Supplementary Information (SI)

Phase evolution in calcium molybdate nanoparticles as a function of synthesis temperature and its electrochemical effect on energy storage

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The supplementary information (SI) contains four figures (Figs. S1 – S4).

Experimental (in-situ powder XRD)

In-situ PXRD experiments were conducted by using a STOE STADI-p diffractometer in transmission geometry with Mo Kα1 radiation (0.70932 Å), equipped with a DECTRIS MYTHEN 1K strip detector and a STOE capillary furnace. The samples were introduced in quartz capillaries and heated at a rate of 10° C min^{-1} from room temperature (RT) to 600 °C and subsequently naturally cooled down to RT. PXRD patterns were recorded every 50 °C with 30 min exposure time after a 10 min rest to ensure that the samples were at the required temperature.

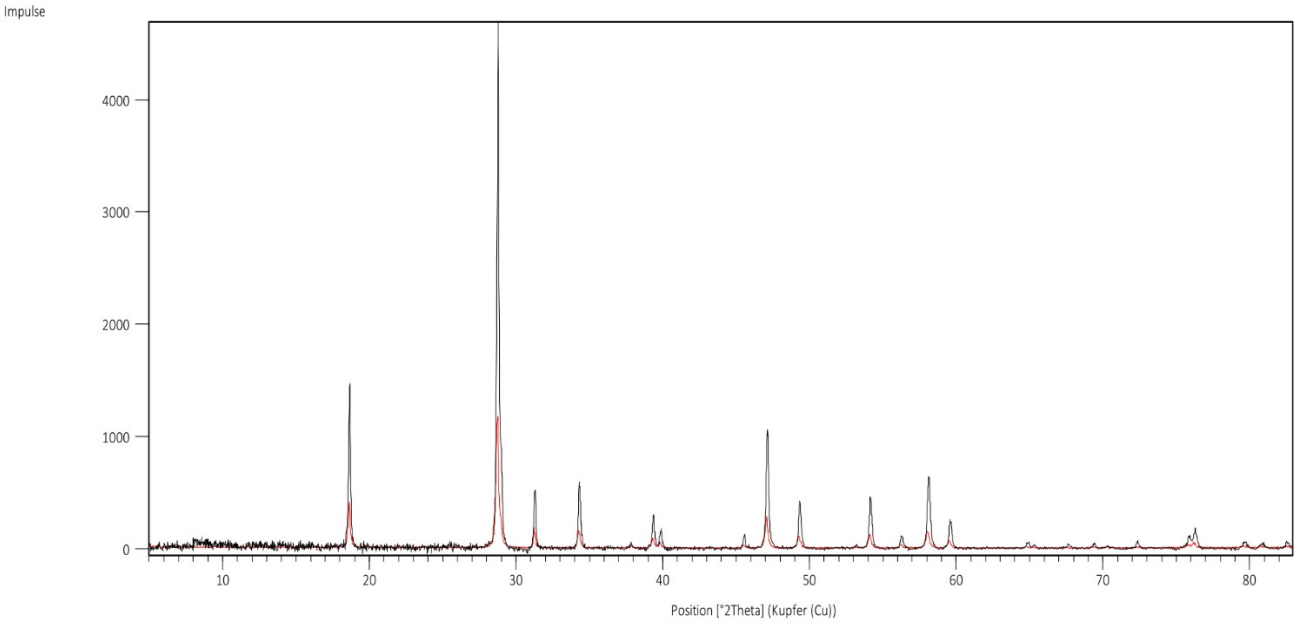


Figure S1 Baseline corrected X-ray diffraction (XRD) patterns of $CaMoO_4$ synthesized at 300 (red) and 500 °C (black), shown in the main article, Fig. 1. After subtracting the pattern from the 500 °C sample, an automatic background is calculated using the X'Pert Highscore software with the following parameters: subdivision = 18, curvature factor = 3.

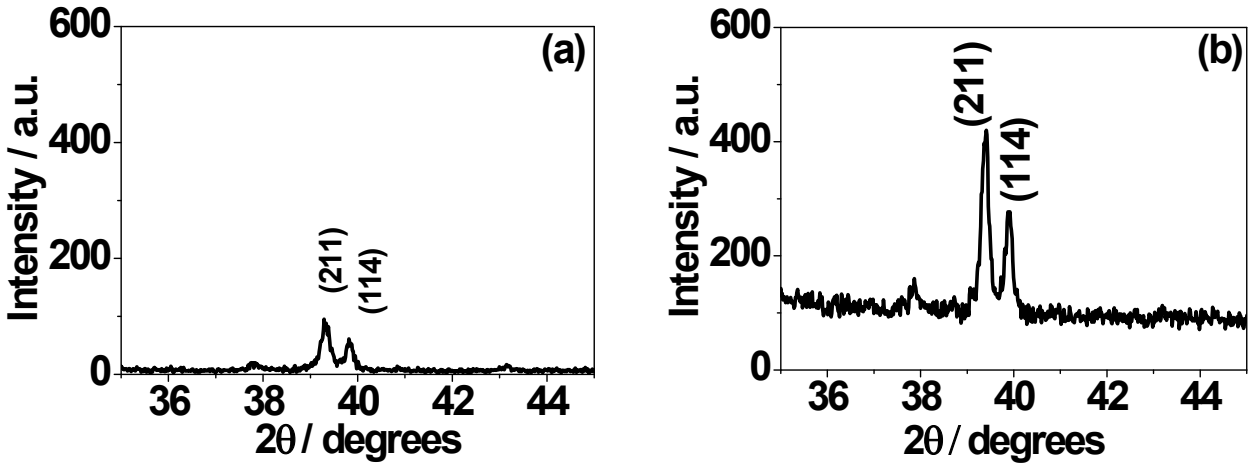
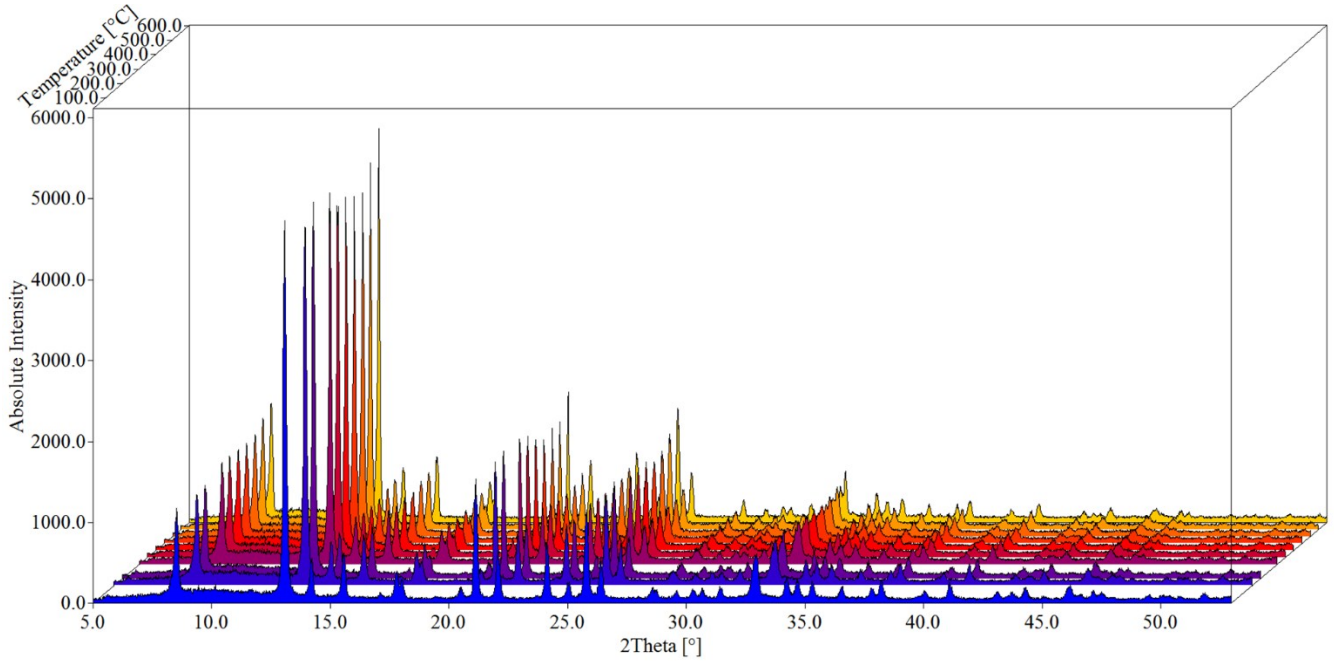
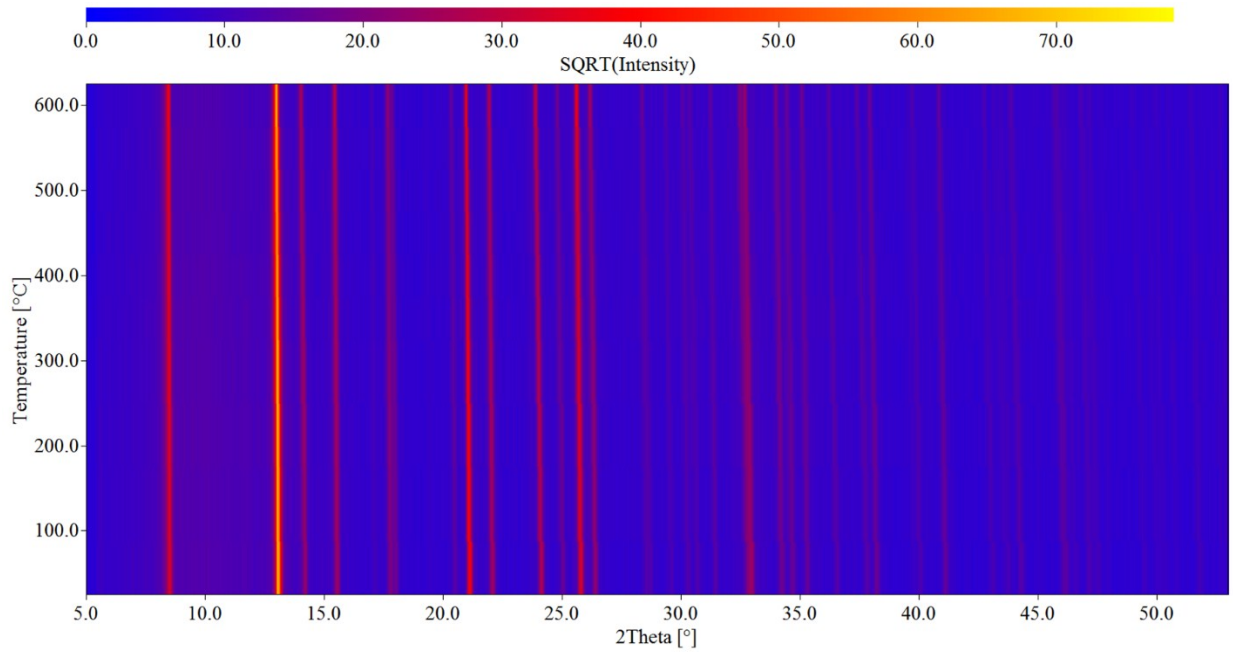


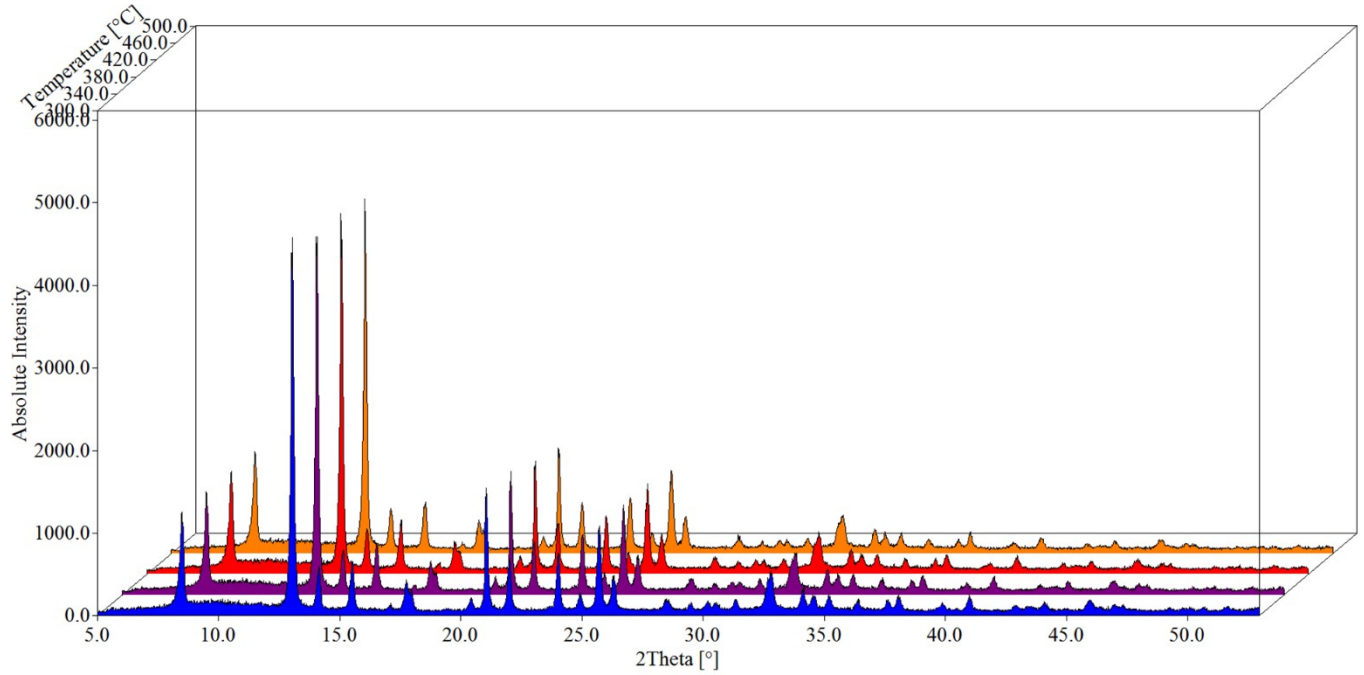
Figure S2 Details of the X-ray diffraction patterns shown in the main article, Fig. 1a and Fig. 1b respectively. The pattern illustrates the (211) and (114) reflections of $CaMoO_4$ in the narrow 2θ region. Minor differences in peak separation and relative intensities were observed.


Temperature [°C]
600.0
500.0
400.0
300.0
200.0
100.0
Absolute Intensity
6000.0
5000.0
4000.0
3000.0
2000.0
1000.0
0.0
5.0
10.0
15.0
20.0
25.0
30.0
35.0
40.0
45.0
50.0
2Theta [°]

(a)


0.0
10.0
20.0
30.0
40.0
50.0
60.0
70.0
SQRT(Intensity)
600.0
500.0
400.0
300.0
200.0
100.0
Temperature [°C]
5.0
10.0
15.0
20.0
25.0
30.0
35.0
40.0
45.0
50.0
2Theta [°]

(b)



(c)

Figure S3 (a) X-ray diffraction (XRD), and (b) corresponding thermal patterns of $CaMoO_4$ synthesized from room temperature to 600 °C, various profiles are stacked in the image. Figure S2 (c) shows a higher resolution patterns for the synthesis temperature of interest, from 300 °C to 500 °C.

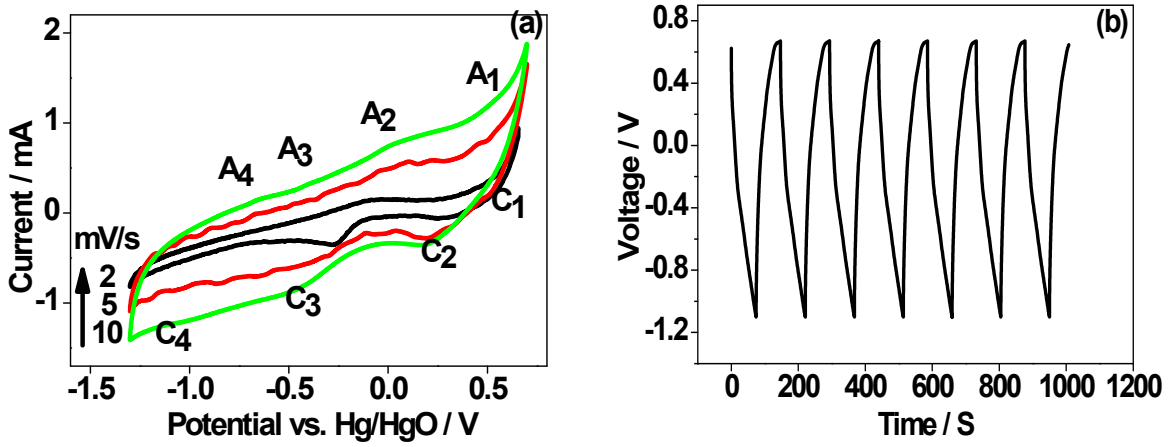


Figure S4 (a) Cyclic voltammetry (CV), and (b) charge-discharge profiles (single electrode study / three-electrode configuration) of $CaMoO_4$ (500 °C) at different potential regions. The electrode is cycled in the whole region 1.6 V window vs. Hg/HgO, respectively. Scan rates are indicated in the figure. Consecutive charge-discharge cycles at 1 A/g are shown for 1000 seconds shows a shorter time to charge and discharge.