Supporting Information (SI)

High capacity gas storage by a microporous oxalamide-functionalized NbO-type metal-organic framework

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Figure S1. The BET plots for HNUST-3 in the chosen range ($P/P_0 = 0.0003 – 0.003$). This range was chosen according to two major criteria established in literatures: (1) The pressure range selected should have values of $Q(P_0-P)$ increasing with $P/P_0$. (2) The $y$ intercept of the linear region must be positive to yield a meaningful value of the $c$ parameter, which should be greater than zero. [(a) Walton, K. S. and Snurr, R. Q. J. Am. Chem. Soc., 2007, 129, 8552. (b) Rouquerol, J.; Llewellyn, P. and Rouquerol, F. Stud. Surf. Sci. Catal., 2007, 160, 49.]

Figure S2. TGA-DSC for as-synthesized samples of HNUST-3.
**Figure S3.** The low-pressure H\textsubscript{2} isotherms collected under 77 and 87 K for HNUST-3.

**Figure S4.** The low-pressure CO\textsubscript{2} sorption isotherms collected under 298 and 273 K for HNUST-3.
Figure S5. The CO₂, CH₄ and N₂ isosteric adsorption enthalpies for HNUST-3 calculated from the adsorption at 298 K and 273 K through Virial method.

Figure S6. The fitting initial slope for CO₂, CH₄ and N₂ isotherms for HNUST-3 collected at 298 K (N_ads = gases uptake; R = related coefficient). The calculated selectivity of CO₂/CH₄ and CO₂/N₂ is 7.9 and 26.1, respectively.
**Figure S7.** Details of virial equation (symbols) fitting to the experimental H₂ adsorption data (solid lines) for HNUST-3 collected at 77 K (red) and 87 K (blue).

**Figure S8.** Details of virial equation (symbols) fitting to the experimental CO₂ adsorption data (solid lines) for HNUST-3 collected at 273 K (red) and 298 K (blue).
**Figure S9.** Details of virial equation (symbols) fitting to the experimental CH\textsubscript{4} adsorption data (solid lines) for HNUST-3 collected at 273 K (red) and 298 K (blue).

**Figure S10.** Details of virial equation (symbols) fitting to the experimental N\textsubscript{2} adsorption data (solid lines) for HNUST-3 collected at 273 K (red) and 298 K (blue).
Figure S11. The reproducibility of the high-pressure CO\textsubscript{2} gas sorption properties for HNUST-3 collected at 273 K and 298 K.

Figure S12. The reproducibility of the high-pressure CH\textsubscript{4} gas sorption properties for HNUST-3 collected at 273 K and 298 K.
**Figure S13.** The reproducibility of the high-pressure excess H$_2$ gas sorption properties for HNUST-3 collected at 77 K.