

## *Supplementary Information*

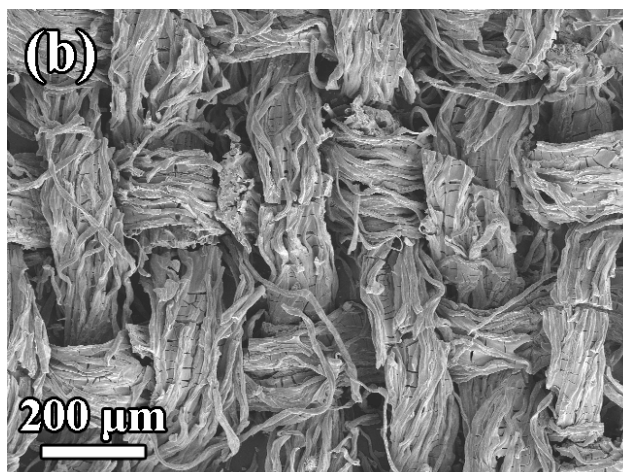
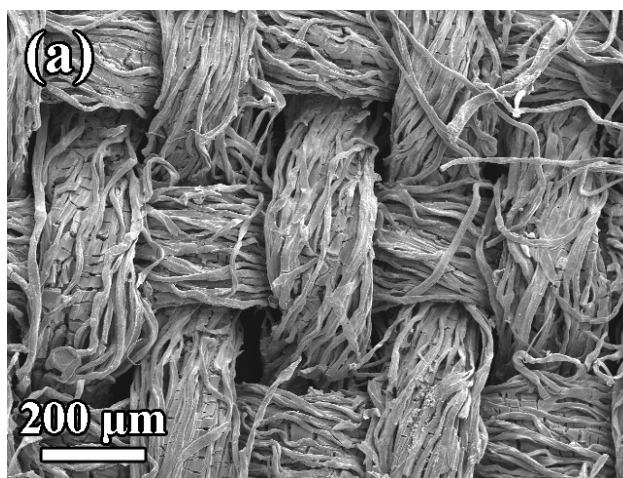
### **Ultrafine MoO<sub>2</sub> nanoparticles embedded in a carbon matrix as a high-capacity and long-life anode for lithium-ion batteries**

Yongming Sun, Xianluo Hu,\* Wei Luo and Yunhui Huang\*

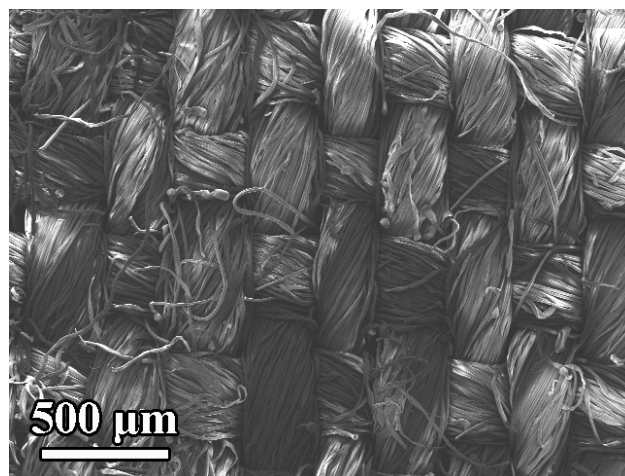
E-mail: huxl@mail.hust.edu.cn (or xlhu07@gmail.com); huangyh@mail.hust.edu.cn

*State Key Laboratory of Material Processing and Die & Mould Technology, School of  
Materials Science and Engineering, Huazhong University of Science and Technology,  
Wuhan 430074, P. R. China*

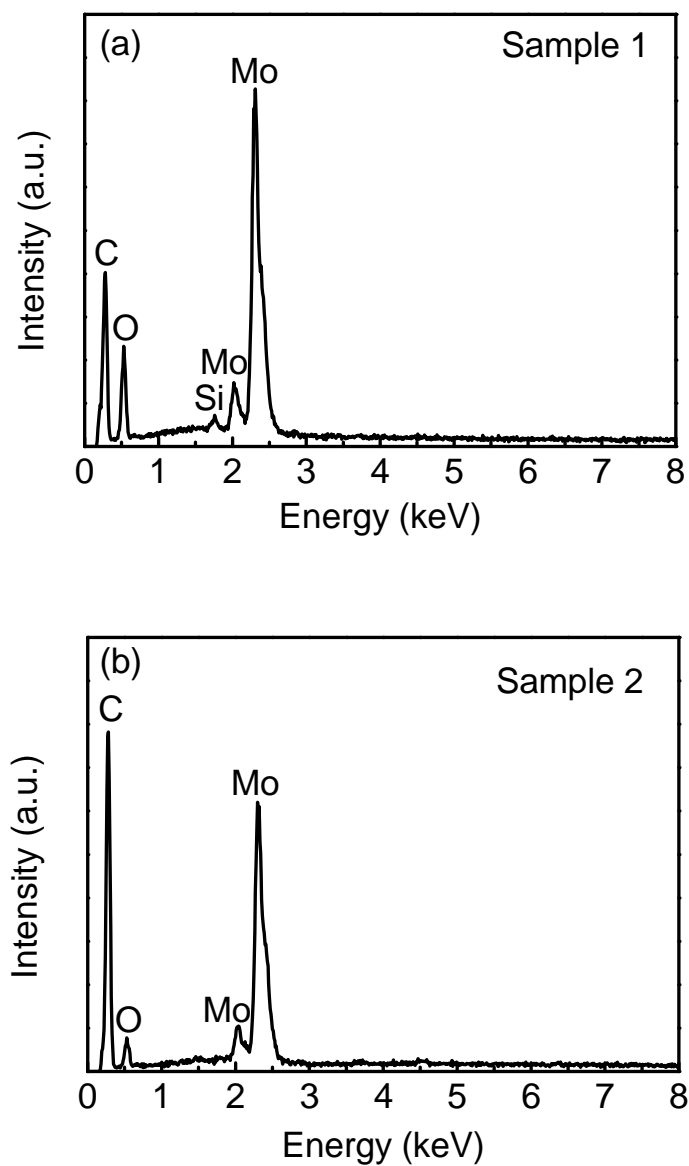
**Fig. S1** SEM images of the MoO<sub>2</sub>/C products prepared at (a) 500 °C and (b) 600 °C for 5 h.



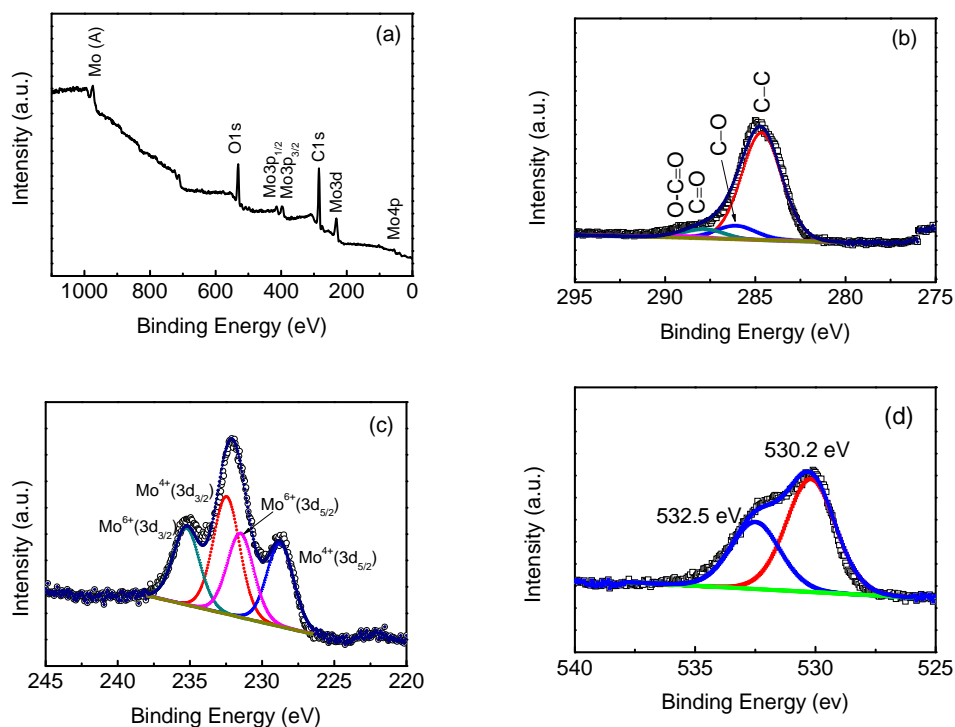
**Fig. S2** SEM image of the cotton cloth showing the fibrous structure.



**Fig. S3** EDX spectra: (a) Sample 1; (b) Sample 2. The signal of Si is generated from the sample holder.

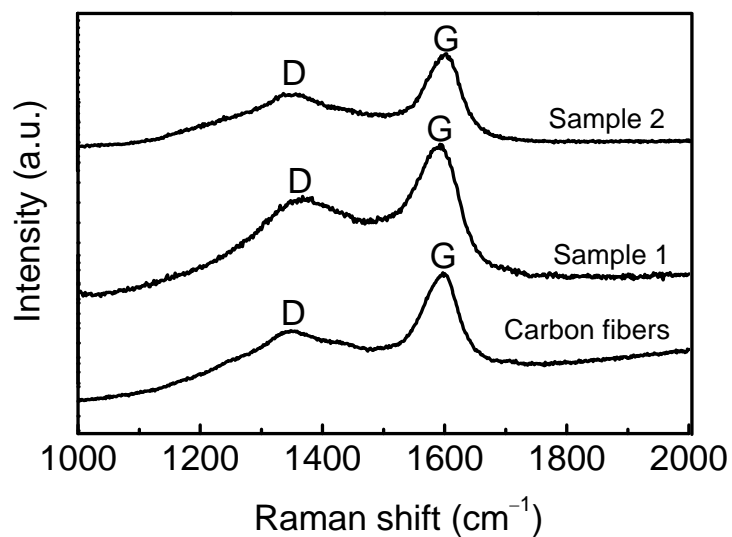


**Fig. S4** XPS spectra of the MoO<sub>2</sub>/C product (Sample 2) prepared at 600 °C for 5 h in 5% H<sub>2</sub>/Ar: (a) Survey XPS spectrum of Sample 2; high-resolution XPS spectra of (b) C 1s, (c) Mo 3d and O 1s. Four distinct peaks at 233.9 (Mo 3d), 398.0 (Mo 3p<sub>3/2</sub>), 415.6 (Mo 3p<sub>1/2</sub>), and 531.9 (O 1s) eV are involved, characteristic of molybdenum oxides. The doublet of core-level Mo 3d<sub>5/2,3/2</sub> indicates the Mo(IV) oxidation state of MoO<sub>2</sub> and Mo(VI) 3d<sub>3/2</sub> of MoO<sub>3</sub>, arising from the surface oxidation of the metastable MoO<sub>2</sub> in air. The degree of oxidation of Sample 2 is much slighter than that of Sample 1 obtained at 500 °C. The small O 1s peak at 532.5 eV was observed, indicating the existence of residual O<sup>2-</sup> species bonded with C atoms in the porous carbon fiber.<sup>1</sup>

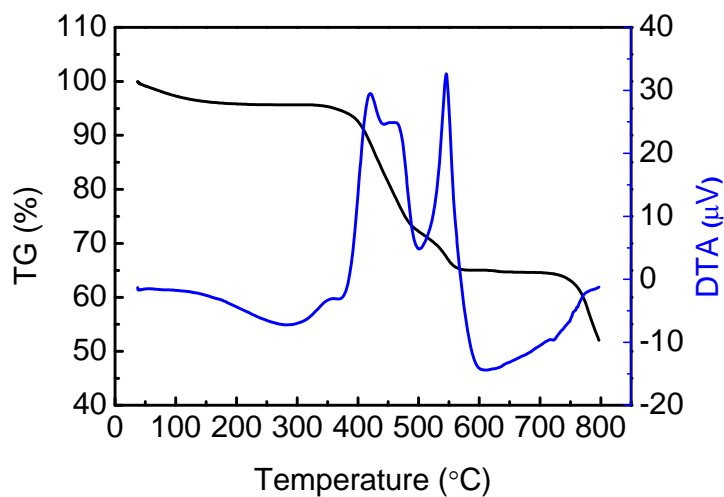


- 1 H. C. Schniepp, J. L. Li, M. J. McAllister, H. Sai, M. HerreraA-lonso, D. H. Adamson, R. K. Prud'homme, R. Car, D. A. Saville and I. A. Aksay, *J. Phys. Chem. B*, 2006, **110**, 8535.

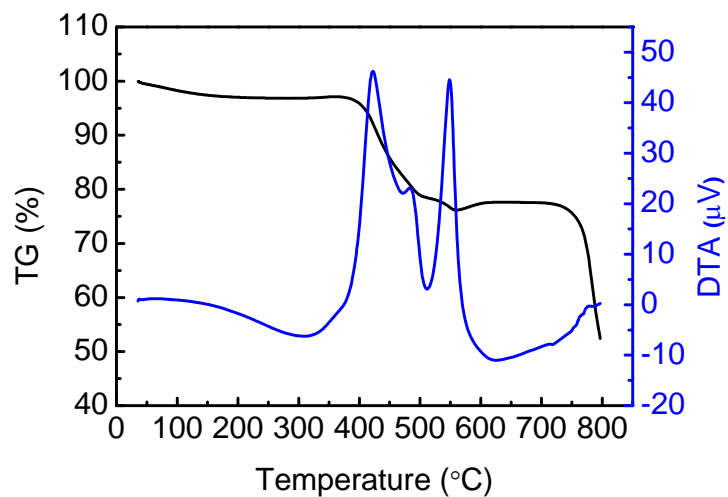
**Fig. S5** Raman spectra of the MoO<sub>2</sub>/C hybrids prepared at 500 °C (Sample 1) and 600 °C (Sample 2) and carbon fibers prepared at 500 °C. The peaks at 1345 and 1600 cm<sup>-1</sup> are attributed to the characteristic D- and G-bands of carbon, respectively.



**Fig. S6** TG/DTA analysis of the MoO<sub>2</sub>/C product (Sample 1) measured at a heating rate of 10 °C min<sup>-1</sup> in a flowing air. The first large weight change from about 200 to 650 °C is attributed to the oxidation of MoO<sub>2</sub> to MoO<sub>3</sub> and the combustion of carbon. The second large weight decrease above 700 °C can be ascribed to the sublimation of MoO<sub>3</sub>. The total weight increase recorded between 200 and 650 °C is 31.1 wt %. According to the theoretical value (12.5 wt %) of the weight increase from MoO<sub>2</sub> to MoO<sub>3</sub>, the residual carbon from the cotton can be calculated to be about 38.3 wt %. The exothermic peak displayed at curve 358 °C in DTA can be associated with the decrystallization of MoO<sub>2</sub> and the oxidation of MoO<sub>2</sub> to MoO<sub>3</sub>. The weight decreases from 300 °C to 575 °C mainly owing to the complete combustion of carbon. In addition, the exothermic peak at 575 °C should be ascribed to the crystallization of MoO<sub>3</sub>.



**Fig. S7** TG/DTA analysis of the MoO<sub>2</sub>/C product (Sample 2) obtained at 600 °C. The amount of carbon in this sample is calculated to be about 28.0 wt %, which is less than that of Sample 1 obtained at 500 °C.





**Fig. S8** Detailed electrochemical data of the MoO<sub>2</sub>/C product (Sample 2) prepared at 600 °C for 5 h in 5% H<sub>2</sub>/Ar: cyclic voltammograms at a scan rate of 0.1 mV s<sup>-1</sup> in the voltage range of 0.01–3.0 V, galvanostatic discharge-charge curves, and cycling performance at a current density of 100 mA g<sup>-1</sup>.

