

# Solvothermal Synthesis of a Novel Calcium Metal-Organic Framework: High Temperature and Electrochemical Behaviour

## Supplementary Material

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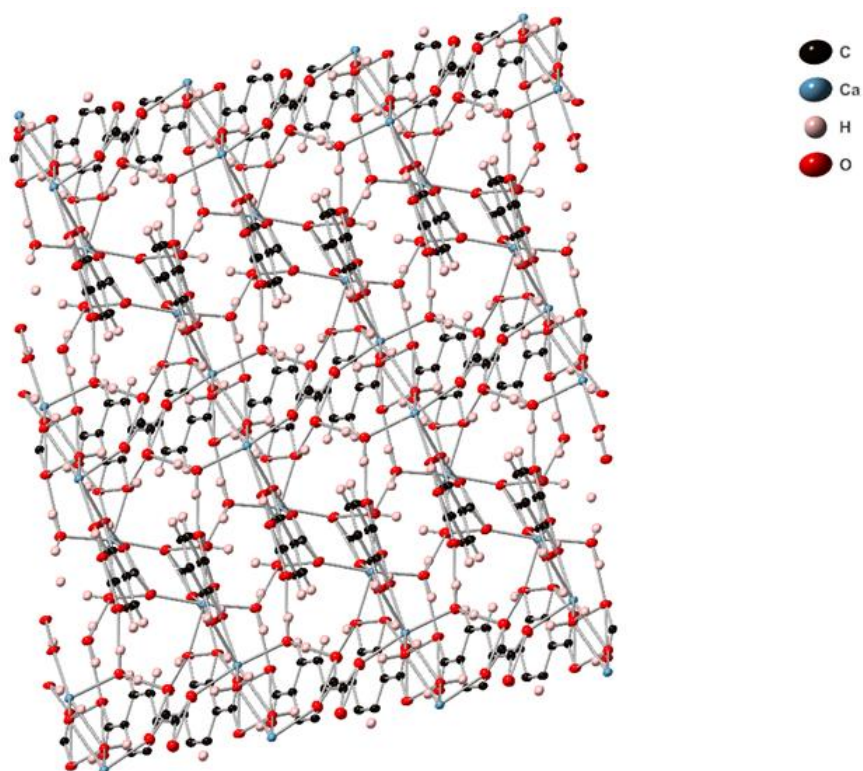


Figure S1: View of the 3D structure of SIMOF-4 (50 % probability ellipsoids) as seen down the crystallographic b-axis, and showing hydrogen bonds.

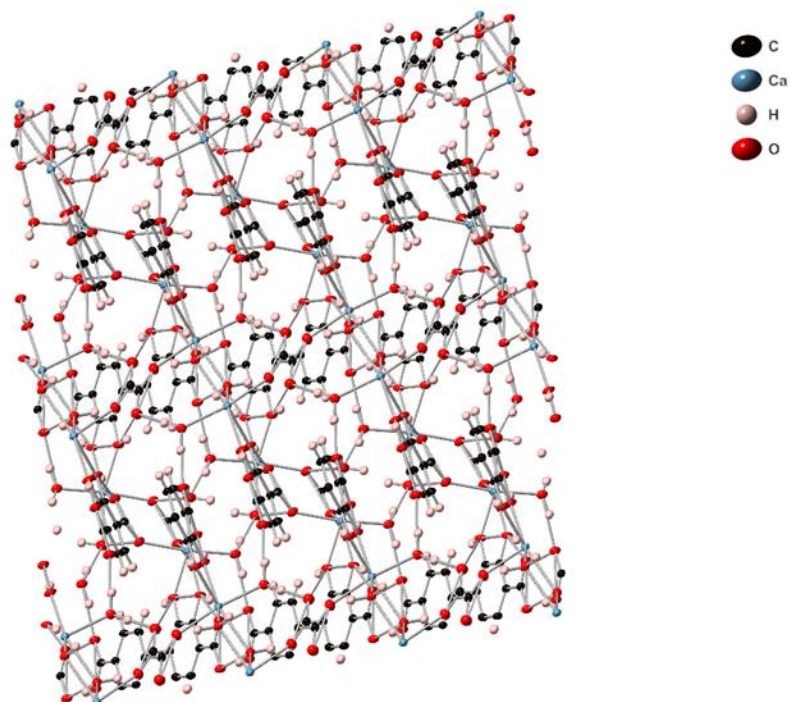


Figure S2: View of the 3D structure of SIMOF-4 (50 % probability ellipsoids) as seen down the crystallographic b-axis, and showing hydrogen bonds.

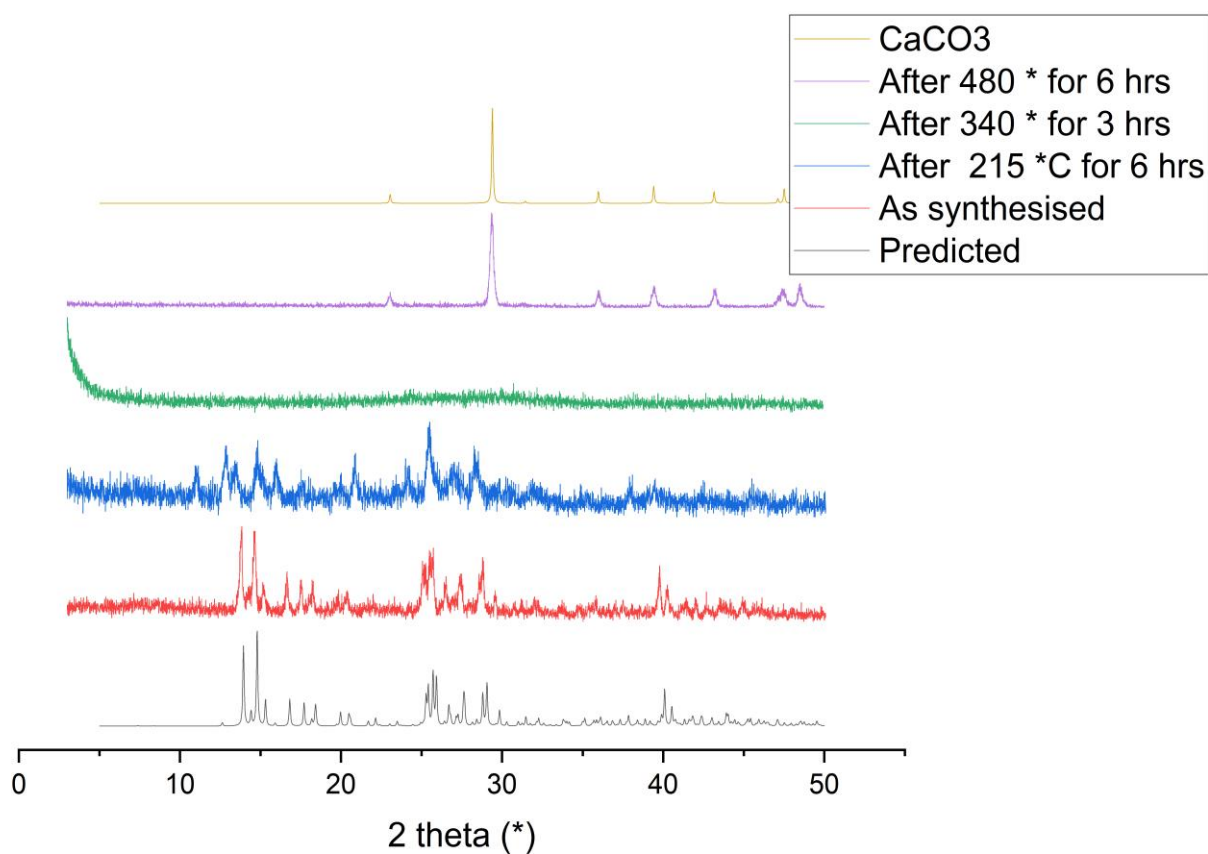


Figure S3: PXRD patterns of SIMOF-4 after different heat treatments, with simulated patterns of CaCO<sub>3</sub> and SIMOF-4 for comparison. All obtained using Cu(K $\alpha$ 1) radiation.

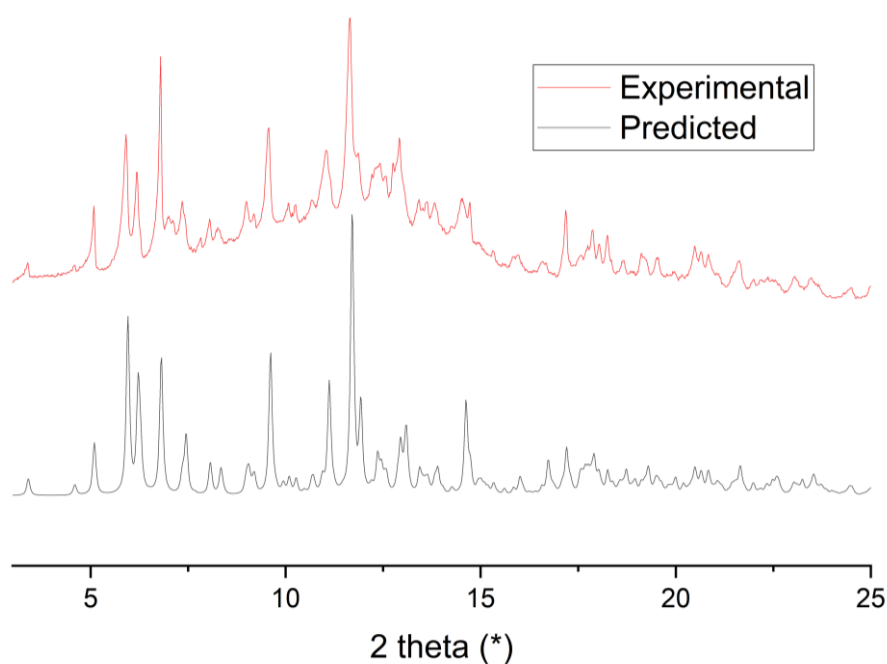


Figure S4: PXRD pattern of SIMOF-4-h simulated from scXRD structure compared with the experimental pattern. Obtained using Mo (K $\alpha$ 1) radiation.

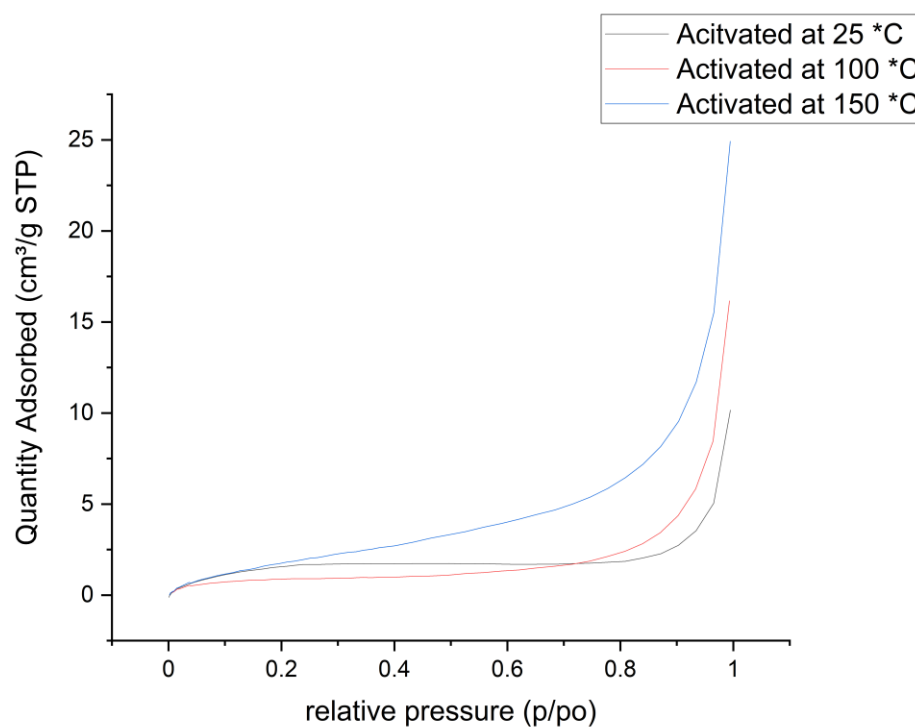


Figure S5:  $N_2$  Adsorption isotherms of SIMOF-4 after 3 different activation protocols of 25 °C, 100 °C and 150 °C all under vacuum.

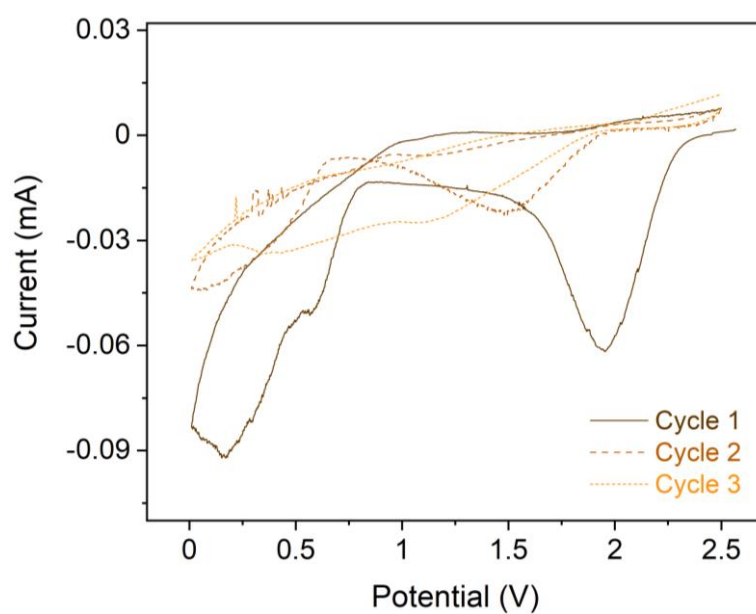


Figure S6: Cyclic voltammogram for SIMOF-4 recorded at a scan rate of  $0.05 \text{ mV s}^{-1}$  between 0.01-2.5 V.

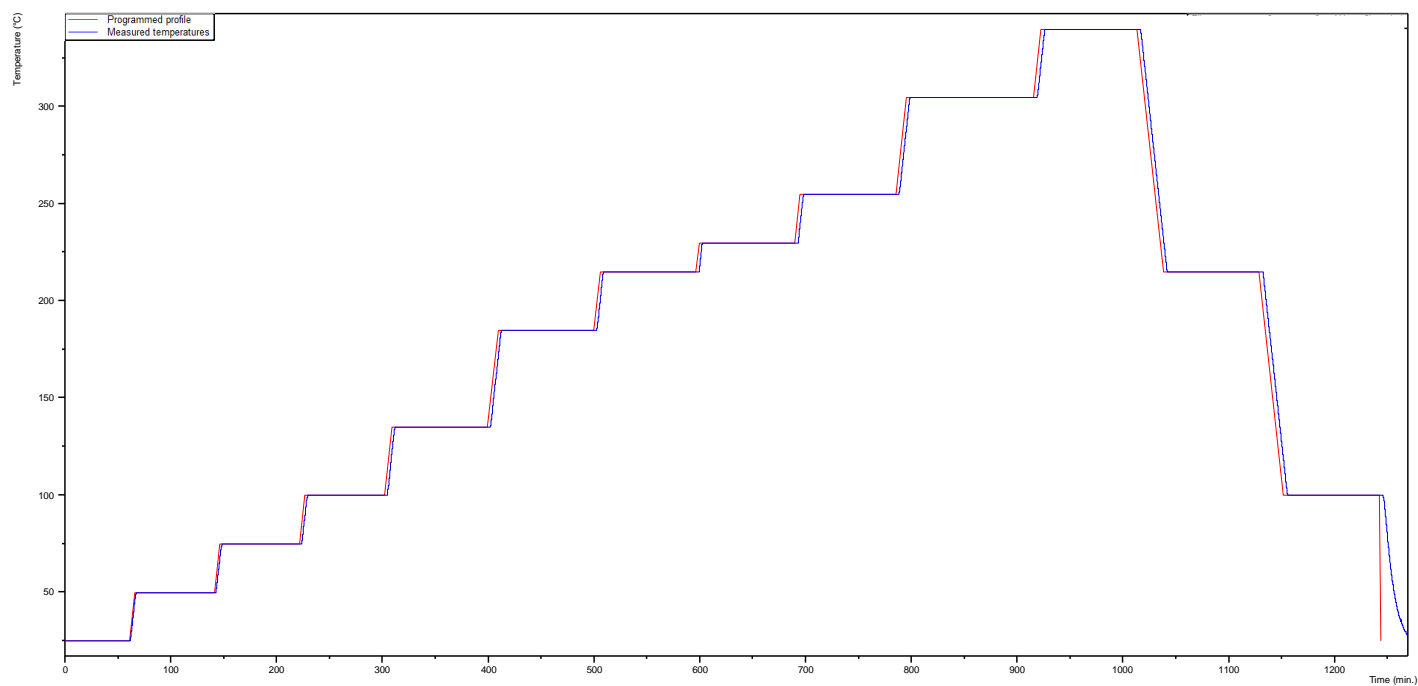


Figure S7: Temperature time profile for the VT-XRD experiment performed on SIMOF-4, showing programmed and measured temperature profiles.