Supplementary information

Microwave Synthesis and Gas Sorption of Calcium and Strontium Frameworks

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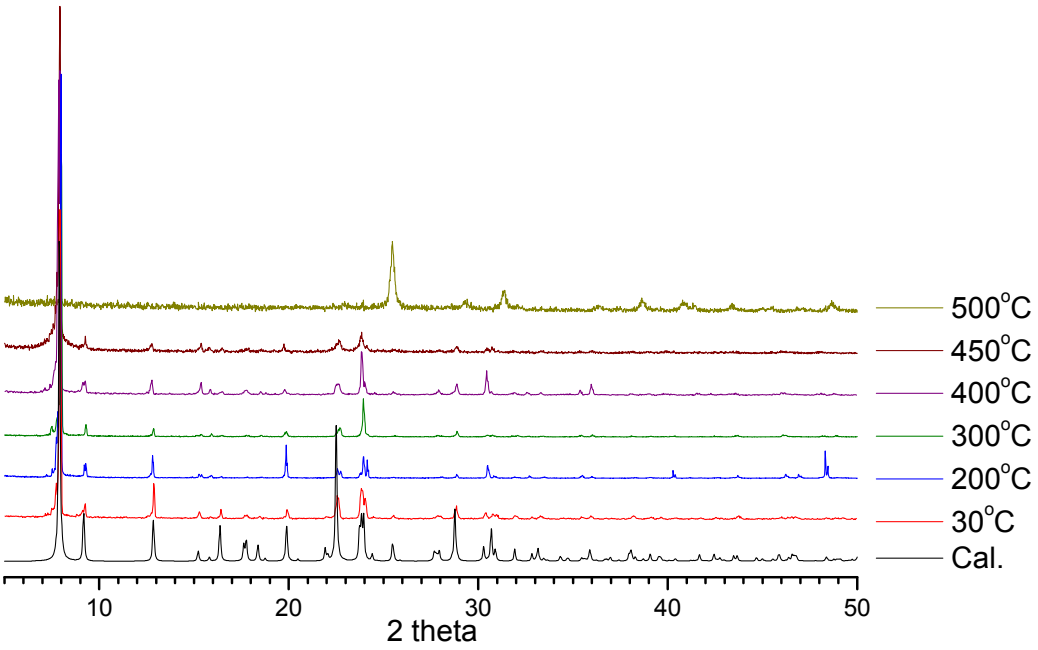


Figure S1. Powder X-ray diffraction patterns with varied temperatures for **CYCU-1**.

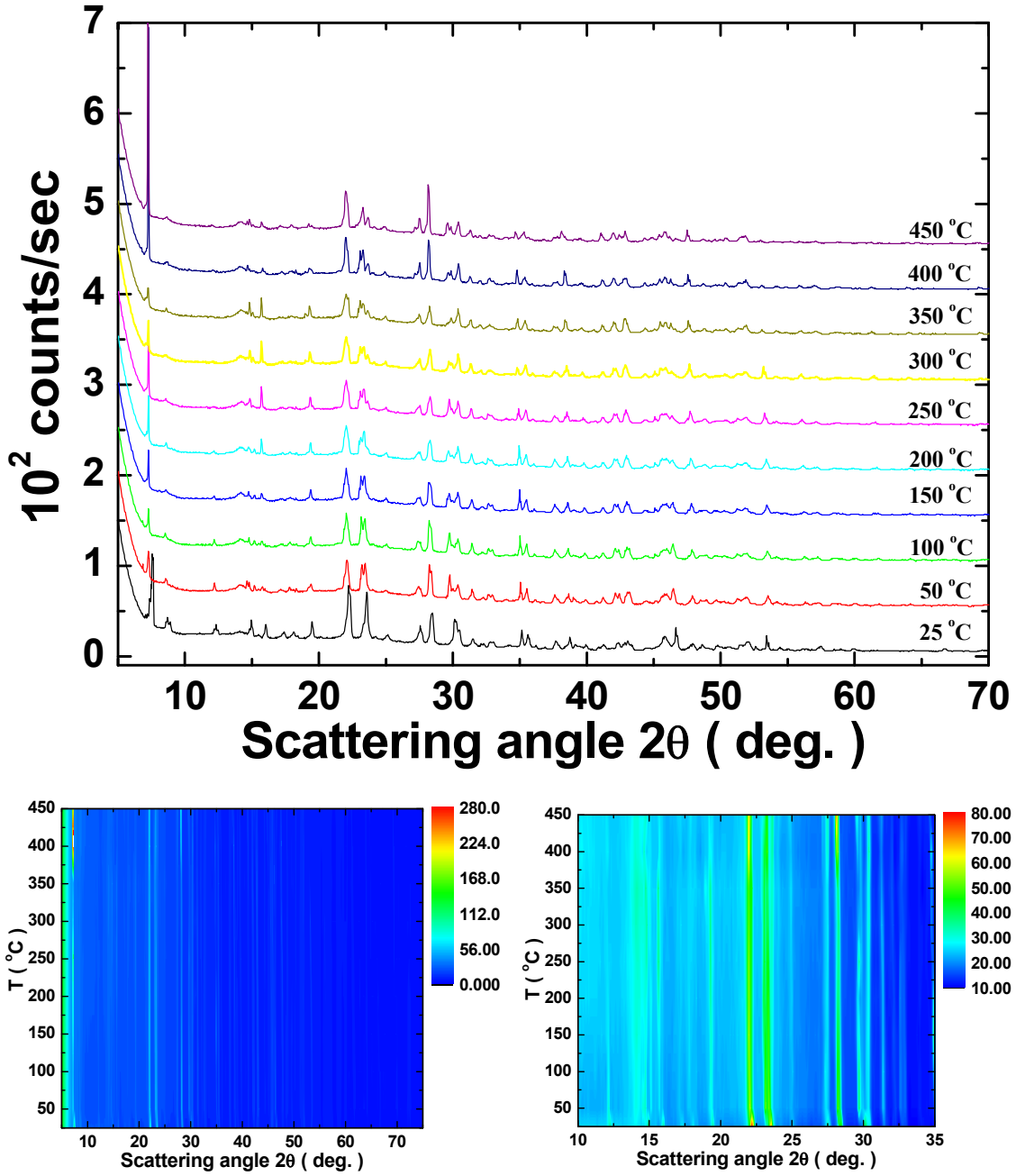


Figure S2. Powder X-ray diffraction patterns under vacuum ($1x10^{-4}$ torr) and varied temperatures for **CYCU-1**.

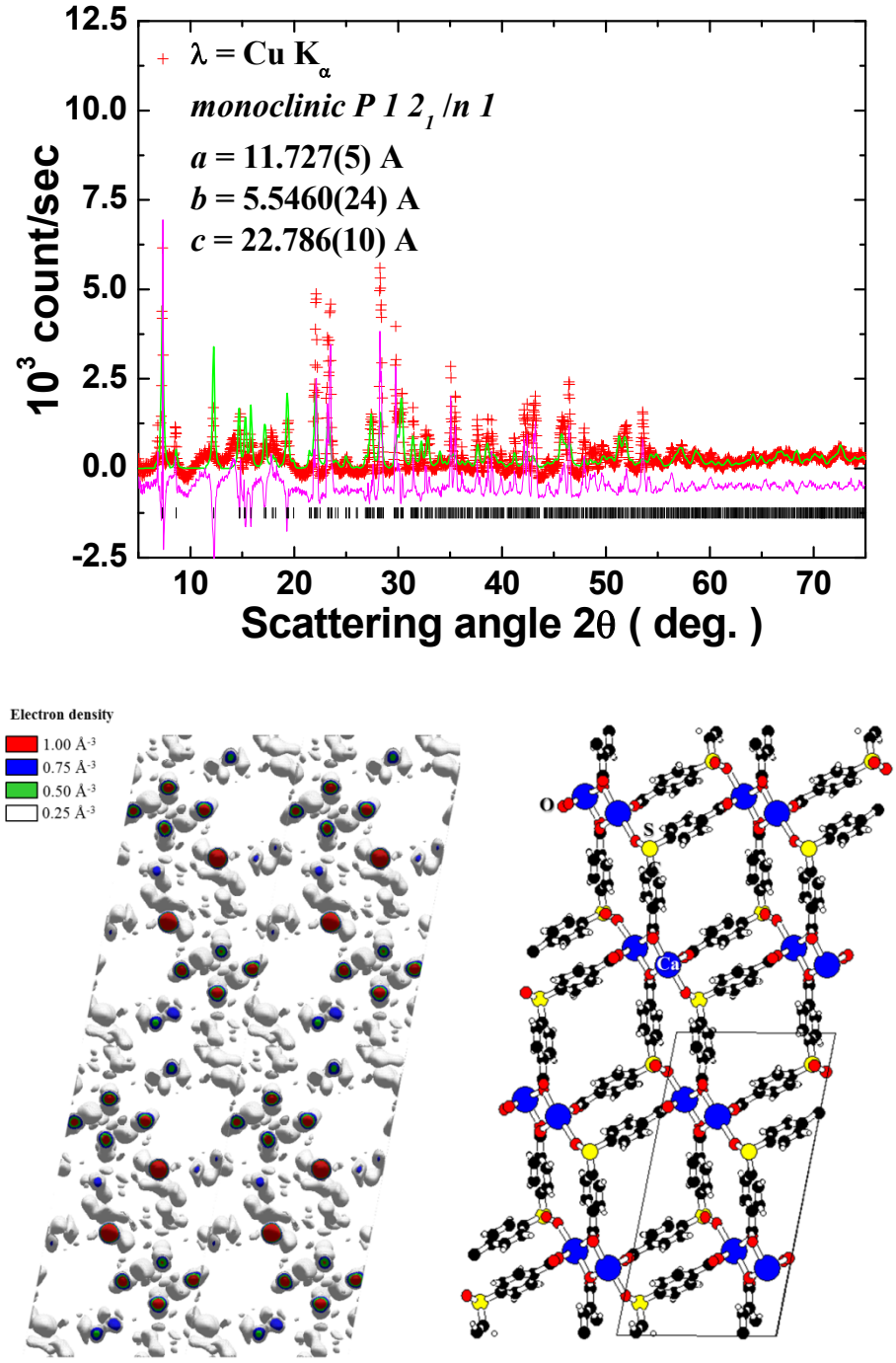


Figure S3. Observed (crosses) and fitted (solid lines) X-ray powder diffraction patterns for **CYCU-1**, assuming a monoclinic symmetry of space group $P2_1/n$. The difference between the calculated and observed is plotted at the bottom. The solid vertical lines mark the calculated positions of Bragg reflections for the proposed crystalline structure. The bottom plots are electron density from X-ray powder diffraction pattern and structure from single crystal X-ray diffraction.

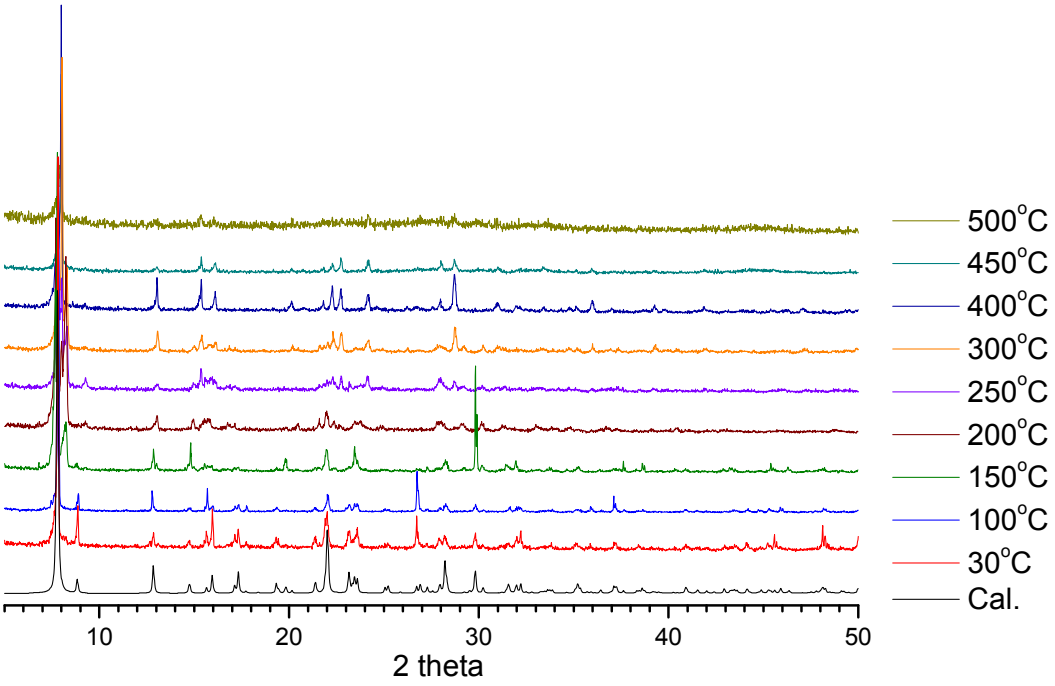


Figure S4. Powder X-ray diffraction patterns with varied temperatures for **CYCU-2**.

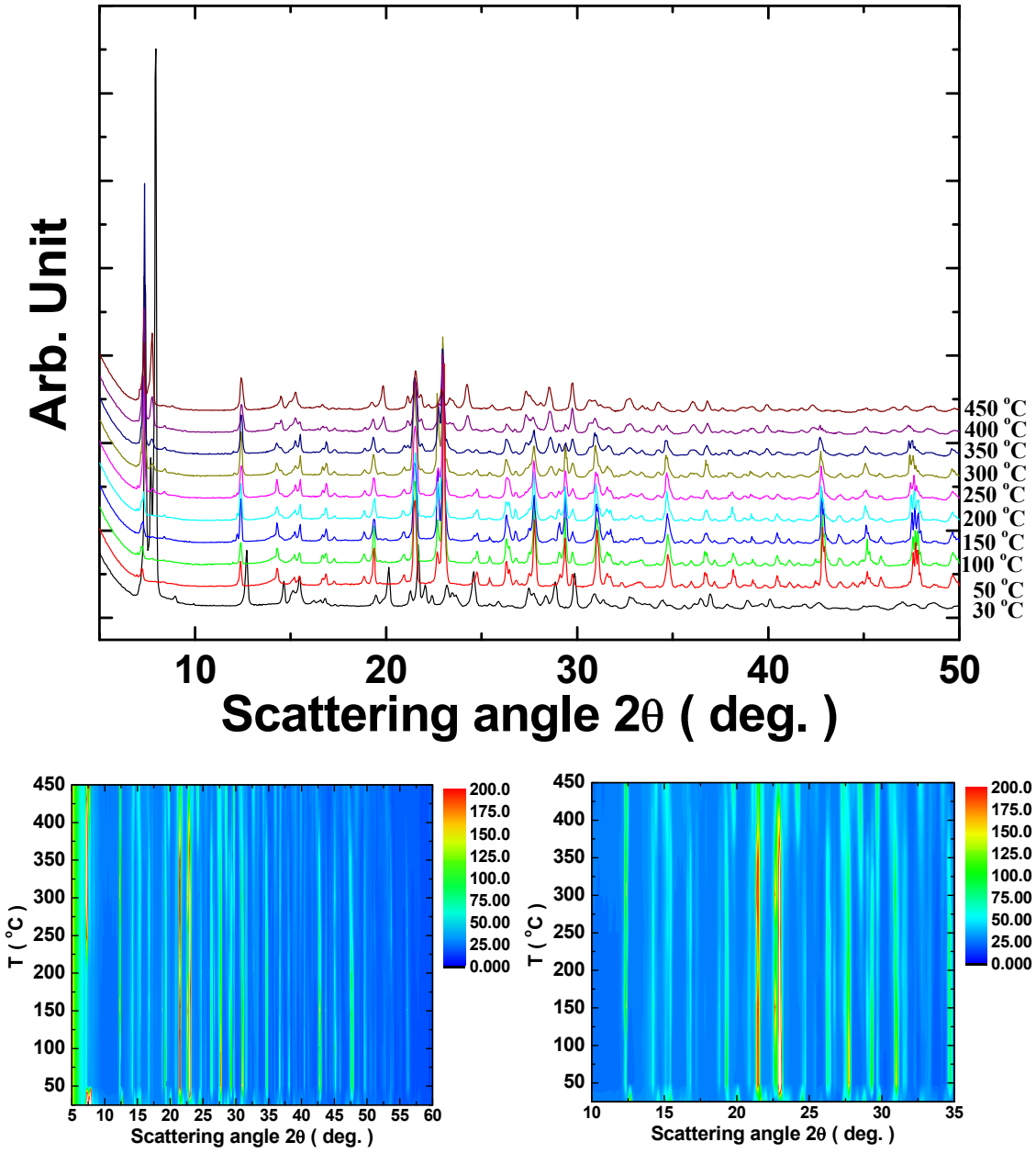


Figure S5. Powder X-ray diffraction patterns under vacuum ($1x10^{-4}$ torr) and varied temperatures for **CYCU-2**.

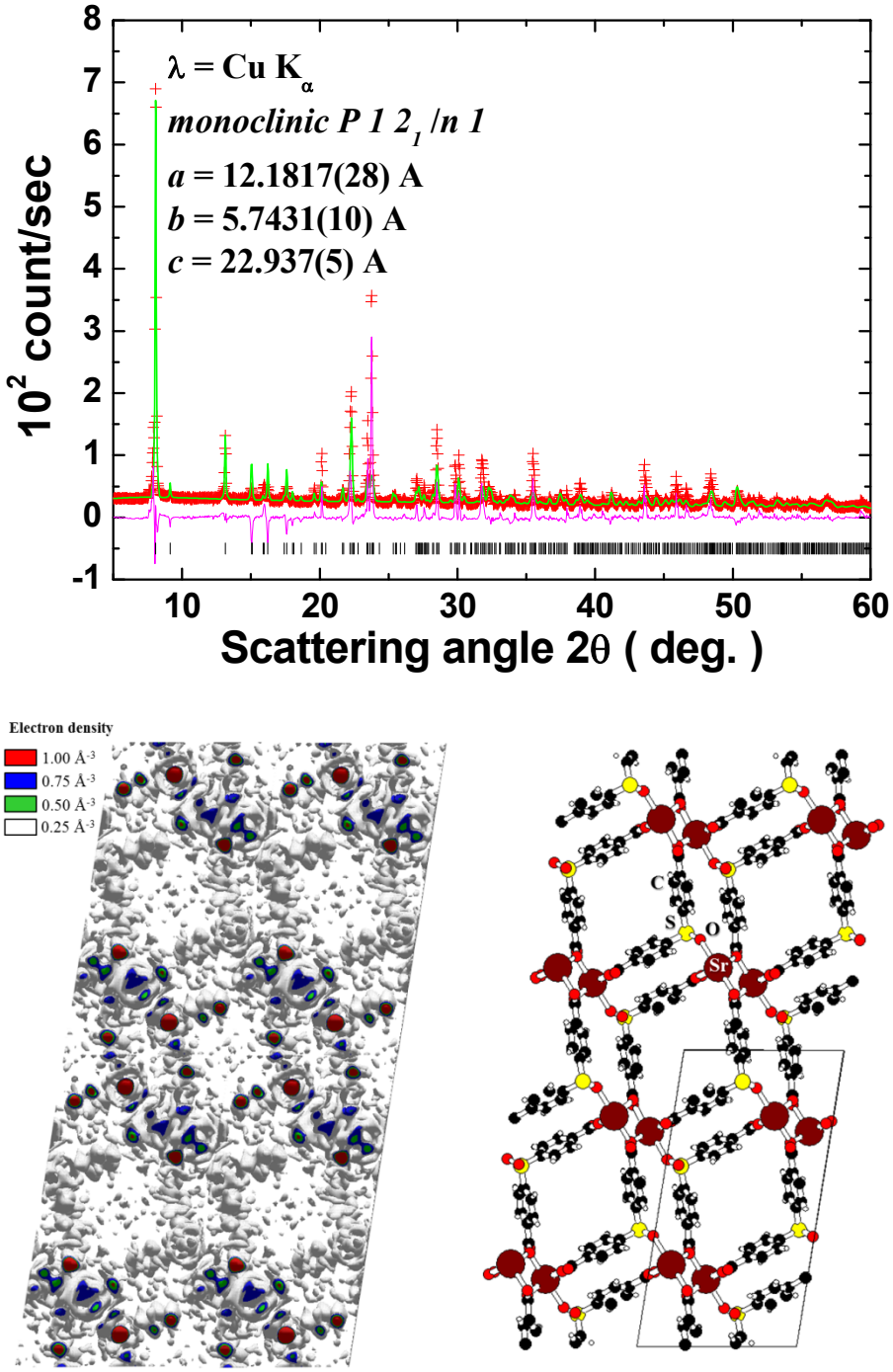
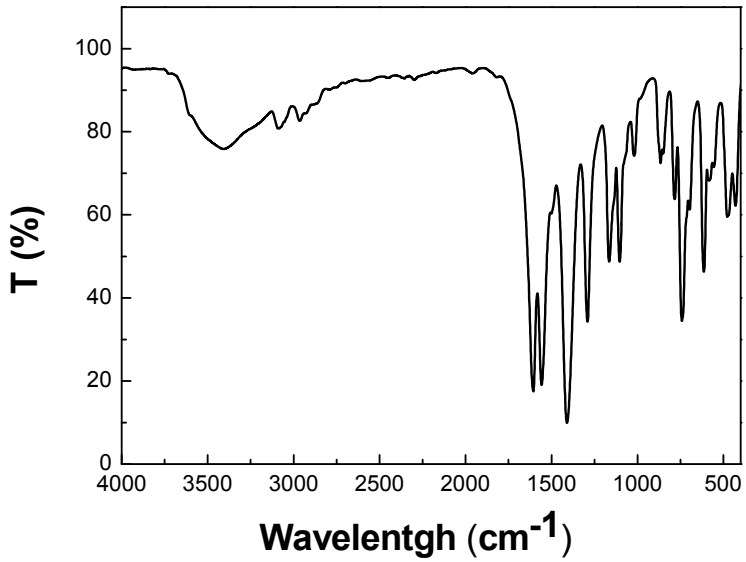


Figure S6. Observed (crosses) and fitted (solid lines) X-ray powder diffraction patterns for **CYCU-2**, assuming a monoclinic symmetry of space group $P2_1/n$. The difference between the calculated and observed is plotted at the bottom. The solid vertical lines mark the calculated positions of Bragg reflections for the proposed crystalline structure. The bottom plots are electron density from X-ray powder diffraction pattern and structure from single crystal X-ray diffraction.

(a) **CYCU-1$_{as}$**



(b) **CYCU-2$_{as}$**

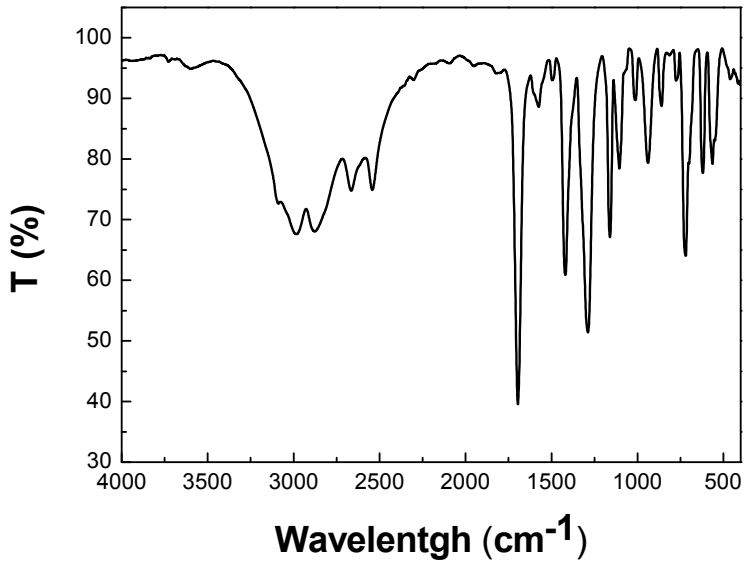
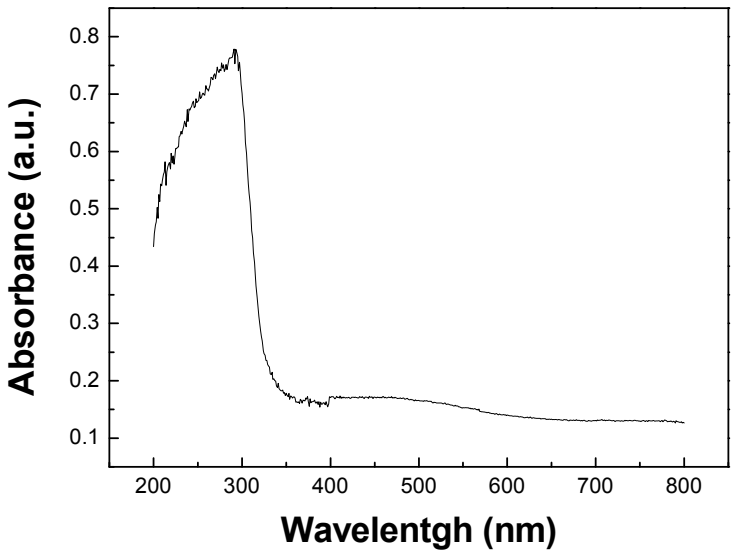


Figure S7. FT-IR spectra.

(a) **CYCU-1$_{as}$**



(b) **CYCU-2$_{as}$**

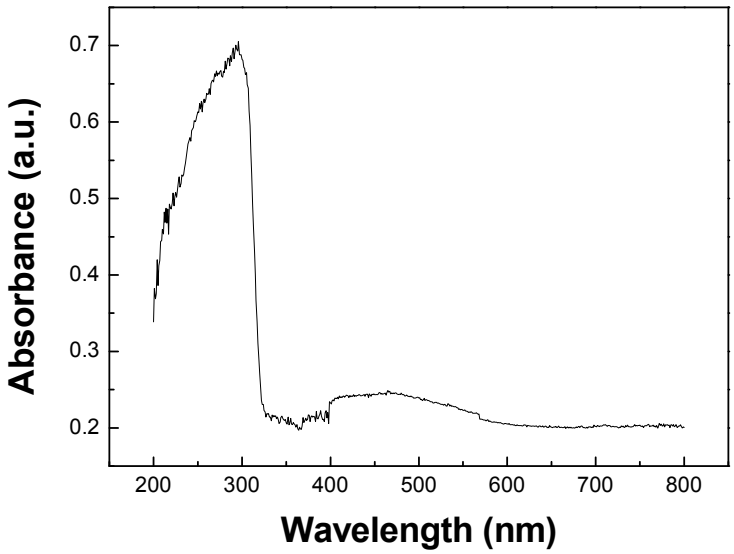
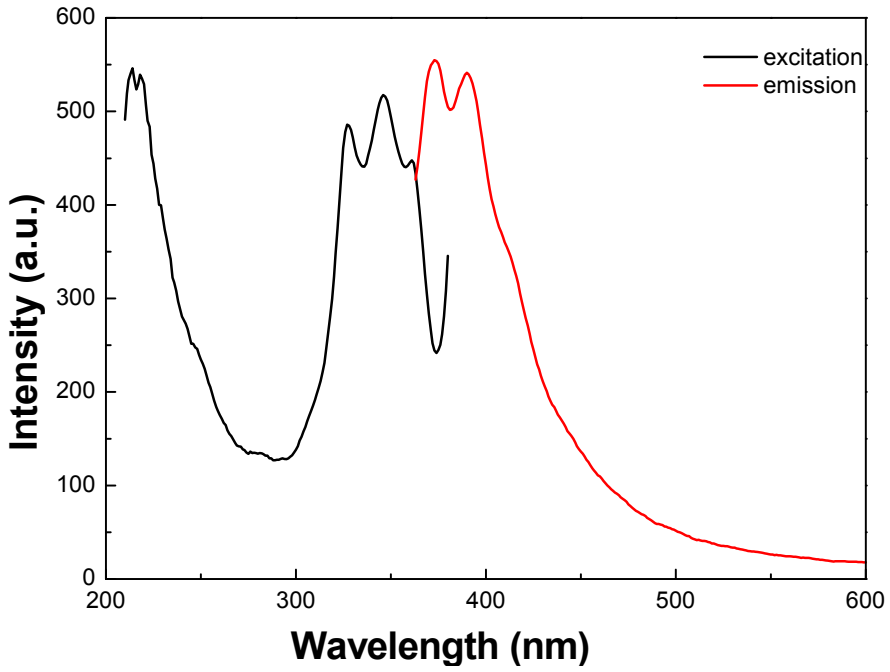


Figure S8. UV-vis absorption spectrua.

(a) **CYCU-1$_{as}$**



(b) **CYCU-2$_{as}$**

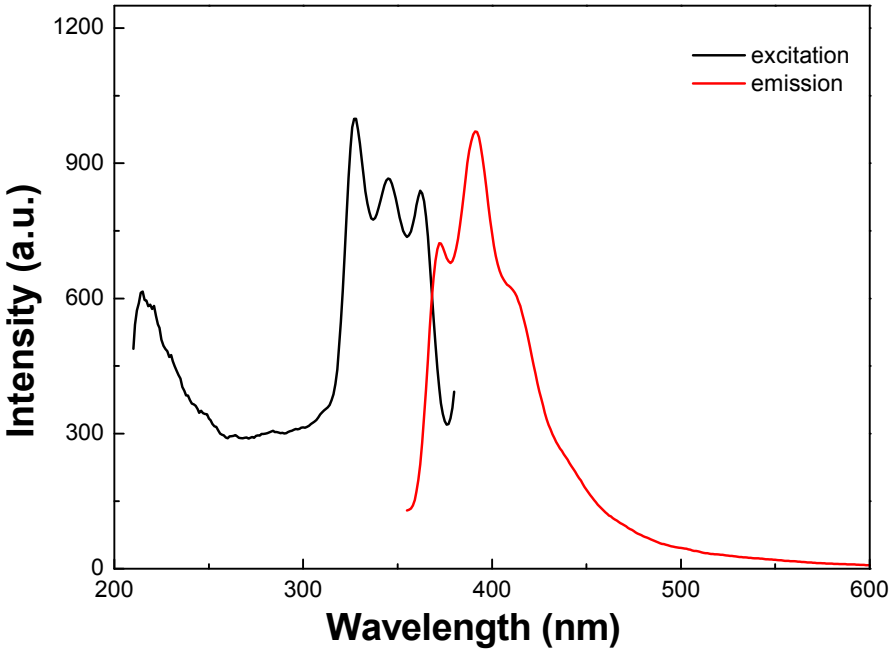
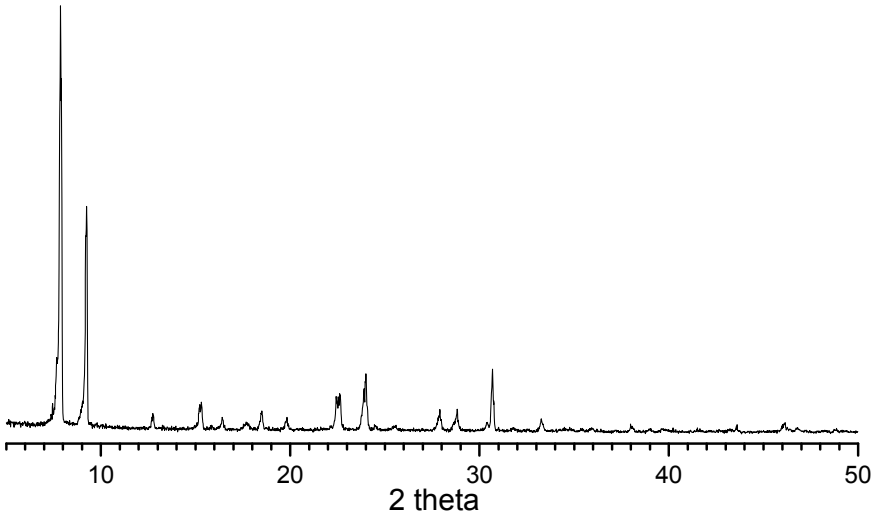


Figure S9. Photoluminescence emission spectra.

(a) **CYCU-1**



(a) **CYCU-2**

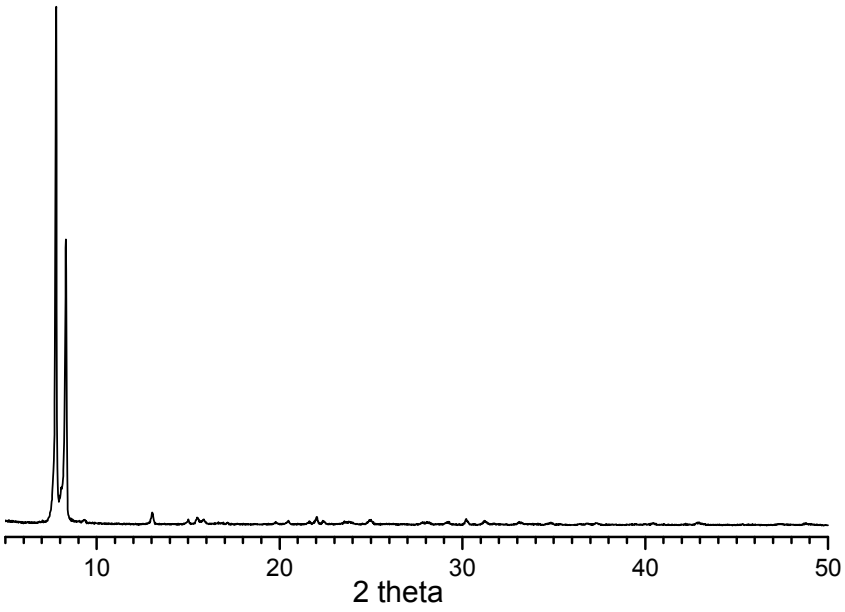
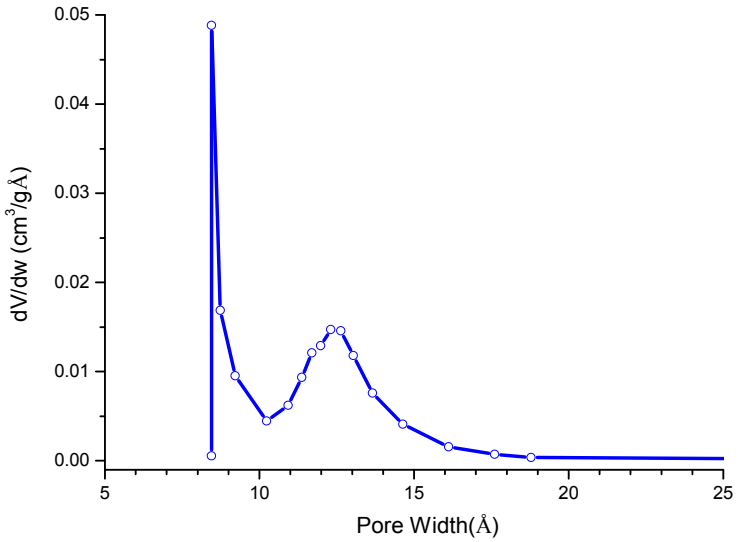


Figure S10. Powder X-ray diffraction patterns after N_2 sorption.

(a) **CYCU-1**



(a) **CYCU-2**

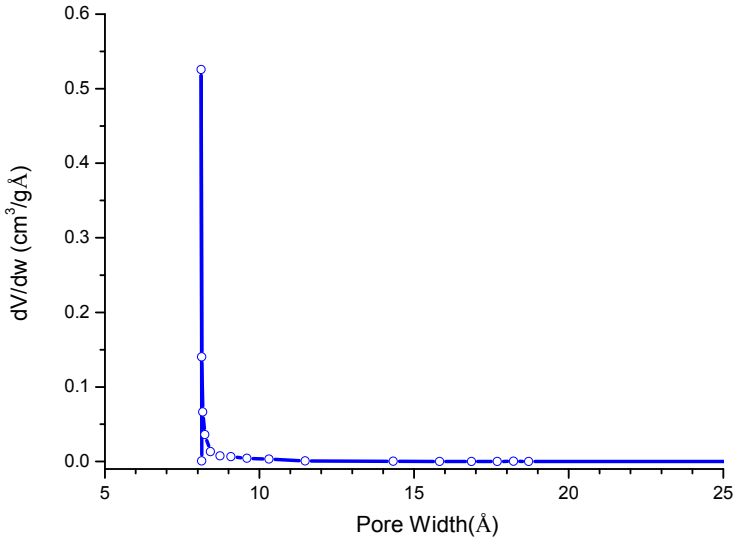
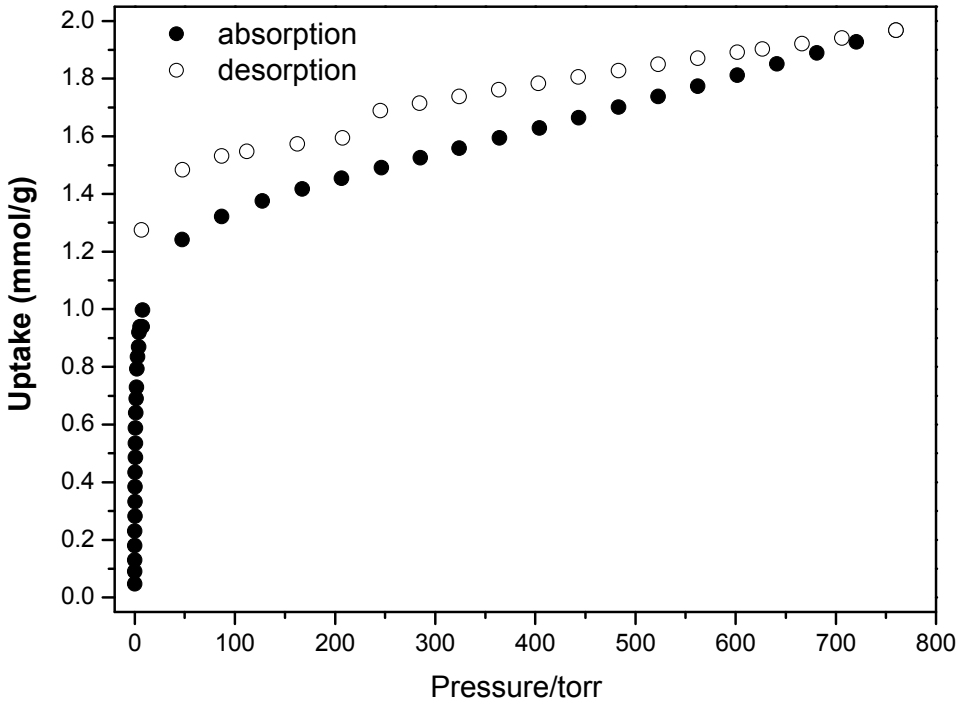


Figure S11. The pore size distributions obtained by the Horvath-Kawazoe (HK) method.

(a)



(b)

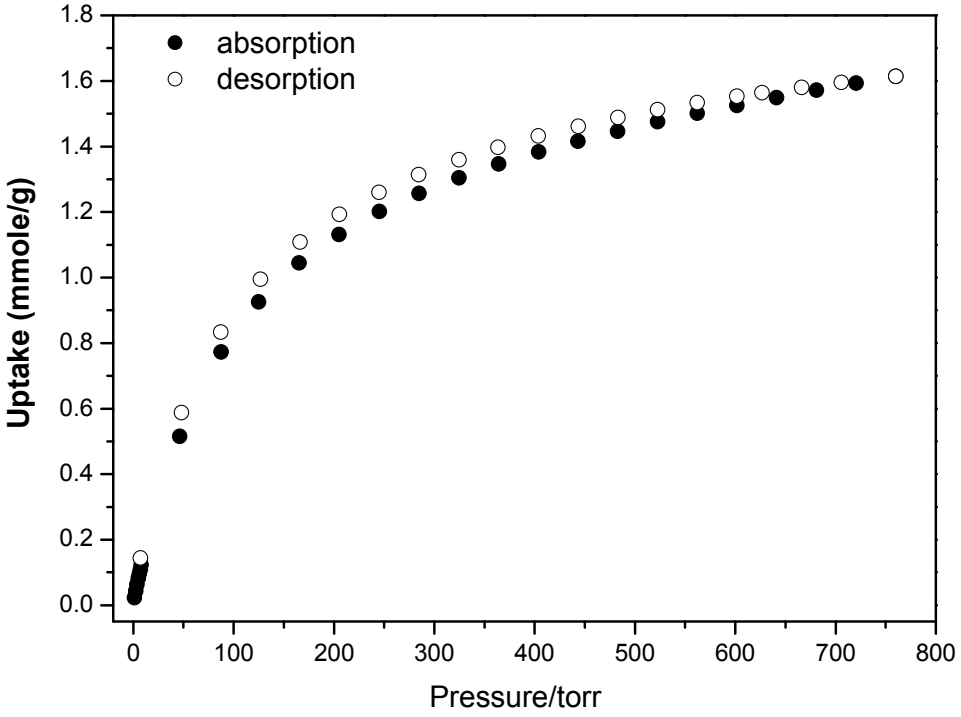


Figure S12. The CO_2 adsorption isotherms at (a) 195 K and (b) 273 K for **CYCU-1**.

The isosteric heat of adsorption for hydrogen and carbon dioxide adsorption on CYCU-1.

The differential heat of adsorption was calculated from the measured carbon dioxide adsorption at 298 K and 273 K by applying the Clausius-Clapeyron equation: [1]

$$\frac{\Delta H_{iso}}{RT^2} = \left(\frac{\partial lnP}{\partial T}\right)_n$$

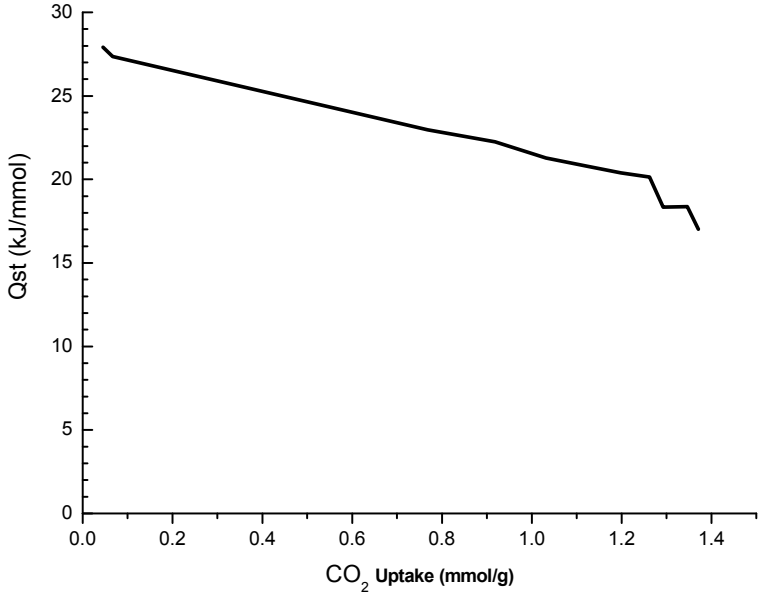


Figure S13. Isosteric heat of adsorption for CO_2 in **CYCU-1**.[1]

Table S1. Selected bond lengths (Å).

CYCU-1$_{as}$			
Ca(1)-O(3)	2.2977(15)	Ca(1)-O(1)#1	2.4367(15)
Ca(1)-O(4)	2.3010(16)	Ca(1)-O(5)	2.4555(14)
Ca(1)-O(2)	2.3604(15)	Ca(1)-O(2)#2	2.8850(17)
Ca(1)-O(1)	2.3772(16)		
CYCU-1			
Ca(1)-O(3)#1	2.2868(17)	Ca(1)-O(1)#4	2.4324(17)
Ca(1)-O(4)#1	2.2873(18)	Ca(1)-O(5)	2.4475(17)
Ca(1)-O(2)#2	2.3439(16)	Ca(1)-O(2)#4	2.8870(18)
Ca(1)-O(1)#3	2.3678(17)		
CYCU-2$_{as}$			
Sr(1)-O(2)	2.4323(19)	Sr(1)-O(4)#1	2.5725(17)
Sr(1)-O(1)	2.4368(18)	Sr(1)-O(5)	2.5882(17)
Sr(1)-O(4)	2.4926(17)	Sr(1)-O(3)#2	2.9326(18)
Sr(1)-O(3)	2.5164(17)		
CYCU-2			
Sr(1)-O(2)	2.431(2)	Sr(1)-O(4)#1	2.573(2)
Sr(1)-O(1)	2.435(2)	Sr(1)-O(5)	2.589(2)
Sr(1)-O(4)	2.491(2)	Sr(1)-O(3)#2	2.937(2)
Sr(1)-O(3)	2.513(2)		

Symmetry transformations used to generate equivalent atoms: for **CYCU-1$_{as}$,** #1 -x+1/2,y+1/2,-z+1/2, #2 -x+1/2,y-1/2,-z+1/2; for **CYCU-1**, #1 -x-1/2,y-1/2,-z+1/2, #2 -x,-y+2,-z, #3 -x,-y+1,-z, #4 x+1/2,-y+3/2,z+1/2; for **CYCU-2$_{as}$** and **CYCU-2,** #1 -x+1/2,y-1/2,-z+3/2, #2 -x+1/2,y+1/2,-z+3/2.

References

S1. P. A. Webb, C. Orr, *Analytical Methods in Fine Particle Technology*; Micromeritics Instrument Corp.: Norcross, USA, 1997; pp 230-231.