# One-dimensional interpenetrated coordination polymers showing step gas sorption properties

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## Supporting Information

**Synthesis of compound 1:** A mixture of adipic acid (0.146 g, 1 mmol), $Cu_2(OH)_2CO_3$ (0.111 g, 0.5 mmol), 2,2'-bipyridine (0.156 g, 1 mmol) was added into a mixture of 10ml water and 10ml methanol. This mixture was heated and stirred on a water bath at 80℃ for 10 h. Then the resulting solution was filtered, the filtrate was evaporated slowly at room temperature. Blue crystals were obtained after 12h, and dried at room temperature 5h to give dark blue blocks.[1]

**Synthesis of compound 2:** A mixture of $Cu(NO_3)_2 \cdot 4H_2O$(0.242 g, 1 mmol), $H_2ipa$ (0.166 g, 1 mmol), 2,2'-bipyridine (0.156 g, 1 mmol), $Et_3N$ (0.3 ml), and water (10 mL) was stirred for 20 min in air, then transferred and sealed in a 20 mL Teflon reactor, which was heated at 150℃ for three days and then cooled to room temperature. Blue block crystals were obtained after washing with water and drying in air.[2]

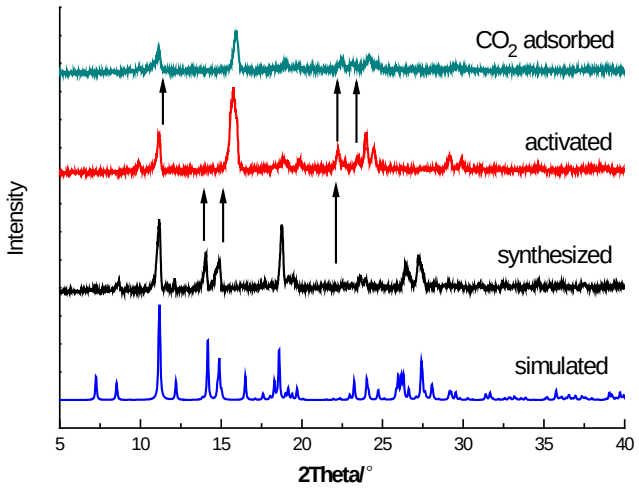


**Figure S1.** The PXRD of sample 1.

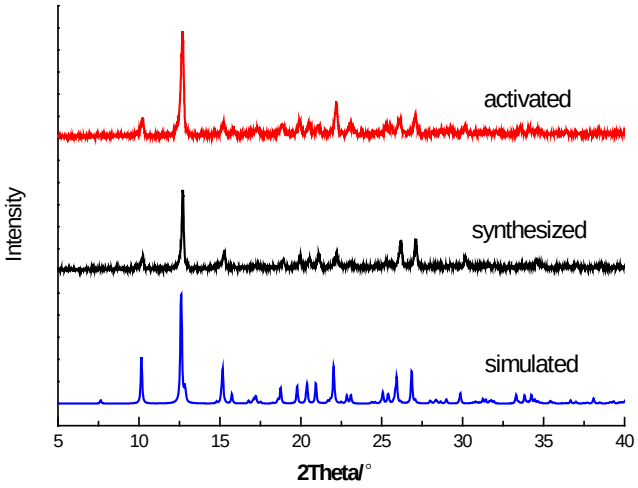


**Figure S2.** The PXRD of sample 2.

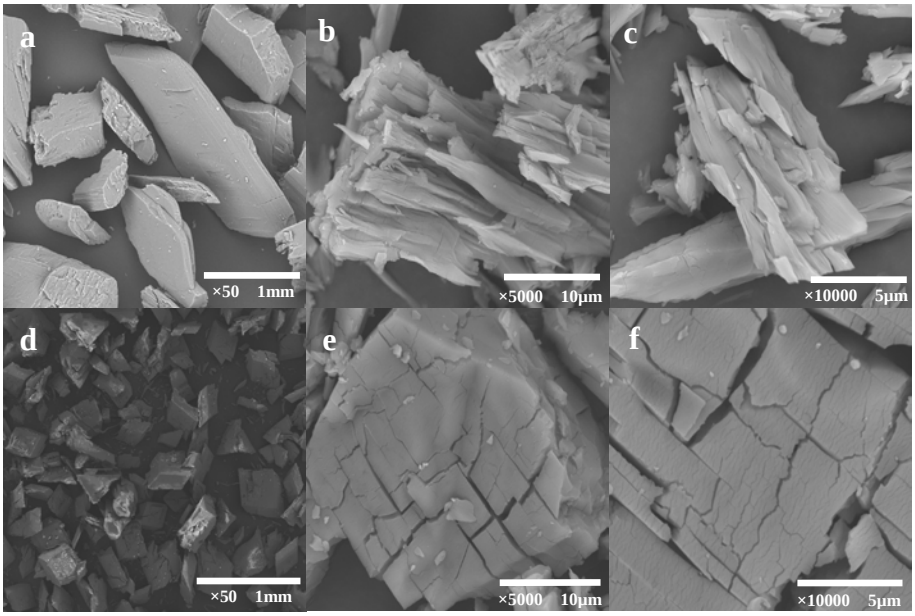


**Figure S3.** SEM images of sample 1(a, synthesized; b, activated; c, after $CO_2$ adsorption) and 2 (d, synthesized; e, activated; f, after $CO_2$ adsorption)

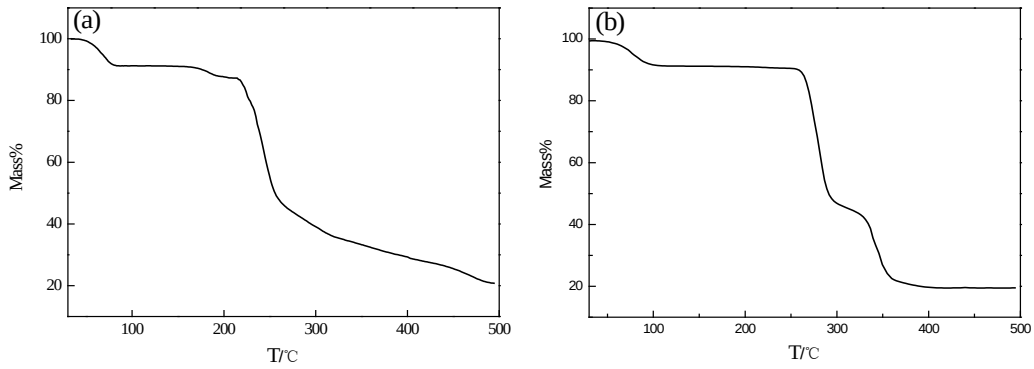


**Figure S4**: TGA curve for sample 1(a) and 2 (b) (NETZSCH STA409C) measured in air with a heating rate of 5 ℃/min.

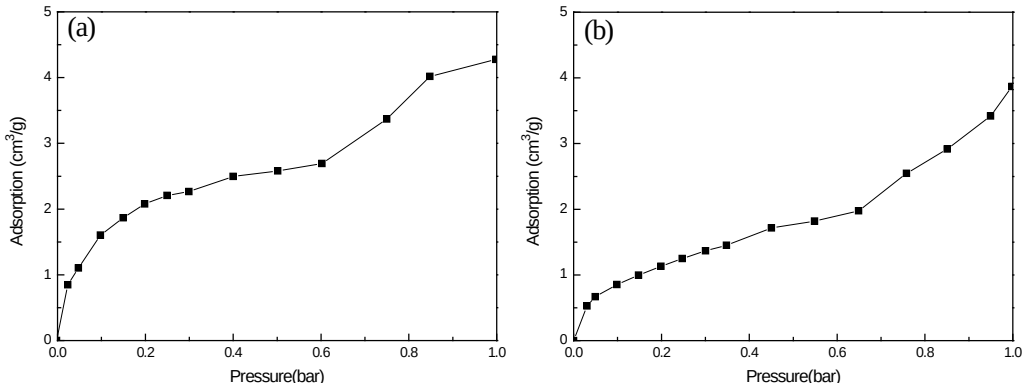


**Figure S5:** $N_2$ adsorption isotherm of sample 1(a) and 2(b) at 77 K.

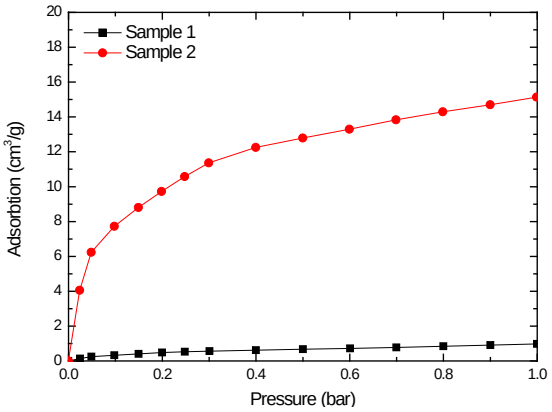


**Figure S6:** $CO_2$ adsorption isotherm of sample 1and 2 at 195 K.

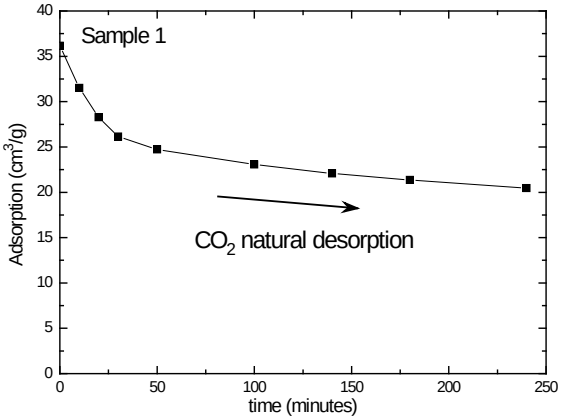


**Figure S7:** $CO_2$ natural desorption isotherms from high pressure (1.8MPa) rapidly decreased to atmospheric of sample 1 at 298 K.

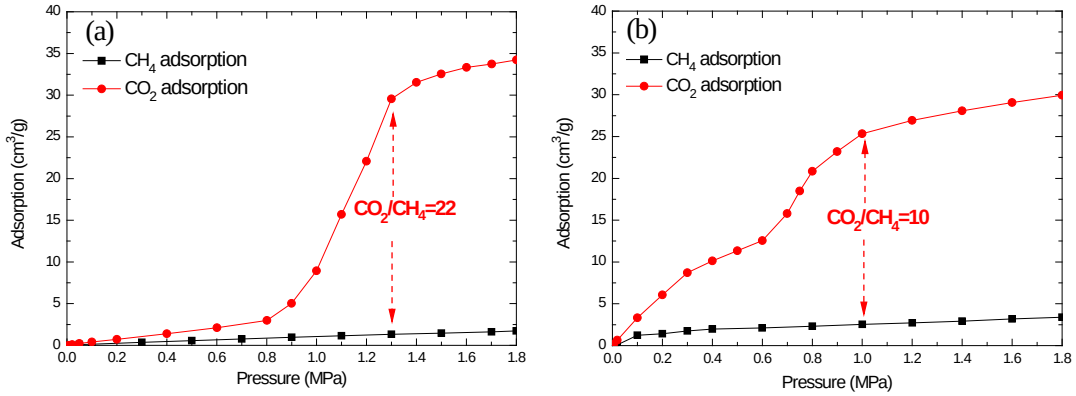


**Figure S8:** $CO_2$, $CH_4$ adsorption isotherms of sample 1(a) and 2(b) at 298 K.

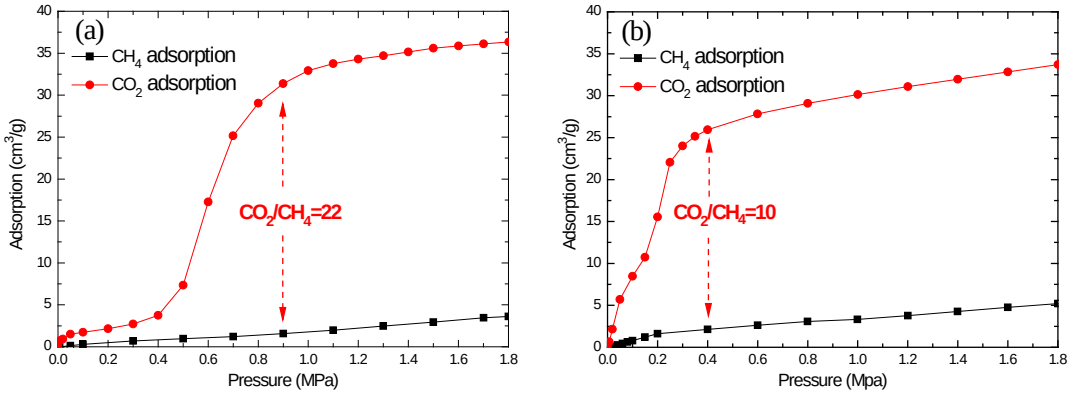


**Figure S9:** $CO_2$, $CH_4$ adsorption isotherms of sample 1(a) and 2(b) at 265 K.

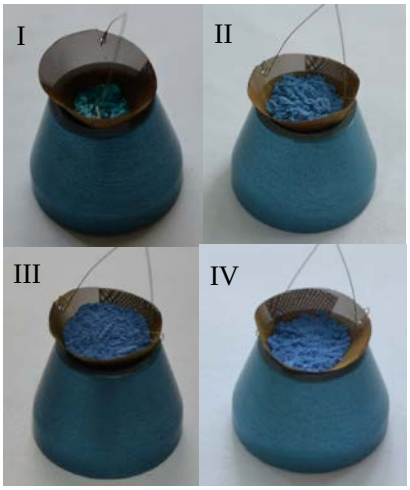


**Figure S10**: Images of the sample 1 morphology change in the gas adsorption process. As-synthesized phase (I), heated and dried at 383K for 6h (II), after $CO_2$ has adsorbed into the sample (III), natural desorption from III (IV).

**Experimental Section:** All commercially available chemicals are of reagent grade and were used as received. The crystallinity and phase purity of the product were measured by the XRD patterns, which were collected using a Rigaku Mini Flex II diffractometer with Cu Kα radiation, operated at 30 kV and 15 mA. The scan range was from 5°to 40°(2 theta) at 4°/min. SEM images were obtained using a JEOS JSM-6700F microscope at 10 kV. The samples were coated with gold in order to increase their conductivity before scanning. The TGA was carried out with a heating rate of 5 K/min using a Netzsch STA-409-C balance. The sorption isotherms for $CO_2$ and $N_2$ were measured using an Intelligent Gravimetric Analyser (IGA001 series, Hiden Analytical Ltd). After pre-drying at a reduced pressure, the system was outgassed at 373 K overnight until no further weight losses were observed; the system temperature was then adjusted to the desired adsorption temperature, and the sample cell was kept under vacuum for 30 min before the first adsorption measurement was taken. Adsorption equilibrium data were collected after a stable pressure and weight had been maintained for 30 min at each point along the isotherm. All the isotherms for each of samples were obtained using a single sample.

All DFT calculations are performed using the Dmol[3] program available in Materials Studio 4.4 package[3,4]. The generalized gradient approximation (GGA) with Perdew-Wang 1991 (PW91) functional[5] is chosen together with the doubled numerical basis set plus D-functions basis sets (DND)[6]. The inner electrons of Cu atoms are kept frozen and replace by an effective core potential (ECP)[7,8], and other atoms are treated with an all electron basis set. The following thresholds are used for the geometry optimization: $2\times10^{-5}$ Hartree for the maximum energy change, $4\times10^{-3}$ Hartree for the maximum force, and $5\times10^{-3}$ Å for the maximum displacement.

## References

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