Electronic Supplementary Information

From Synthetic Montroseite VOOH to Topochemical Paramontroseite VO₂ and Their Applications in Aqueous Lithium Ion Batteries

Yang Xu, Lei Zheng and Yi Xie*

*Division of Nano-materials and Nano-chemistry, Hefei National Laboratory for Physical Sciences at Microscale, University of Science & Technology of China, Hefei, Anhui 230026, P. R. China. Fax: 86-551-3606266, E-mail: yxie@ustc.edu.cn

S1. EDX spectrum of the as-obtained montroseite VOOH hollow nanourchins.



Figure S1. EDX spectrum of the as-obtained montroseite VOOH hollow nanourchins, showing that only vanadium and oxygen signals were observed (copper and carbon signals arise from the TEM grid).

S2. XRD analysis of the intermediate precursor V₁₀O₁₄(OH)₂.

In this approach, the intermediate precursor $V_{10}O_{14}(OH)_2$ is self-produced and then acts as the self-sacrificed template. The close resemblance of XRD pattern of the intermediate precursor, as shown in **Figure 7B** in the manuscript, to that of hexagonal ferrihydrite Fe₁₀O₁₄(OH)₂ indicates that these two materials possess the similar crystal structure. First, on the basis of the crystallographic lattice constants a=4.9370 Å and c=9.2549 Å which are obtained according to the *d*-values of the obtained XRD pattern and the borrowed corresponding indices of (300) and (112) from hexagonal ferrihydrite Fe₁₀O₁₄(OH)₂, respectively, we used the following equation to confirm that the other four peaks in the obtained XRD pattern can be all indexed to the hexagonal system with the crystallographic lattice constants given above:

$$d = \frac{1}{\left(\frac{3}{4} * \frac{h^2 + hk + k^2}{a^2} + \frac{l^2}{c^2}\right)^{1/2}}$$

The results are summarized in Table S1, from which one can see that the experimental *d*-values agree with the theoretical *d*-values, confirming that the XRD pattern of the intermediate precursor here can be indexed to the hexagonal system with the crystallographic lattice constants a=4.9370 Å and c=9.2549 Å. On the basis of the close resemblance, the formula for the intermediate precursor is $V_{10}O_{14}(OH)_2$ from the crystallographic point of view.

Table S1. Summary of the experimental and theoretical *d*-values calculated according to the indices of the crystallographic planes of hexagonal $Fe_{10}O_{14}(OH)_2$ for the intermediate precursor.

(hkl)	Theoretical <i>d</i> -value [Å]	Experimental <i>d</i> -value [Å]
(110)	2.4647	2.4685
(113)	1.9307	1.9274
(114)	1.6865	1.6881
(115)	1.4866	1.4809