.*, 2019, **23**, 149-163.
- 5. H. Li and Z. Du, ACS Appl. Mater. Inter., 2019, 11, 45930-45938.