

Morphology-controlled synthesis of novel nanostructured Li₄P₂O₇ with enhanced Li-ion conductivity for all-solid-state battery applications

Hany El-Shinawi,^{a,b*} Edmund J. Cussen^a and Serena A. Cussen^a

^a Department of Materials Science and Engineering, University of Sheffield, Sir Robert Hadfield Building, Sheffield, S1 3JD, UK.

^b Department of Chemistry, Mansoura University, Mansoura, 35516, Egypt.

Supporting Information:

Table S1. Refined structural parameters from Rietveld fit against XRD data for Li₄P₂O₇-400 at room temperature.

atom	site	occupation	x	y	z	U _{iso} (Å ²)
P1	4e	1	0.133(2)	0.714(2)	0.377(1)	0.127(4)
P2	4e	1	0.894(2)	0.758(2)	0.133(1)	0.127(4)
O1	4e	1	0.017(3)	0.784(4)	0.101(3)	0.166(5)
O2	4e	1	0.876(3)	0.136(4)	0.124(2)	0.166(5)
O3	4e	1	0.695(3)	0.792(5)	0.160(3)	0.166(5)
O4	4e	1	0.770(3)	0.734(4)	0.039(2)	0.166(5)
O5	4e	1	0.511(4)	0.196(4)	0.099(3)	0.166(5)
O6	4e	1	0.411(3)	0.617(4)	0.114(2)	0.166(5)
O7	4e	1	0.262(3)	0.227(5)	0.163(3)	0.166(5)
Li1	4e	1	0.729(3)	0.220(4)	0.185(2)	0.088(2)
Li2	4e	1	-0.020(3)	0.380(4)	0.081(2)	0.088(2)
Li3	4e	1	0.256(3)	0.313(4)	0.329(2)	0.088(2)
Li4	4e	1	0.374(3)	0.906(4)	0.122(2)	0.088(2)

^aSpace group $P2_1/n$, $a=8.6181(6)$ Å, $b=5.1863(2)$ Å, $c=13.1373(1)$ Å, and $\beta=103.624(5)$; fit statistics: $\chi^2=2.243$; $wRp=0.0837$, $Rp=0.0612$.

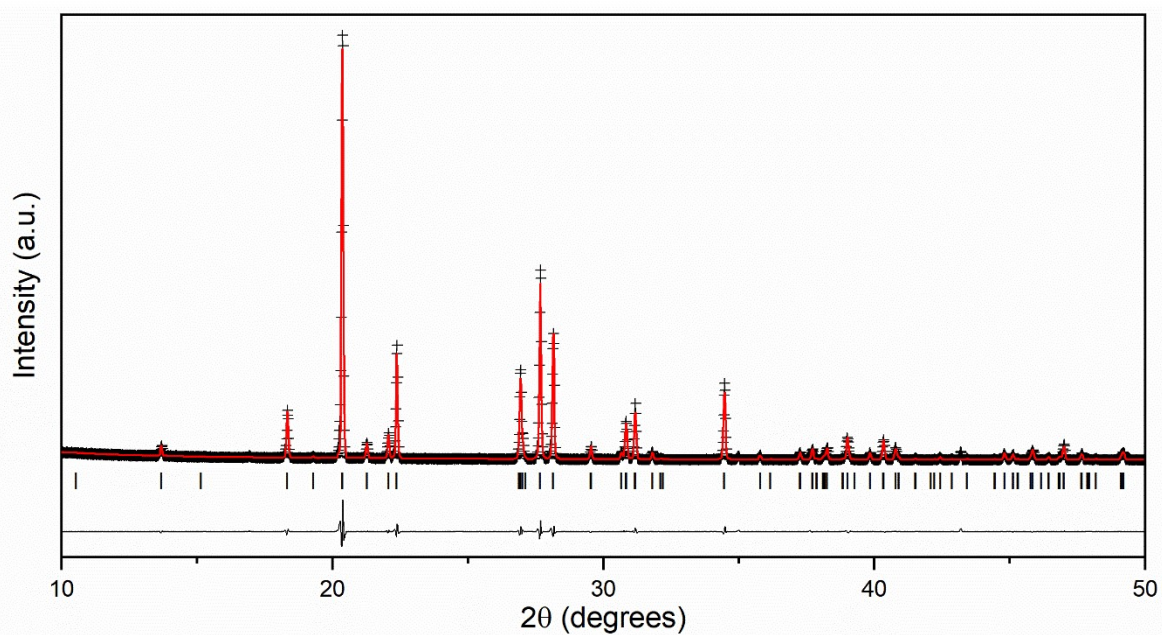


Figure S1. Observed (+), calculated (red) and difference (black) patterns of the Rietveld analysis of the XRD data collected from $\text{Li}_4\text{P}_2\text{O}_7$ -800. The structural model in reference 9 was adopted. Space group $P\bar{1}$; $a=8.5642(3)$, $b=7.1061(3)$, $c=5.1847(2)$, $\alpha=111.400(3)^\circ$, $\beta=89.987(3)^\circ$, and $\gamma=103.050(2)^\circ$.

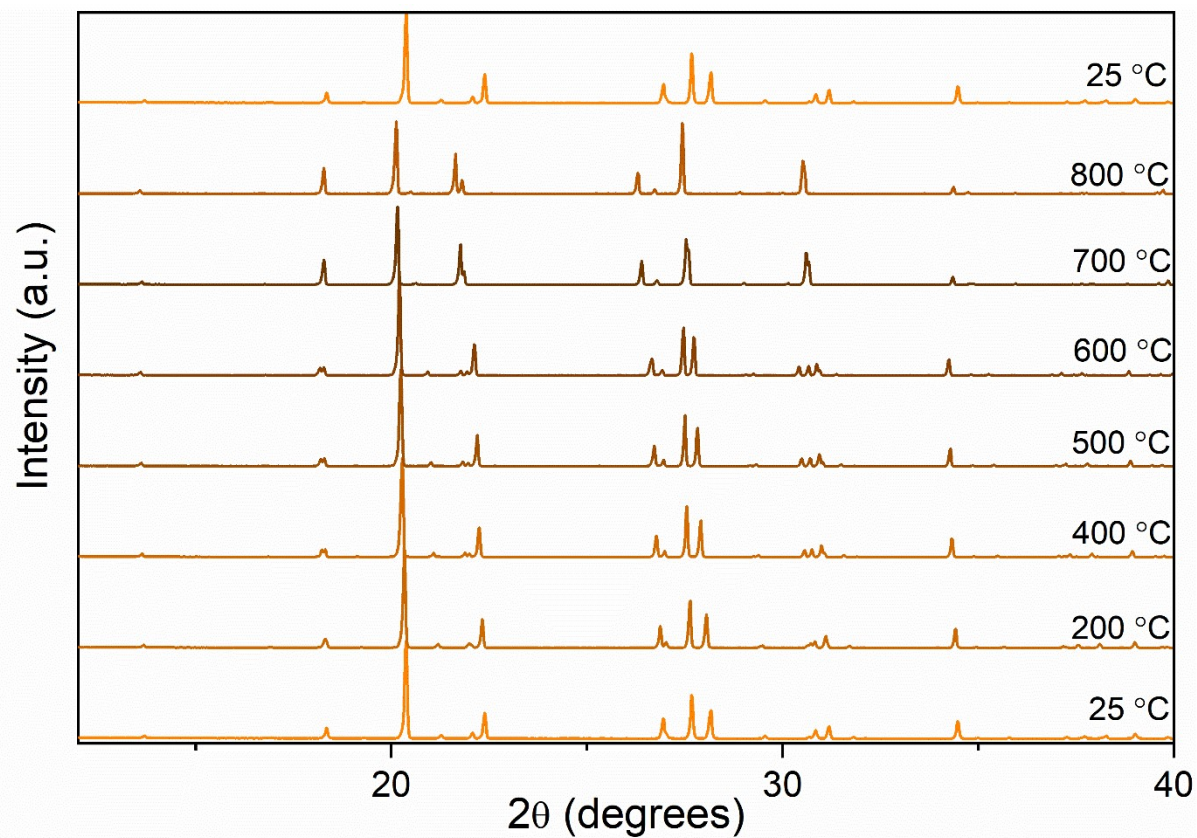


Figure S2. In situ XRD patterns of $\text{Li}_4\text{P}_2\text{O}_7$ -800 (previously heated to 800°C) through heating from room temperature to 800°C, then cooling back to room temperature. This is the second heating/cooling cycle of $\text{Li}_4\text{P}_2\text{O}_7$ -400; the first heating/cooling cycle is shown in Figure 2.

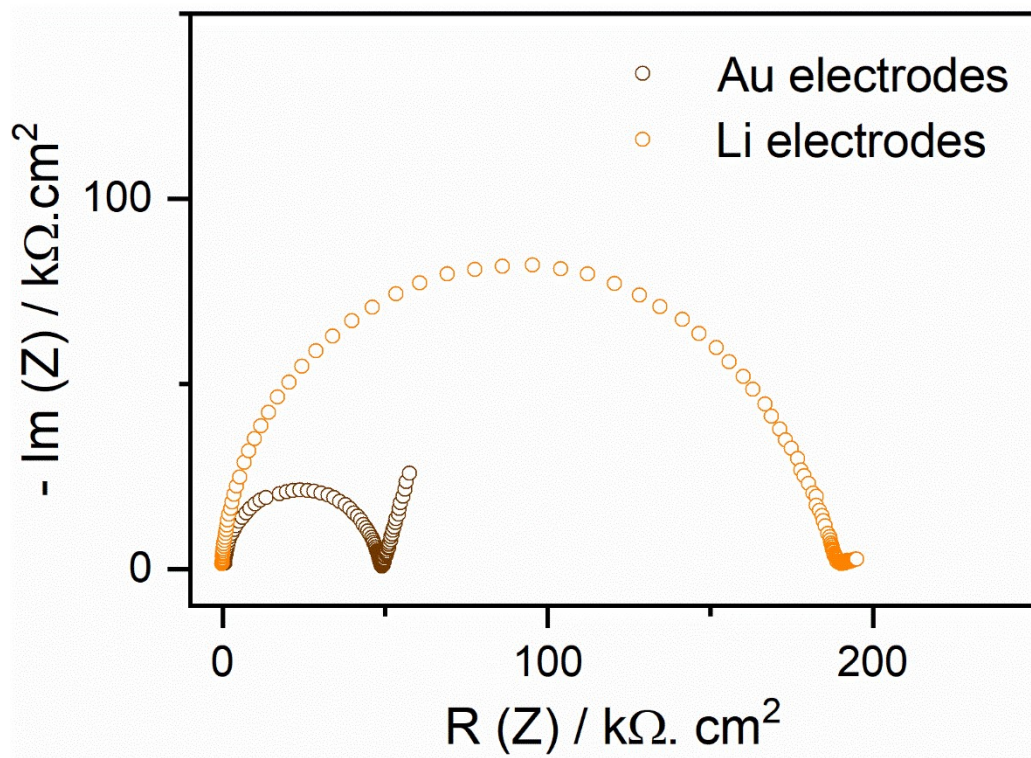


Figure S3. Impedance collected from $\text{Li}_4\text{P}_2\text{O}_7$ -400 using Au and Li electrodes (at 80°C).