Electronic Supplementary Material (ESI) for RSC Advances.

A 2D metal-organic framework composed of bi-functional ligand with ultra-micropores for post-combustion CO_2 capture

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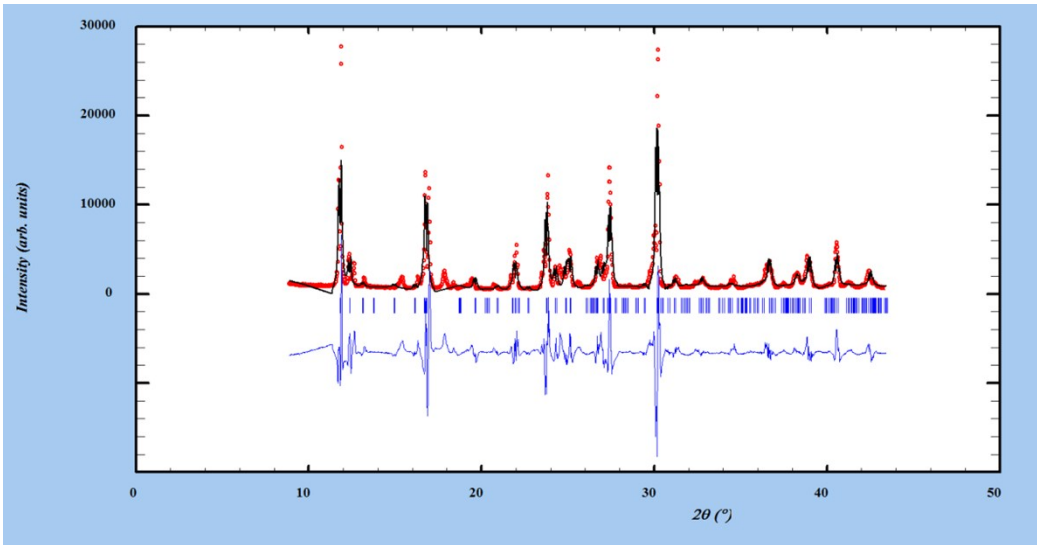

Figure S1 LeBail fitting for as-synthesized NUS-5

Monoclinic system, P 2(1)/n

a = 8.8226(1) Å, b = 10.5468(2) Å, c = 10.6916(2) Å,

α = 90.0° , β = 96.249(2), γ = 90.0°

Bragg R-factor: 3.60 Vol: 988.950(0.126) Å ^{3}

Rf-factor= 3.24

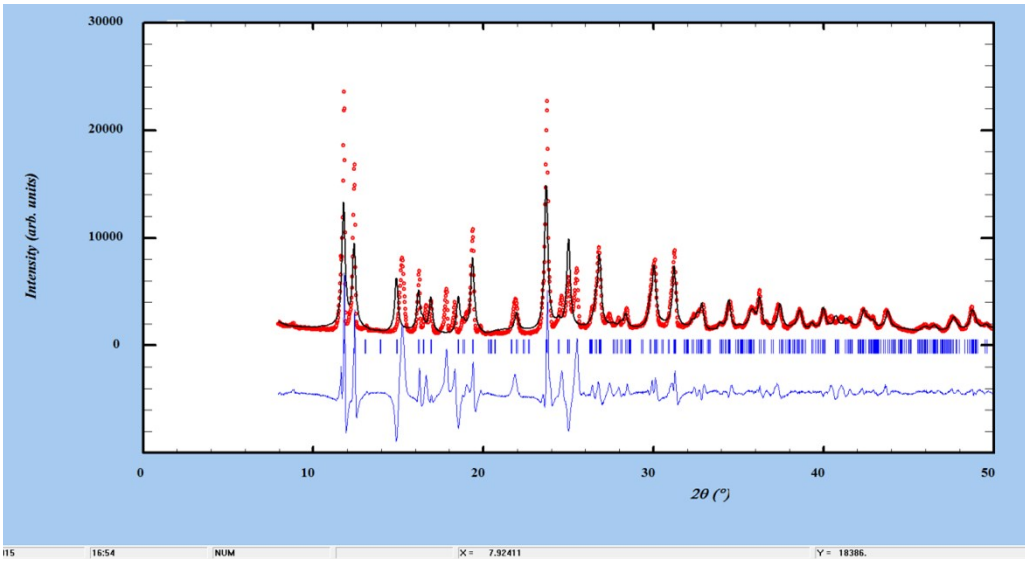

Figure S2 LeBail fitting for activated NUS-5

Monoclinic system, P 2(1)/n

a = 8.8000(3) Å, b = 10.7646(7) Å, c = 10.5532(6) Å,

α = 90.0° , β = 96.7364(5), γ = 90.0°

Bragg R-factor: 2.26 Vol: 992.784(0.340) $Å^3$

Rf-factor= 1.33

The LeBail refinements for the powder X-ray diffraction (PXRD) patterns of the as-synthesized and activated NUS-5 were conducted and the results are depicted in Figure S1 and Figure S2, respectively. There are some unidentified phases presented in the XRD patterns especially for the activated sample. This is likely due to the decomposition of the crystal upon water adsorption. The compound was found unstable in water. The high humidity of Singapore coupled with the inability to isolate the sample from the air in the PXRD measurement process makes it difficult to avoid water adsorption from the air. Nevertheless, the unidentified phase is only a small proportion in the as-synthesized sample. It is important to note here that the synthesized crystals were not exposed to the air during the activation and the gas measurement processes. Therefore, the results of gas adsorption reported here were primarily from the crystal itself.