Supporting Information

Synthesis and characterization of a SWCNT@HKUST-1 composite: Enhancing the CO_2 adsorption properties of HKUST-1

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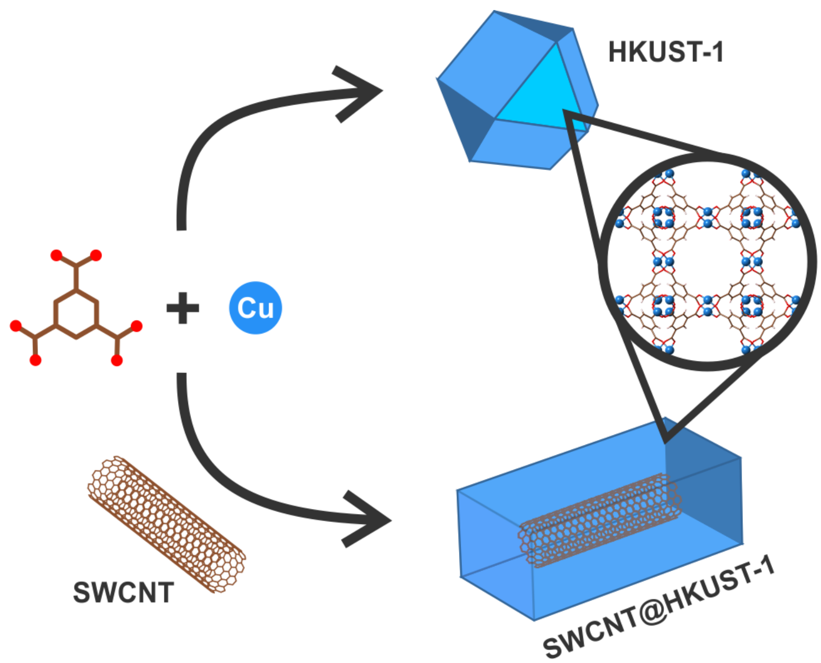

Scheme S1. Synthetic strategy for SWCNT@HKUST-1. HKUST-1 synthesis consists of the dropwise addition of a copper ethanolic solution into an aqueous solution of the deprotonated ligand, affording cuboctahedral crystals. When the SWCNT are added into the mixture, the SWCNT@HKUST-1 composite is obtained.

1. Thermogravimetric Analysis

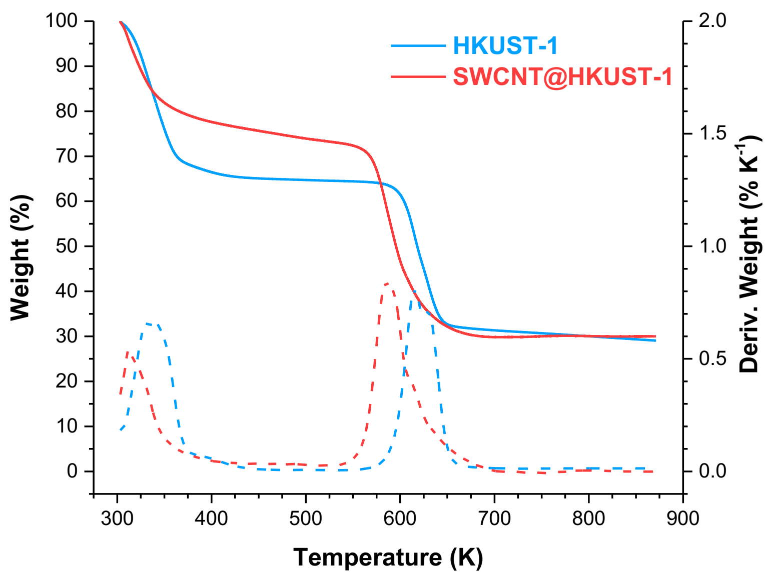

Figure S1. TGA trace for the HKUST-1 (blue) and SWCNT@HKUST-1 composite (red), dashed line represents the derivate of weight.

2. Powder X-Ray Diffraction

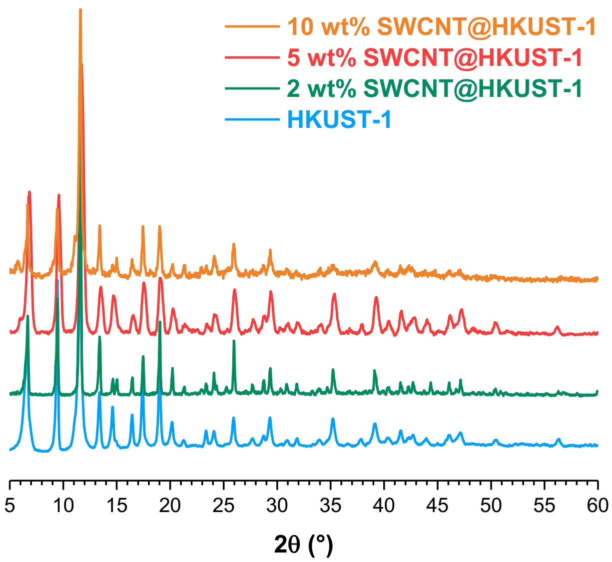

Figure S2. PXRD patterns of the HKUST-1 and SWCNT@HKUST-1 samples (2, 5 and 10 wt% of SWCNT).

3. Electron Microscopy

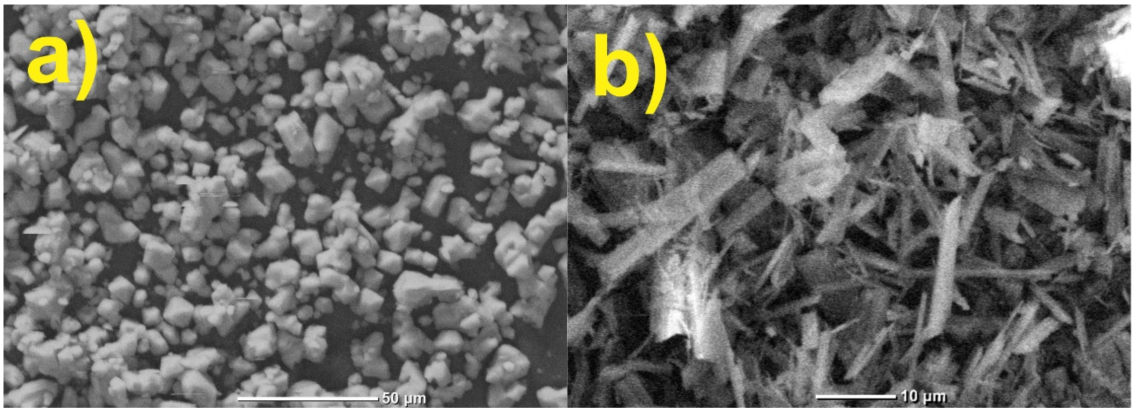

Figure S3. SEM micrographs of HKUST-1 a) and 5 wt% SWCNT@HKUST-1 b), featuring the rod-like crystals of the composite.

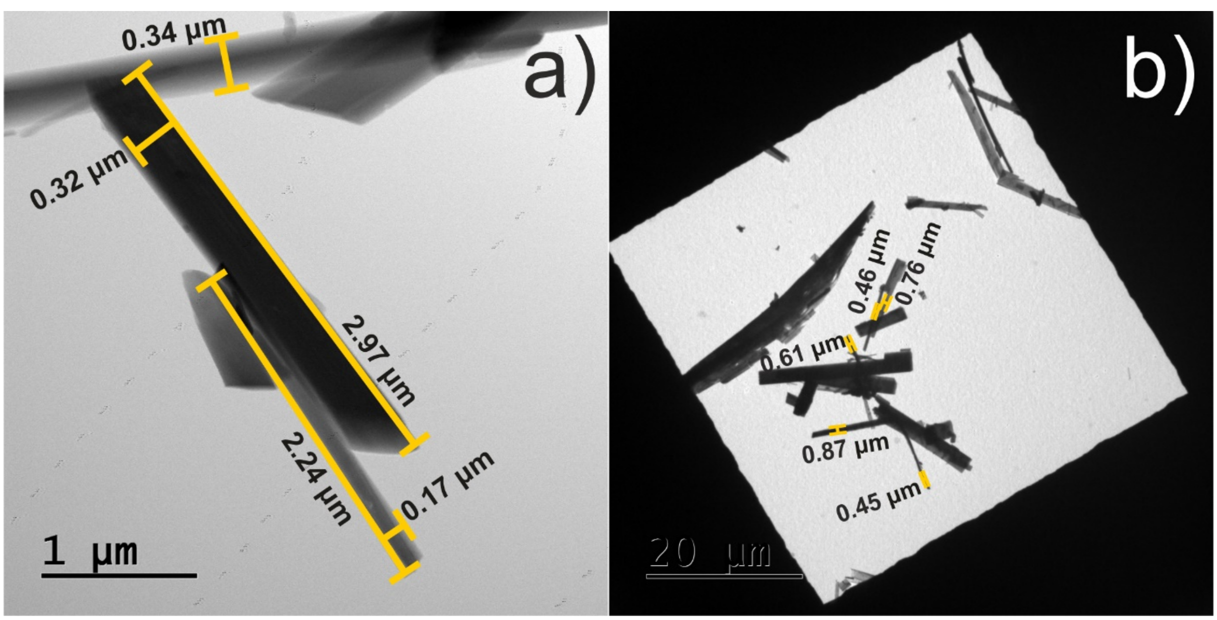

Figure S4. TEM micrographs of 5 wt% SWCNT@HKUST-1 a) rod-like crystals and b) conglomerate, marked length and width of the crystals.

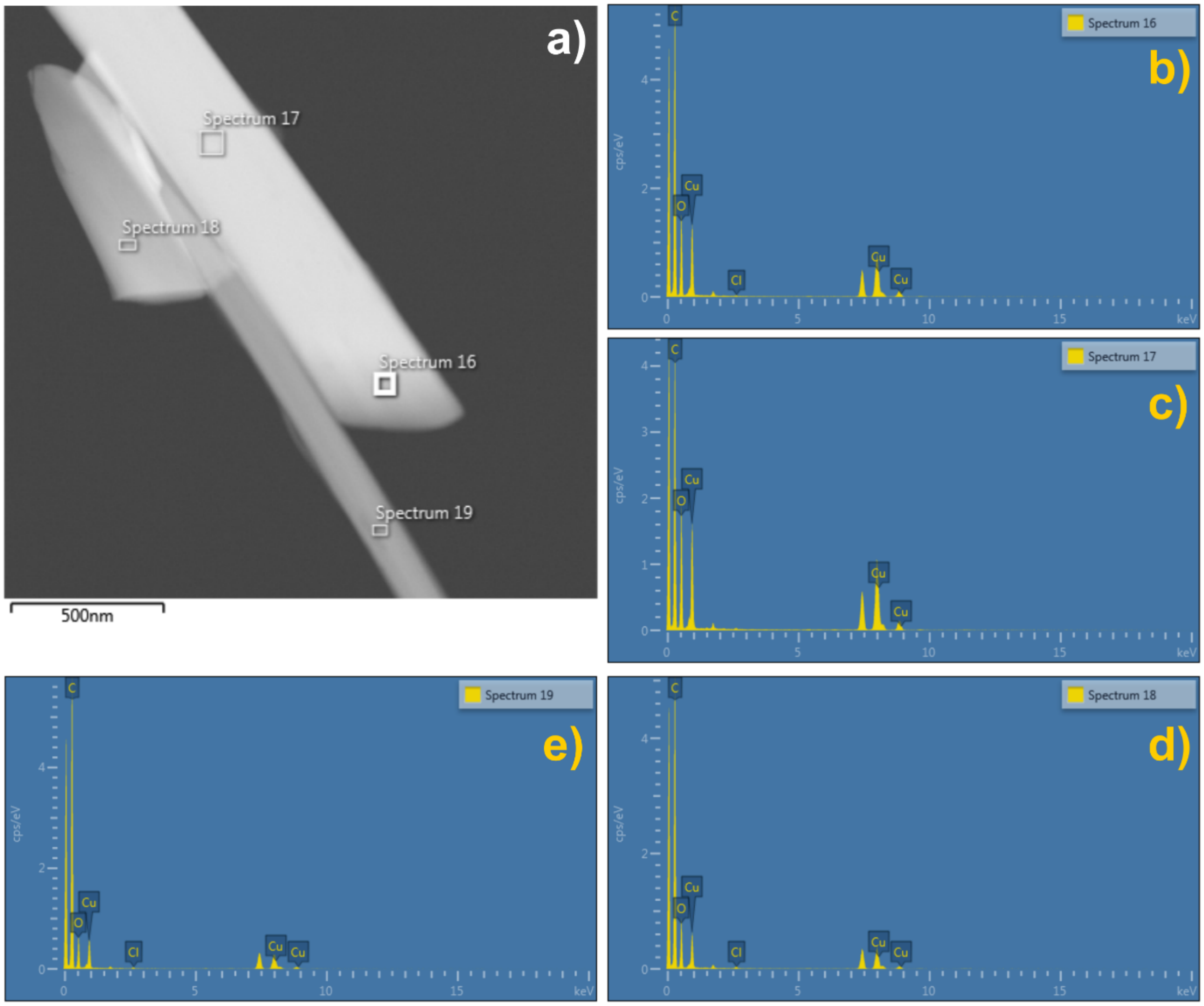

Figure S5. a) TEM micrograph of 5 wt% SWCNT@HKUST-1 b), c), d) and e) EDX spectra of different crystals of the composite.

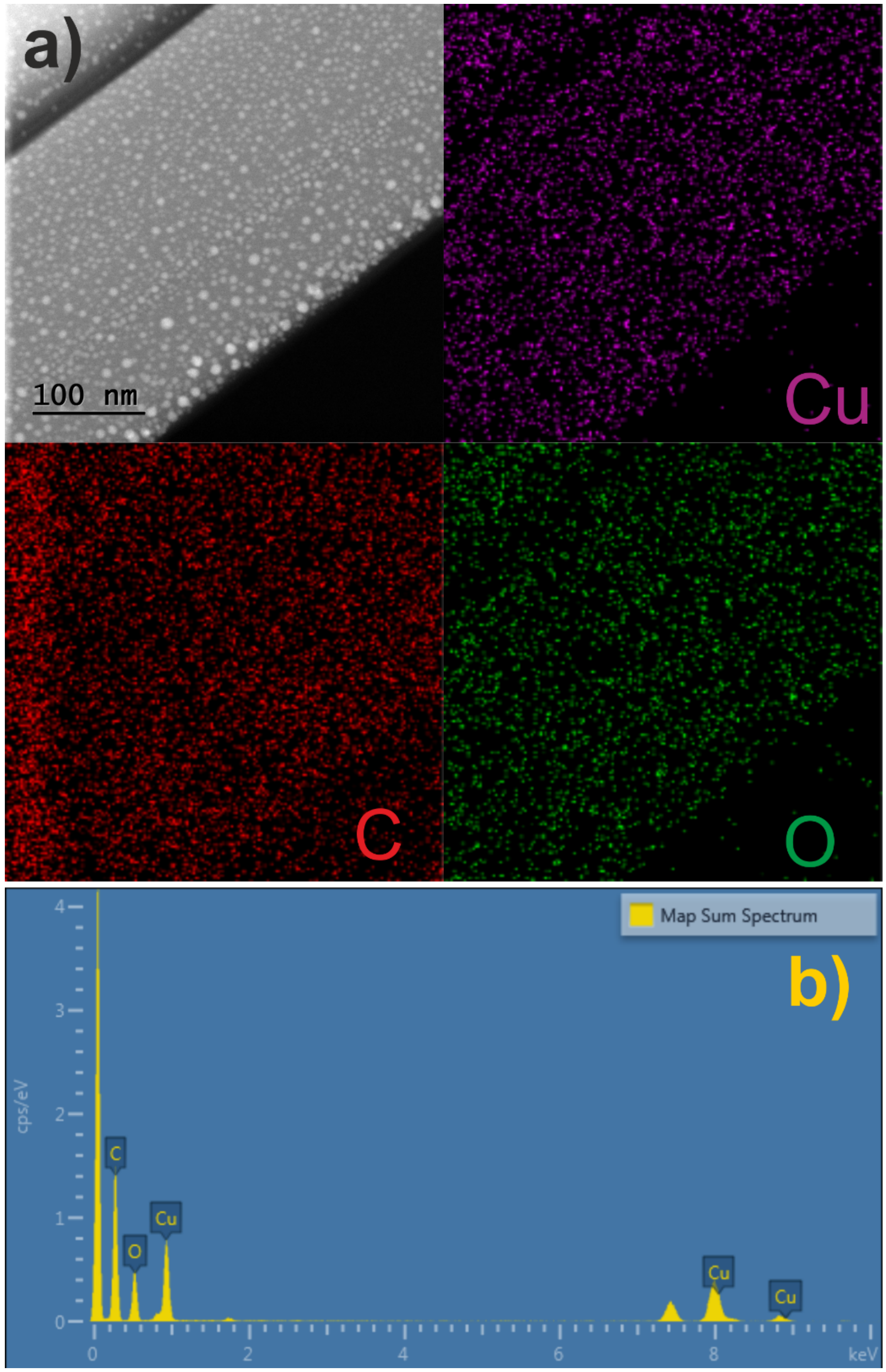

Figure S6. a) TEM micrograph of HKUST-1 with elemental mapping (purple: copper; red: carbon; green: oxygen), and b) EDX spectra.

4. RAMAN

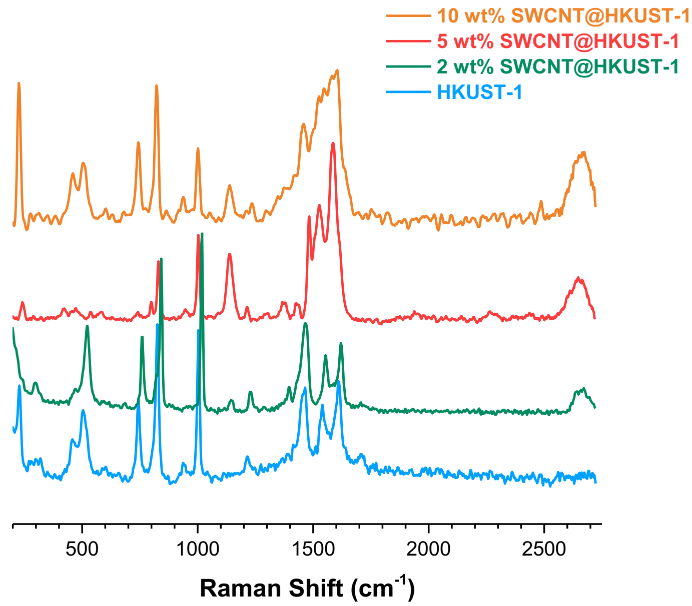

Figure S7. Raman spectra for HKUST-1 and the SWCNT@HKUST-1 composites with 2, 5 and 10 wt% of SWCNT.

5. Isosteric Heat of Adsorption

The CO_2 heat of adsorption, ΔH, was calculated by the isosteric method for the 5 wt% SWCT@HKUST-1 composite, using the CO_2 adsorption isotherms at 212 and 231 K (Figure S8, left). A virial-type equation was used to fit the adsorption isotherms:

$$ln\left(\frac{n}{p}\right) = A_0 + A_1 n + A_2 n^2 + \cdots \qquad \textbf{Equation S1}$$

where p is the pressure, n is the amount adsorbed and A_0, A_1, ... are the virial coefficients (A_2 and higher terms can be ignored at lower coverage values). A plot of $ln(n/p)$ versus n should give a straight line at low surface coverage (Figure S8, right).

Using the Clausius Clapeyron equation (Equation S2) for a fixed surface coverage (θ), the Equation S3 is obtained. By the substitution of p in Equation S3 with Equation S1, results an expression of the isosteric heat of adsorption (Equation S4). From the linear fittings, the virial coefficients are used to estimate the isosteric heat of adsorption.

$$\left(\frac{\partial ln(p)}{\partial T}\right)_\theta = \frac{Q_{ST}}{RT^2}$$ **Equation S2**

$$ln\left(\frac{p_1}{p_2}\right) = \frac{Q_{ST}}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)$$ **Equation S3**

$$Q_{ST} = R\left[\left(A_0^{T_2} - A_0^{T_1}\right) + \left(A_1^{T_2} - A_1^{T_1}\right)n\right]\left(\frac{T_1T_2}{T_1 - T_2}\right)$$ **Equation S4**

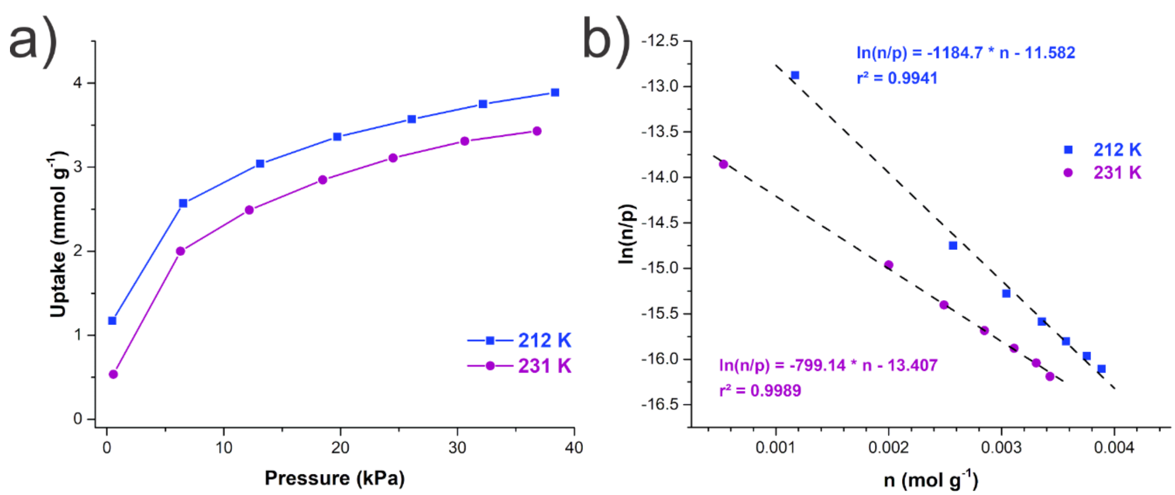

Figure S8. 5 wt% SWCNT@HKUST-1 a) CO_2 adsorption isotherms at 212 and 231 K, and b) virial plots for the CO_2 adsorption.