

ELECTRONIC SUPPLEMENTARY INFORMATION

CO₂ capture in the presence of water vapour in MIL-53(Al)

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1. Materials and measurements

All reagents and solvents were used as received from commercial suppliers without further purification. Powder X-ray diffraction (PXRD) data were collected under ambient conditions on a Bruker AXD D8 Advance diffractometer operated at 160 W (40 kV, 40 mA) for Cu K α_1 ($\lambda = 1.5406 \text{ \AA}$). Thermal gravimetric analysis (TGA) was performed under N₂ at a scan rate of 2 °C/min using a TA Instruments Q500HR analyser. N₂ adsorption was carried out in a conventional volumetric technique by a Micromeritics ASAP 2020 sorptometer. The surface area was calculated using the BET method based on adsorption data in the partial pressure (p/p_0) range 0.01 to 0.04. Dynamic and isothermal experiments were performed using a humidity-controlled thermobalance (TA Instruments, model Q5000SA) at 30 and 50 °C and a relative humidity (RH) of 20 and 40%.

2. Experimental

CO₂ capture experiments

Kinetic uptake experiments were performed by using a thermobalance (Q500 HR, from TA) at different temperatures with a constant CO₂ flow (60 mL min⁻¹). Then, samples of MIL-53(Al) and MCM-41 were placed into the thermobalance and activated by heating from room temperature to 180 °C for 1h and under a flow of N₂ gas. After the activated sample was cooled down, the desired temperature was set and a constant CO₂ flow (60 mL min⁻¹) was started. With a humidity-controlled thermobalance (Q5000 SA, from TA) kinetic uptake experiments at 30 and 50 °C with a constant CO₂ flow (60 mL min⁻¹) were carried out on activated samples (180 °C for 1h and under a flow of N₂ gas) of MIL-53(Al) and only at 30 °C on activated samples (180 °C for 1h and under a flow of N₂ gas) of MCM-41.

3. TGA plot

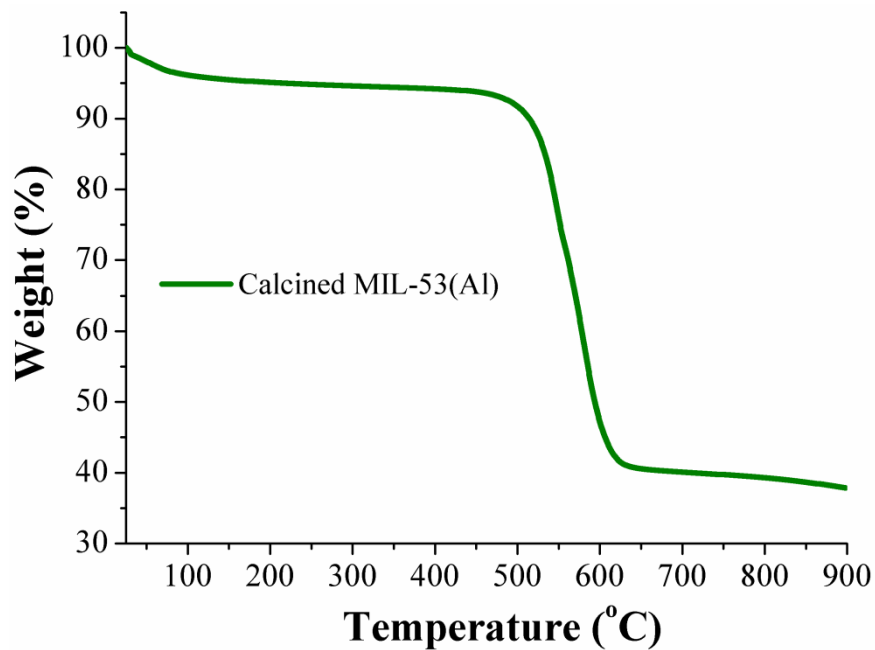


Fig. S1: TGA analysis of calcined MIL-53(Al).

4. Powder X-ray diffraction patterns of MIL-53(Al)

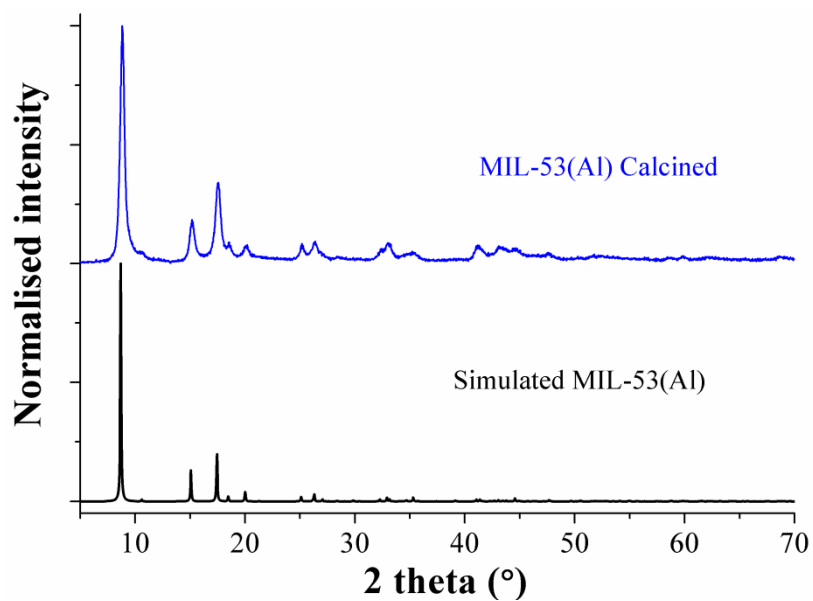


Fig. S2: PXRD patters of simulated (black) and calcined (blue) MIL-53(Al).

5. Dynamic and isothermal CO₂ anhydrous experiments on MCM-41

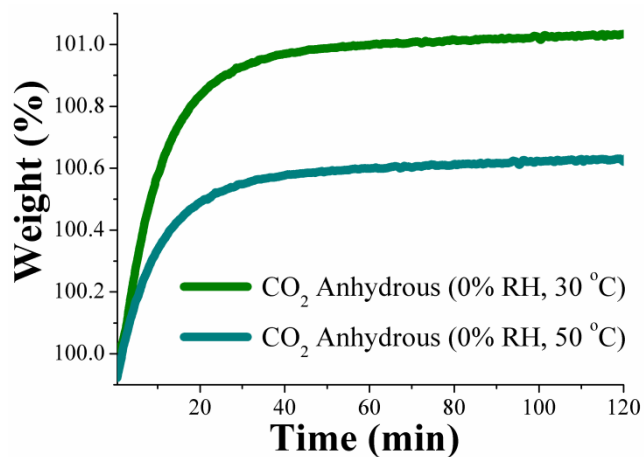


Fig. S3 Kinetic uptake experiments performed at different temperatures (30 and 50 °C) with a CO₂ flow of 60 mL/min on MCM-41.

6. PXRD of anhydrous MCM-41

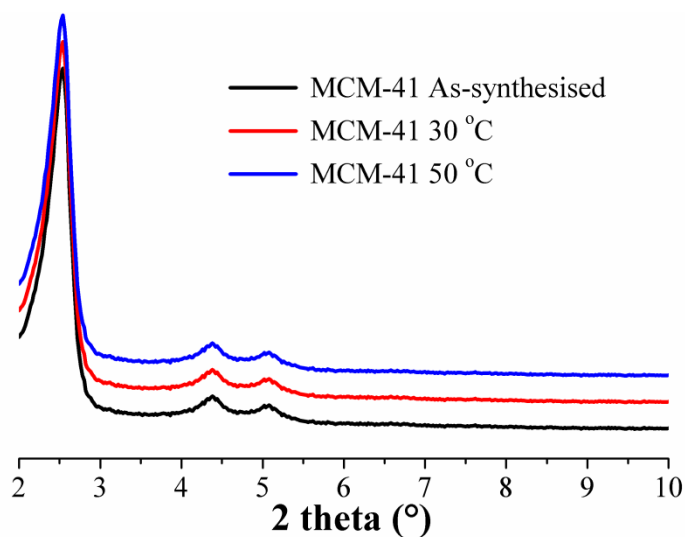


Fig. S4: PXRD patterns of each MCM-41 samples after the kinetic CO₂ isotherms were carried out at different temperatures.

7. PXRD of each MIL-53(Al) samples after the kinetic CO₂ isotherms.

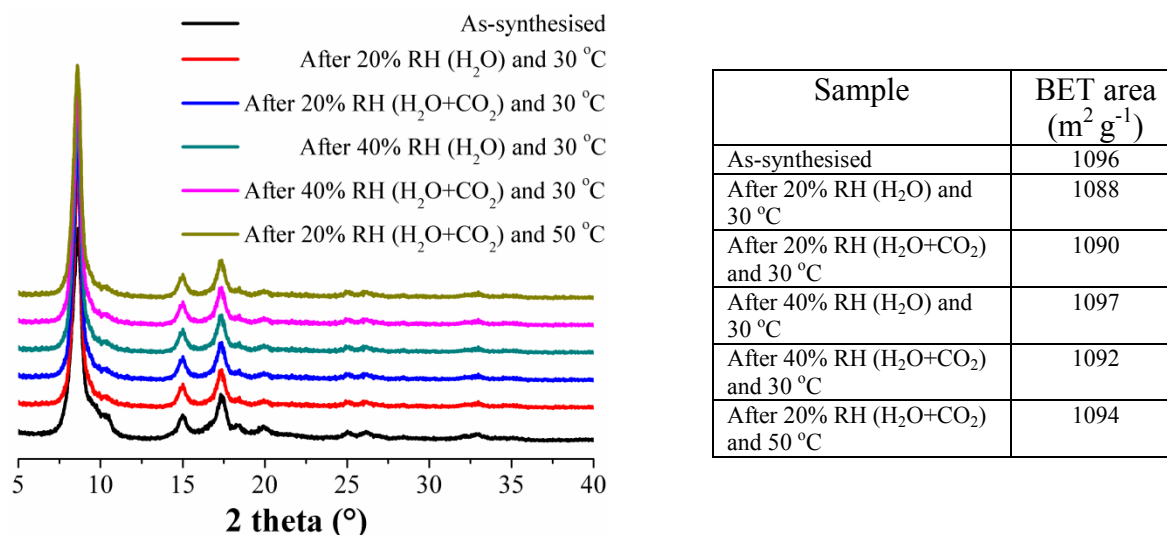


Fig. S5: (left) PXRD patterns of each MIL-53(Al) samples after the kinetic CO₂ isotherms were carried out at different relative humidities and temperatures; (right) BET areas of each MIL-53(Al) samples after the kinetic CO₂ isotherms were carried out at different relative humidities and temperatures.

8. Dynamic and isothermal CO₂ experiments on MCM-41

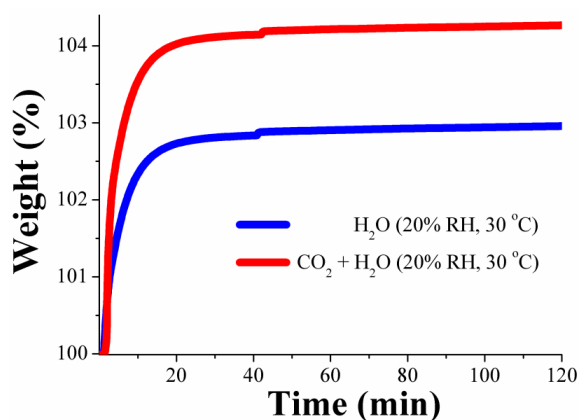


Fig. S6: Kinetic uptake experiments carried out at 30 °C and 20% RH with CO₂+H₂O (red line) and only H₂O (blue line).

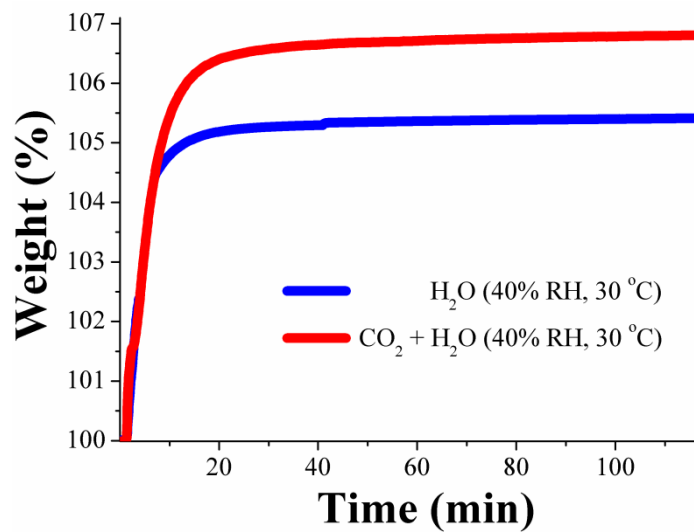


Fig. S7: Kinetic uptake experiments carried out at 30 °C and 40% RH with CO₂+H₂O (red line) and only H₂O (blue line).

9. PXRD of each MCM-41 samples after the kinetic CO₂ isotherms.

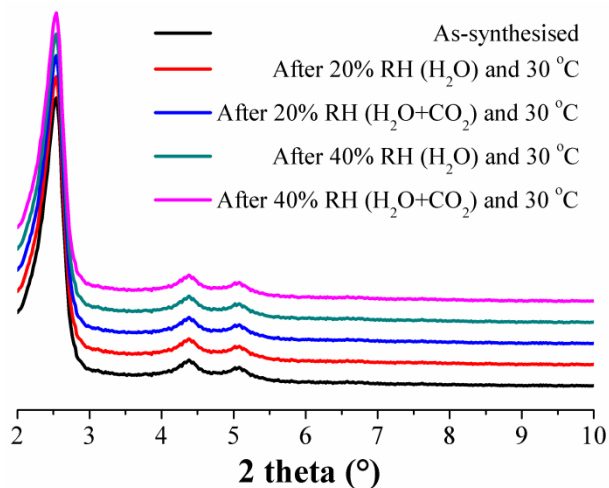


Fig. S8: PXRD patterns of each MCM-41 samples after the kinetic CO₂ isotherms were carried out at different relative humidities.

10. Dynamic and isothermal CO₂ experiments on PCM-14

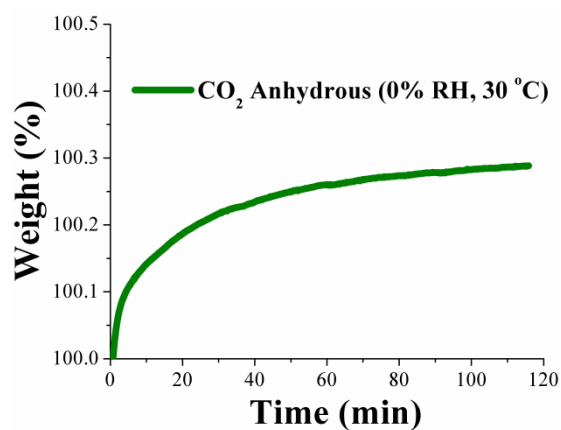


Fig. S9: Kinetic isotherms carried out at 30 °C and 0% RH with a CO₂ flow of 60 mL/min in PCM-14.

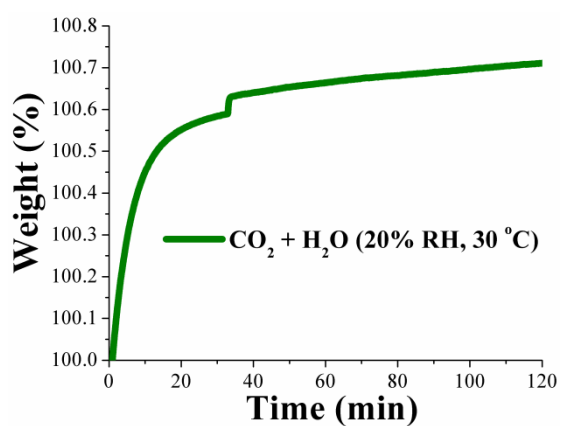


Fig. S10: Kinetic isotherms carried out at 30 °C and 20% RH with a CO₂ flow of 60 mL/min in PCM-14.

11. Static and isothermal adsorption experiments on MIL-53

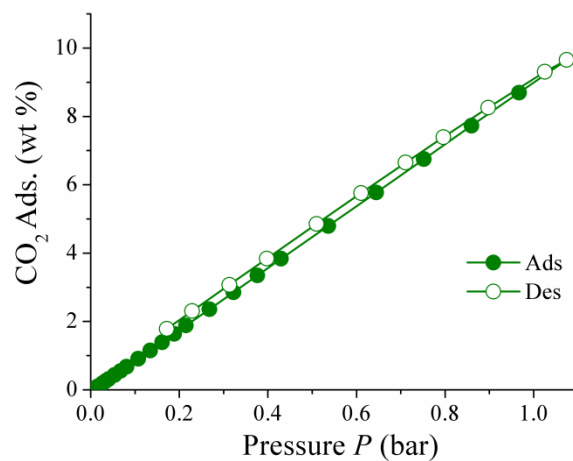


Fig. S11: Static CO₂ isotherm carried out at 30 °C in MIL-53.

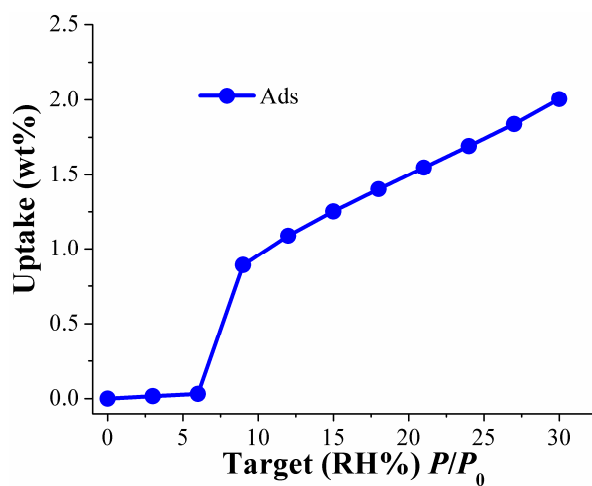


Fig. S12: Static H₂O isotherm carried out at 30 °C in MIL-53.