

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

Supplementary Material

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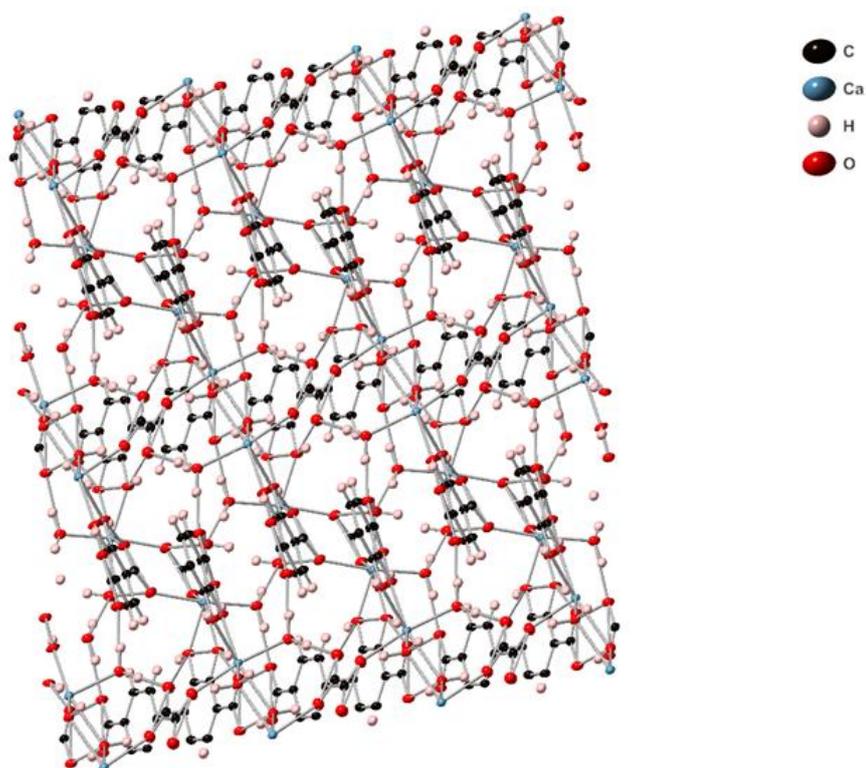


Figure S1: View of the 3D structure of SIMOF-4 (50 % probability ellipsoids) as seen down the crystallographic b-axis, and showing hydrogen bonds.

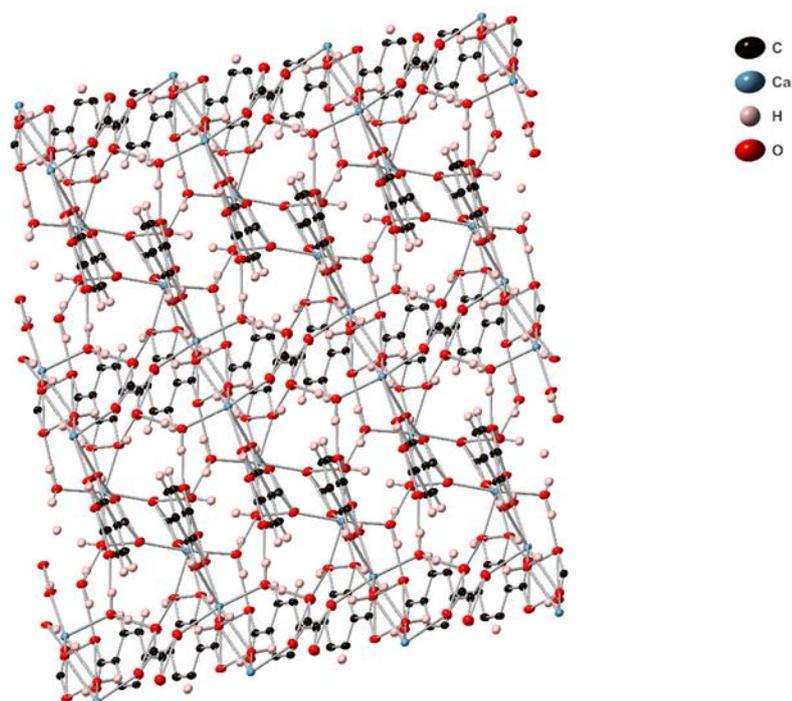


Figure S2: View of the 3D structure of SIMOF-4 (50 % probability ellipsoids) as seen down the crystallographic b-axis, and showing hydrogen bonds.

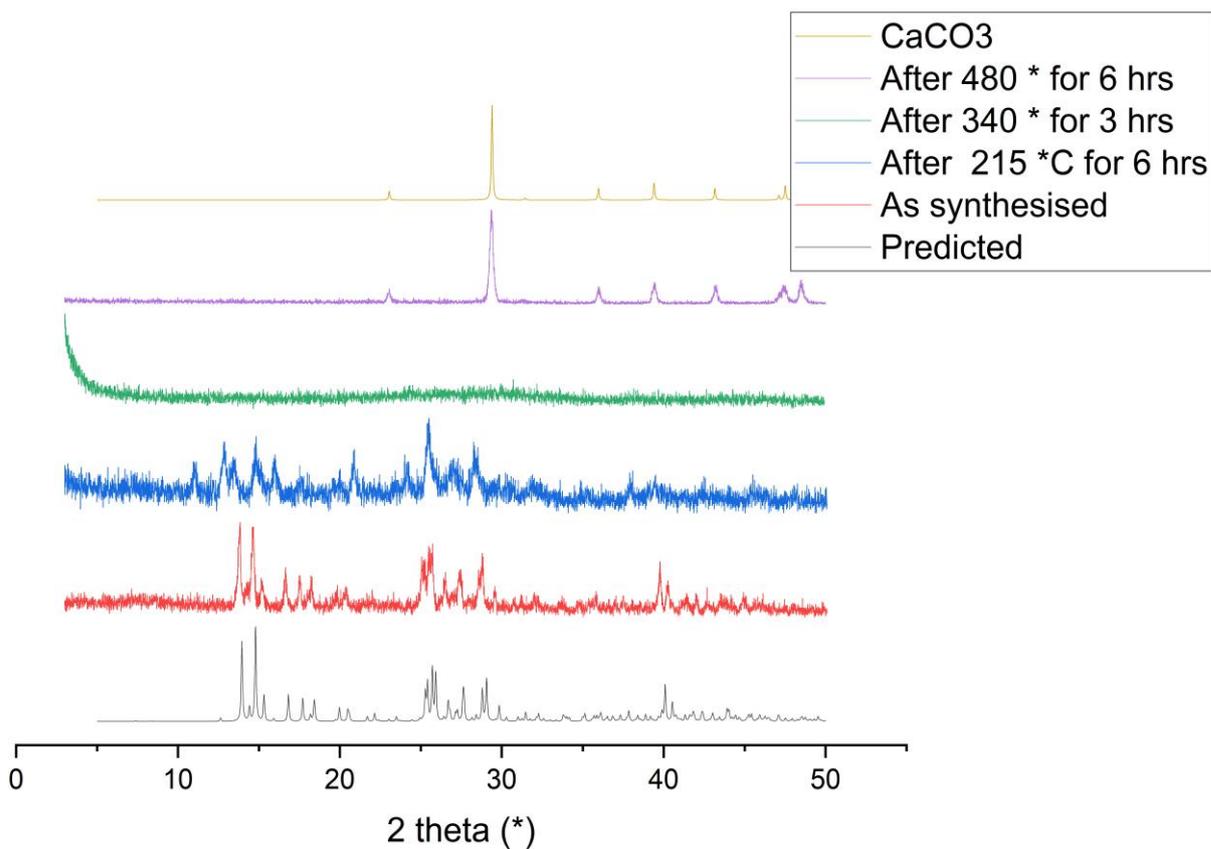


Figure S3: PXRD patterns of SIMOF-4 after different heat treatments, with simulated patterns of CaCO₃ and SIMOF-4 for comparison. All obtained using Cu(K α 1) radiation.

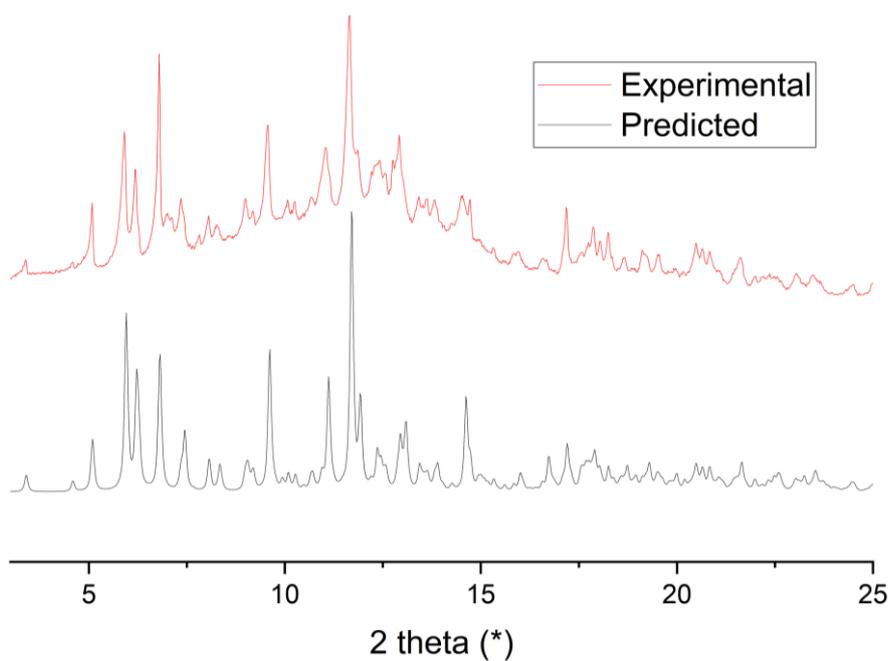


Figure S4: PXRD pattern of SIMOF-4-h simulated from scXRD structure compared with the experimental pattern. Obtained using Mo (K α 1) radiation.

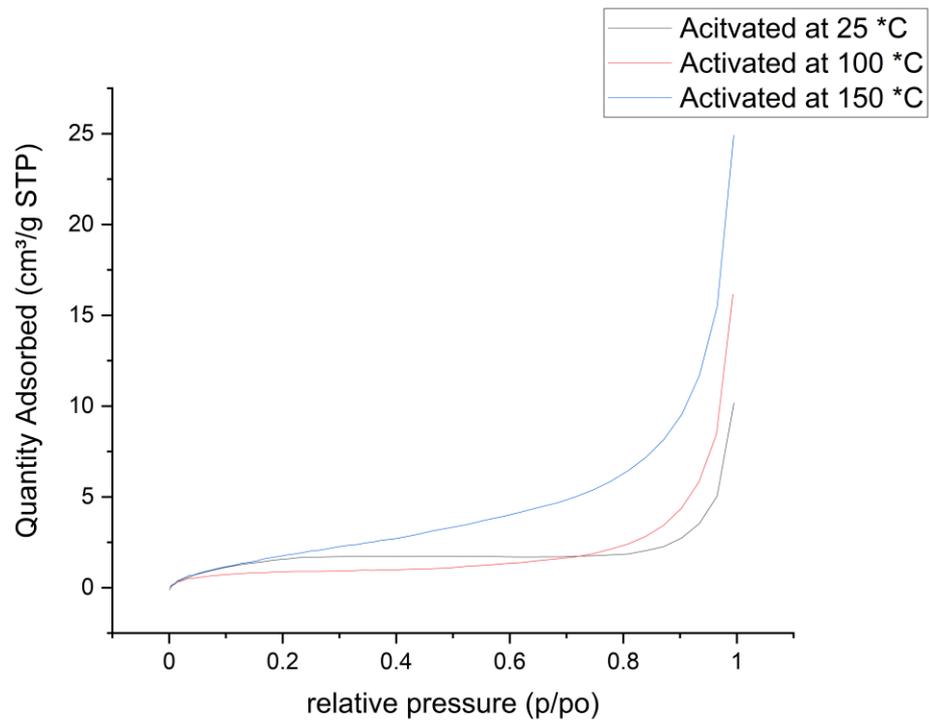


Figure S5: N_2 Adsorption isotherms of SIMOF-4 after 3 different activation protocols of 25 °C, 100 °C and 150 °C all under vacuum.

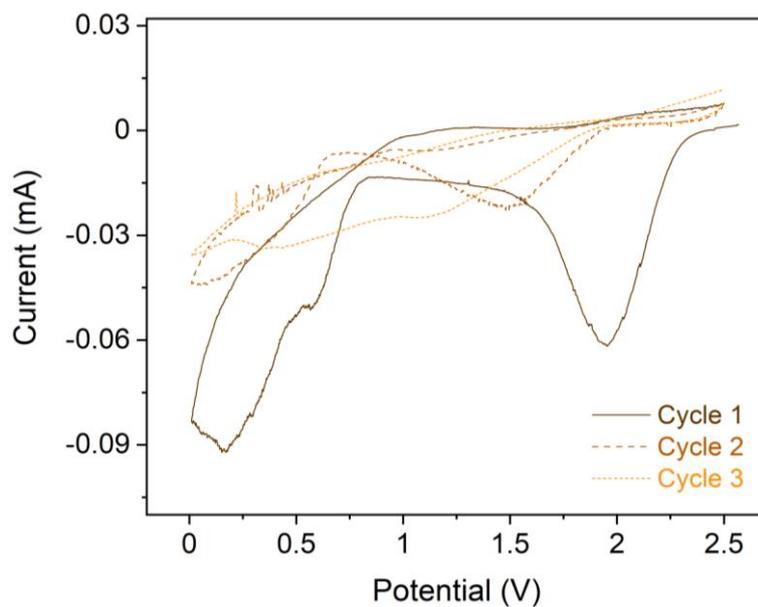


Figure S6: Cyclic voltammogram for SIMOF-4 recorded at a scan rate of 0.05 mV s^{-1} between 0.01-2.5 V.

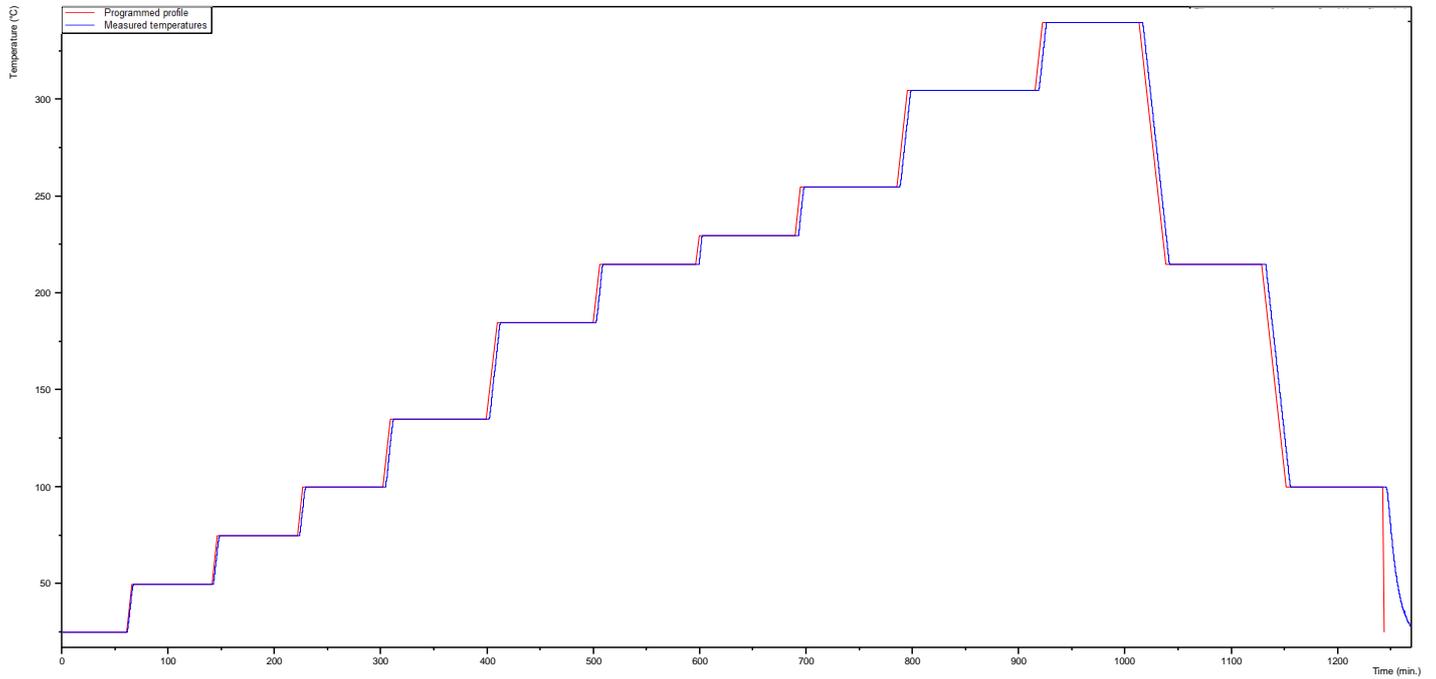


Figure S7: Temperature time profile for the VTXRD experiment performed on SIMOF-4, showing programmed and measured temperature profiles.