

Supplementary Information

Experimental and First-principle Study of Metal-Organic Framework with Sulfur Embedding Cathode for Enhanced Performance Lithium- Sulfur Battery

Yan Feng,^{*,1} *Yuliang Zhang*,¹ *Guixiang Du*,¹ *Jingbo Zhang*,¹ and *Xiaohui Qu*,^{*,2,3}

¹ College of Chemistry, Tianjin Normal University, Tianjin 300387, P. R. China

² Energy Storage and Distributed Resources Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, United States

³ College of Engineering Research, University of California, Berkeley, California 94720, United States

* Corresponding authors: hxyfy@mail.tjnu.edu.cn (Y. F.); xqu1981@gmail.com (X. Q.)

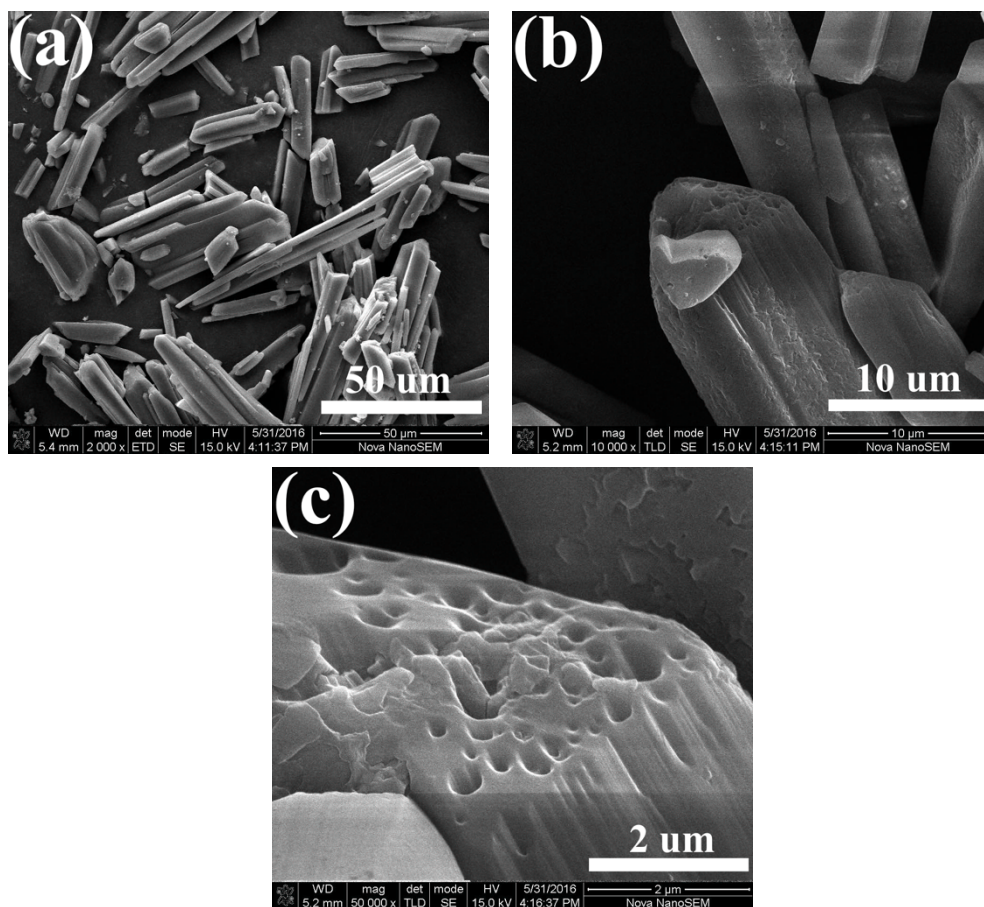


Figure S1. SEM images of pristine CoMOF after 155 °C heating.

Compared the SEM images of the pristine CoMOF before (Figure 1a-c) and after 155 °C heating (Figure S1a-c), the crystal structure has no change after heating, with porous and defective structure still remain on the surface of CoMOF crystal. The result consists with the XRD pattern in Figure S2, which shows the MOF structure is as excellent as before without any damage during the 155 °C heating process.

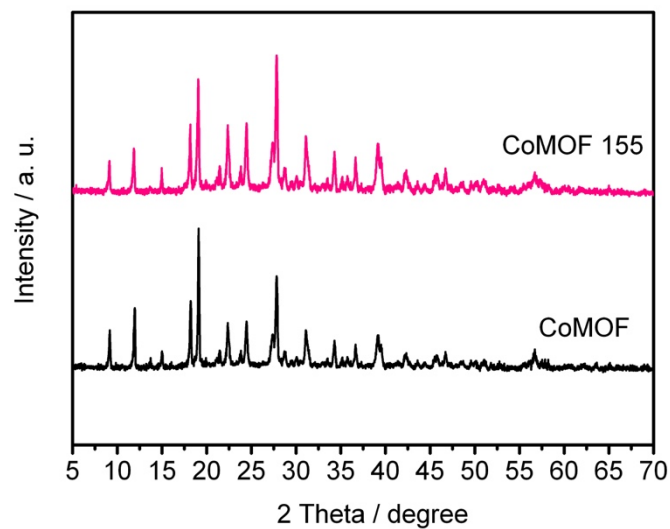


Figure S2. XRD patterns of pristine CoMOF before (CoMOF) and after 155 °C heating (CoMOF 155).

Compared the XRD patterns of pristine CoMOF before and after heating at 155 °C shown in Figure S2, the CoMOF structure is intact and remain robustly, which indicates the MOF structure was not destroyed in the heating process.

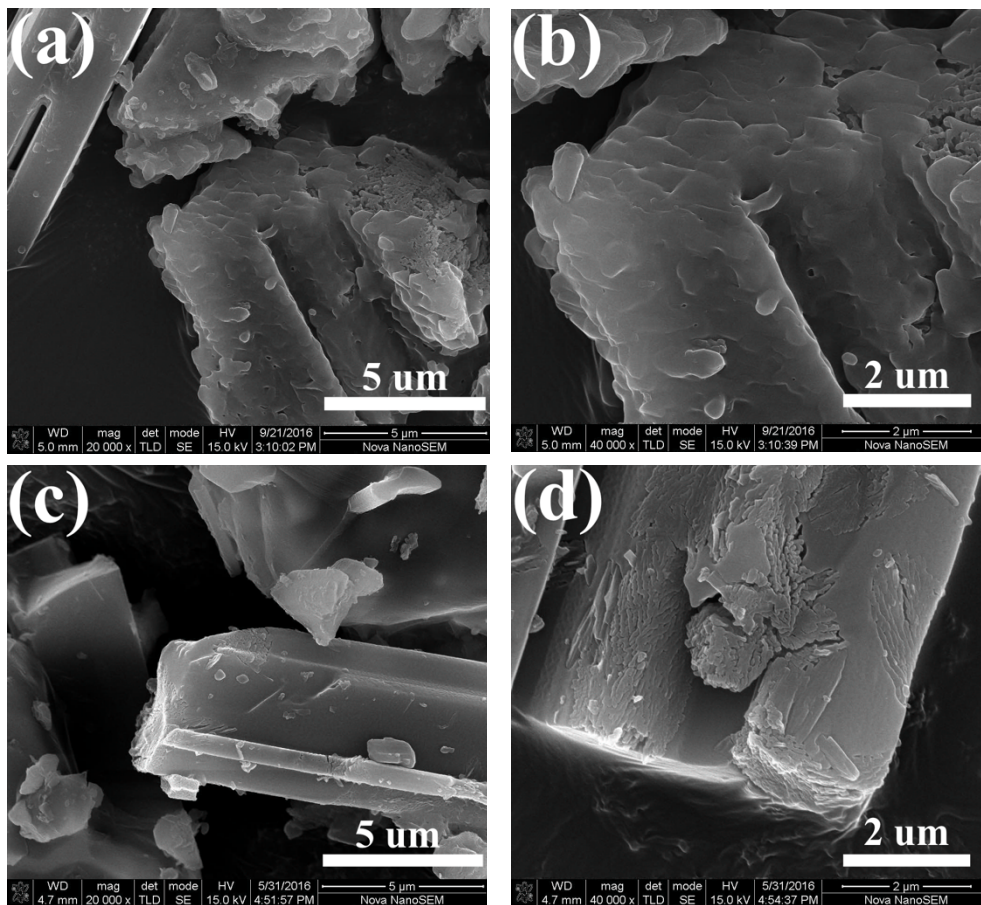


Figure S3. SEM images of the CoMOFS1 (a, b) and CoMOFS3 (c, d) materials.

From Figure S3, we can see the CoMOFS1 and CoMOFS3 composites have the same structures as CoMOFS2.

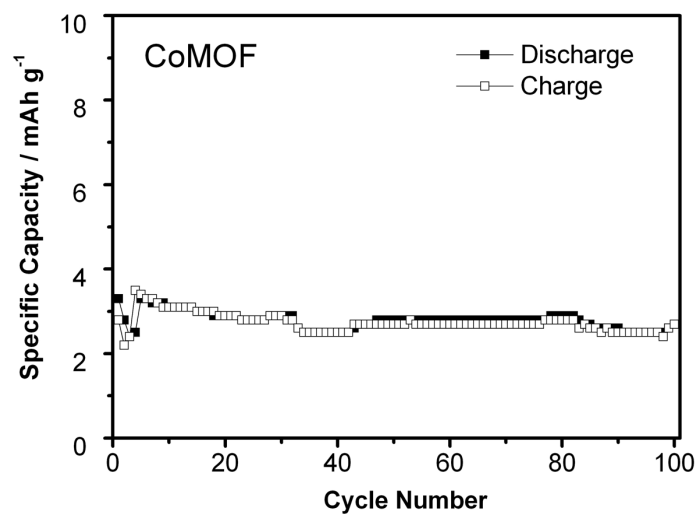


Figure S4. Cycle performance of pristine CoMOF (without S) cathode at a charge/discharge current density of 167.5 mAh g^{-1} .

The role of the CoMOF structure only is the sulfur host, it provide almost no capacity in the CoMOFS cathode, which can be proven by the cycle performance of pristine CoMOF in Figure S4 of the Supplementary Information.