Electronic Supplementary Information

A highly porous acylamide decorated MOF-505 analogue exhibiting large and selective CO_2 gas uptake capability

Baishu Zheng,*[a] Lu Huang,‡[a] Xiyang Cao,‡[a] Shaohua Shen,[a] Haifei Cao,[b] Cheng Hang,[c] Wenjiang Zeng[a] and Zhaoxu Wang*[a]

[a] *Key Laboratory of Theoretical Organic Chemistry and Function Molecule of Ministry of Education, Hunan Provincial Key Laboratory of Controllable Preparation and Functional Application of Fine Polymers, School of Chemistry and Chemical Engineering, Hunan University of Science and Technology, Xiangtan, 411201, China. E-mail: zbaishu@163.com (B. S. Zheng); hnust_chem@163.com (Z. X. Wang). Tel: +86 731 58290137.*

[b] *State Key Laboratory of Materials-Oriented Chemical Engineering, Nanjing Tech University, Nanjing, 210009, China*

[c] *State Key Laboratory of Coordination Chemistry, Nanjing University, Nanjing, 210023, China.*

‡ These authors contributed equally to this work.

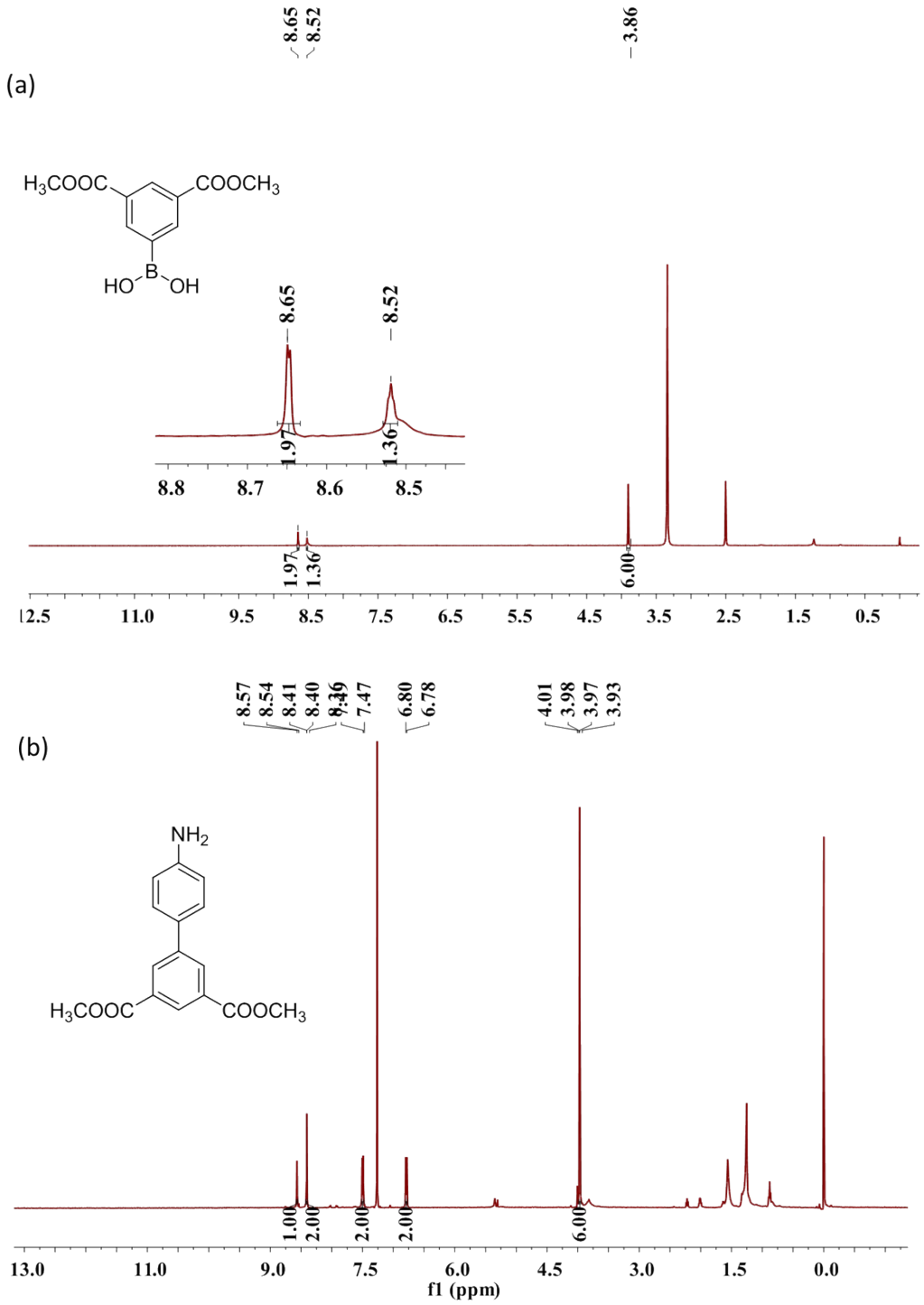

Fig. S1 ^{1}H NMR spectrum of 3,5-bis(methoxycarbonyl)phenyl)boronic acid in DMSO-d_6 (a) and Dimethyl 4'-amino-[1,1'-biphenyl]-3,5-dicarboxylate in $CDCl_3$ (b).

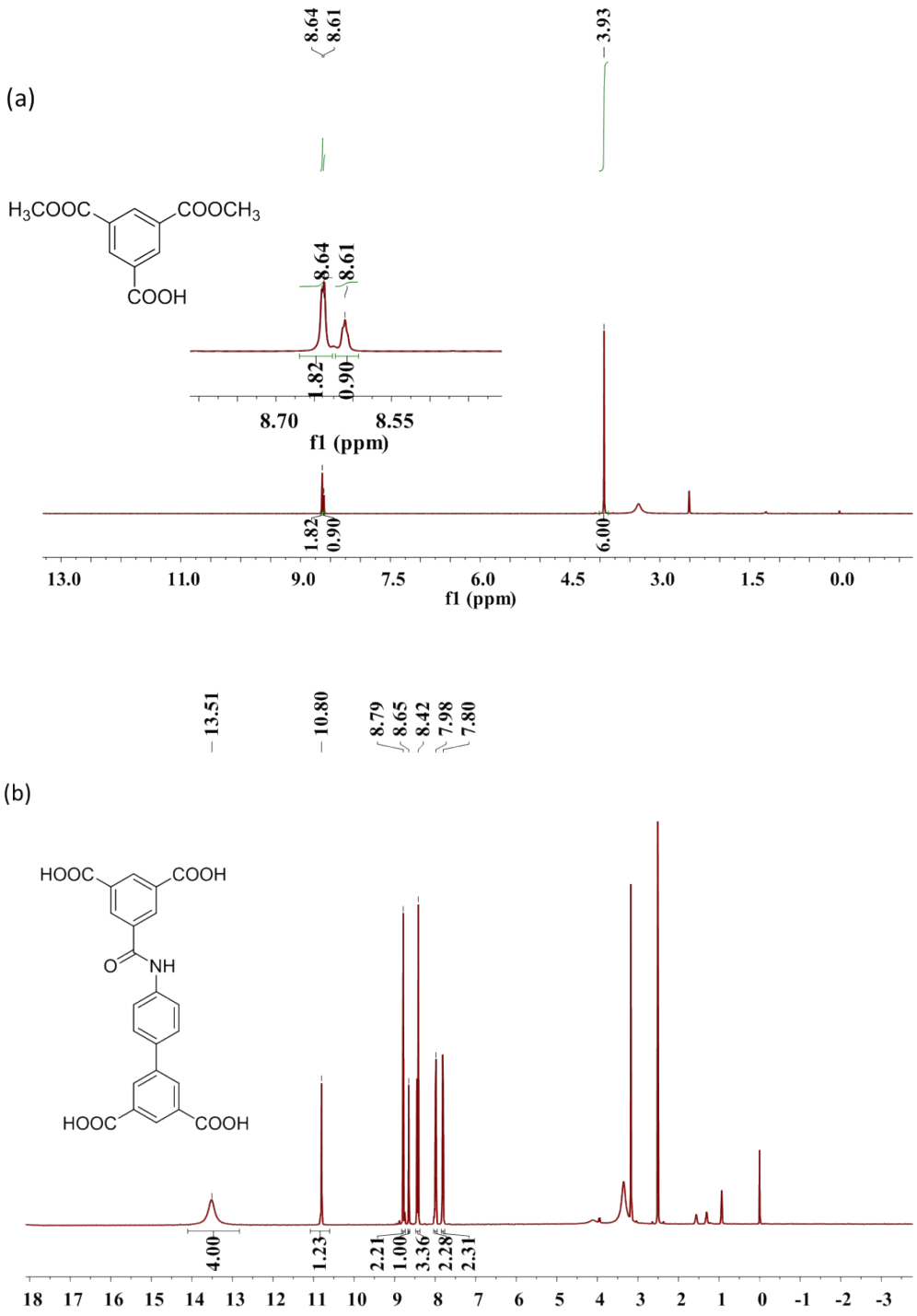

Fig. S2 ^{1}H NMR spectrum of 3,5-bis(methoxycarbonyl)benzoic acid in DMSO-d_6 (a) and 4'-(3,5-dicarboxybenzamido)-[1,1'-biphenyl]-3,5-dicarboxylic acid (H_4DBBD, H_4L) in DMSO-d_6 (b).

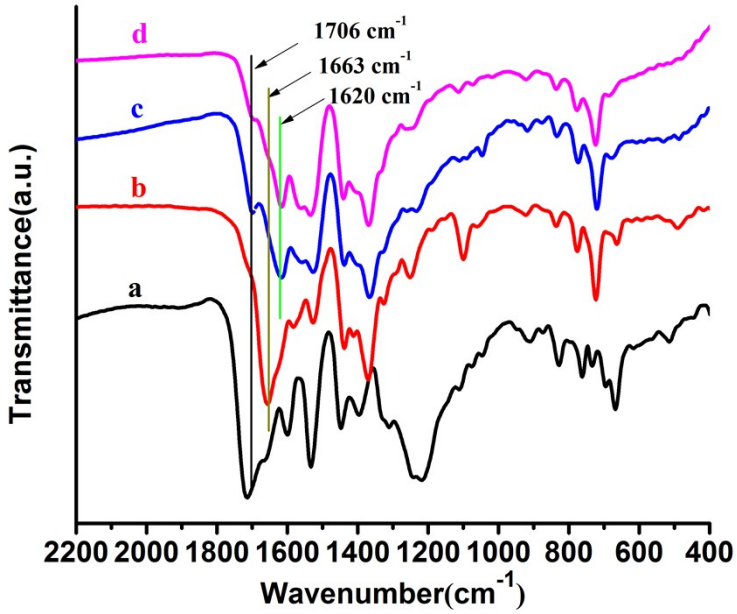

Fig. S3 The infrared spectra for **HNUST-7**: (a) ligand, (b) as-synthesized, (c) acetone-exchanged and (d) activated MOF materials. Note the absence of the vibration frequencies of the solvent DMF and acetone molecules in activated samples. The frequencies at 1663 cm^{-1} in (b) and 1706 cm^{-1} in (c) attribute to the v (CO) vibration of the DMF and acetone, respectively. The presence of the v (OH) stretching frequencies at 1620 cm^{-1} in both (c) and (d) may result from the rapid re-adsorption of trace moisture during the IR measurements.

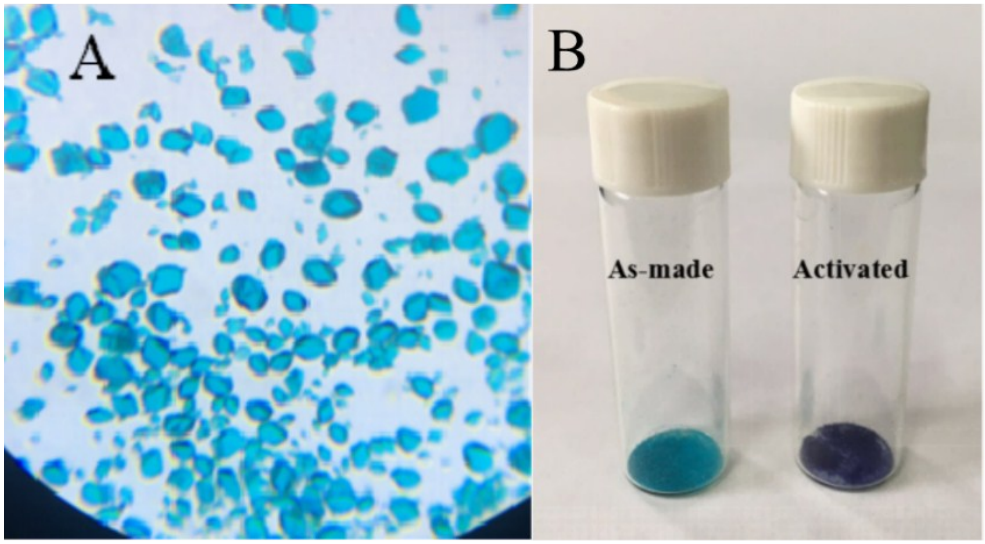

Fig. S4 Photographic image of as-synthesized **HNUST-7** (A, the crystal size has been magnified about 80 times), and visual color change of **HNUST-7** upon activation (B).

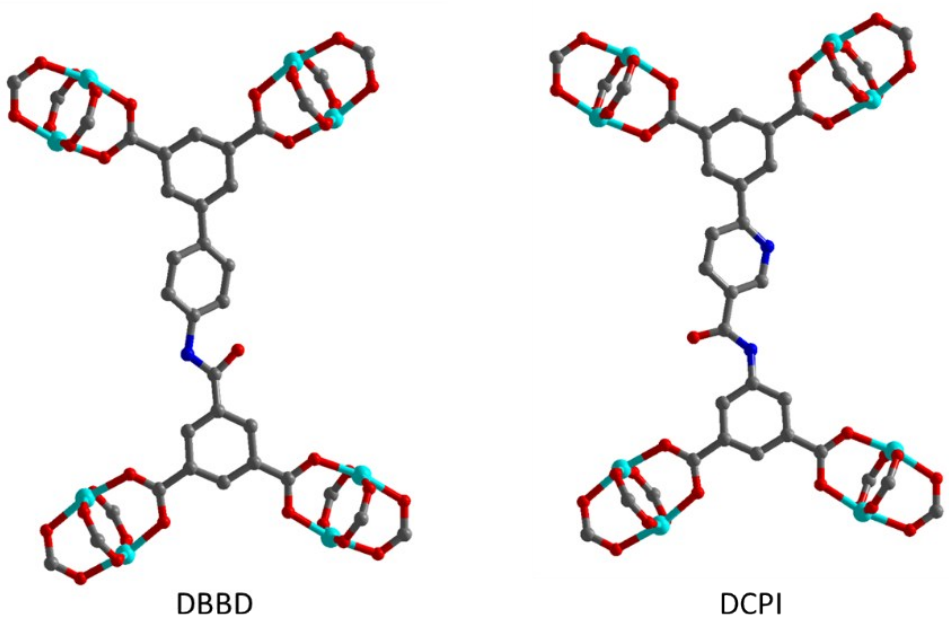

Fig. S5 The comparison of structural geometry, size and coordination motif between organic linker DBBD in **HNSUT-7** and DCPI in **NJU-Bai43**.

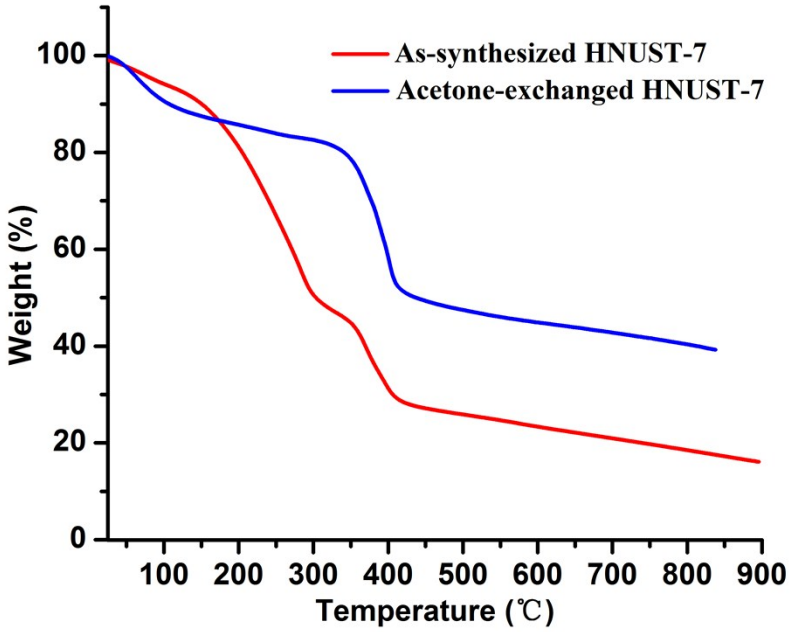

Fig. S6 TGA data of as-synthesized and acetone-exchanged **HNUST-7**.

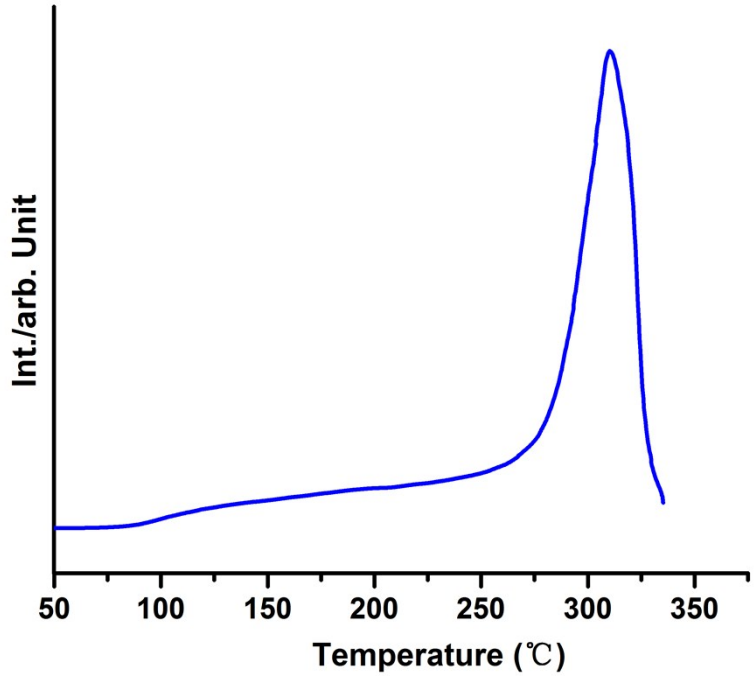

Fig. S7 NH_3-TPD profile of **HNUST-7**.

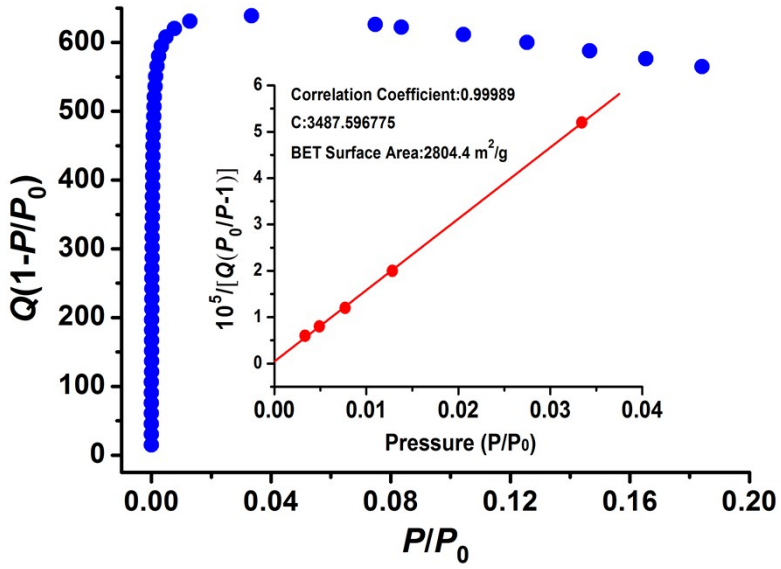

Fig. S8 The BET plots for **HNUST-7** in the chosen range (P/P_0 = 0.002 – 0.04). This range was chosen according to two major criteria established in literatures[1]: (1) The pressure range selected should have values of $Q(P_0\text{-}P)$ increasing with P/P_0. (2) The y intercept of the linear region must be positive to yield a meaningful value of the C parameter, which should be greater than zero.

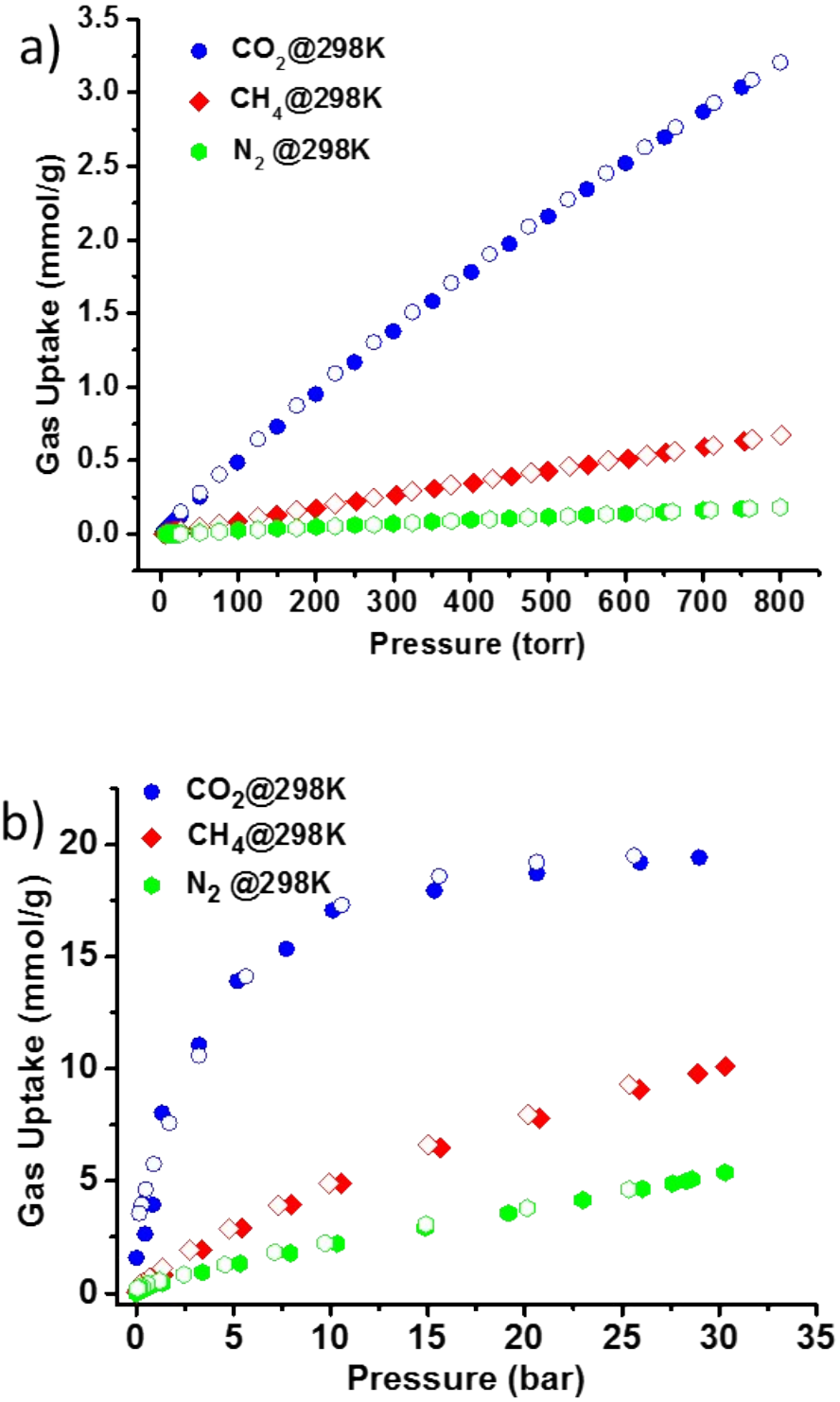

Fig. S9 Low- and high-pressure gas (CO_2, CH_4 and N_2) sorption isotherms of **HNUST-7** at 298 K (filled symbols, adsorption; open symbols, desorption).

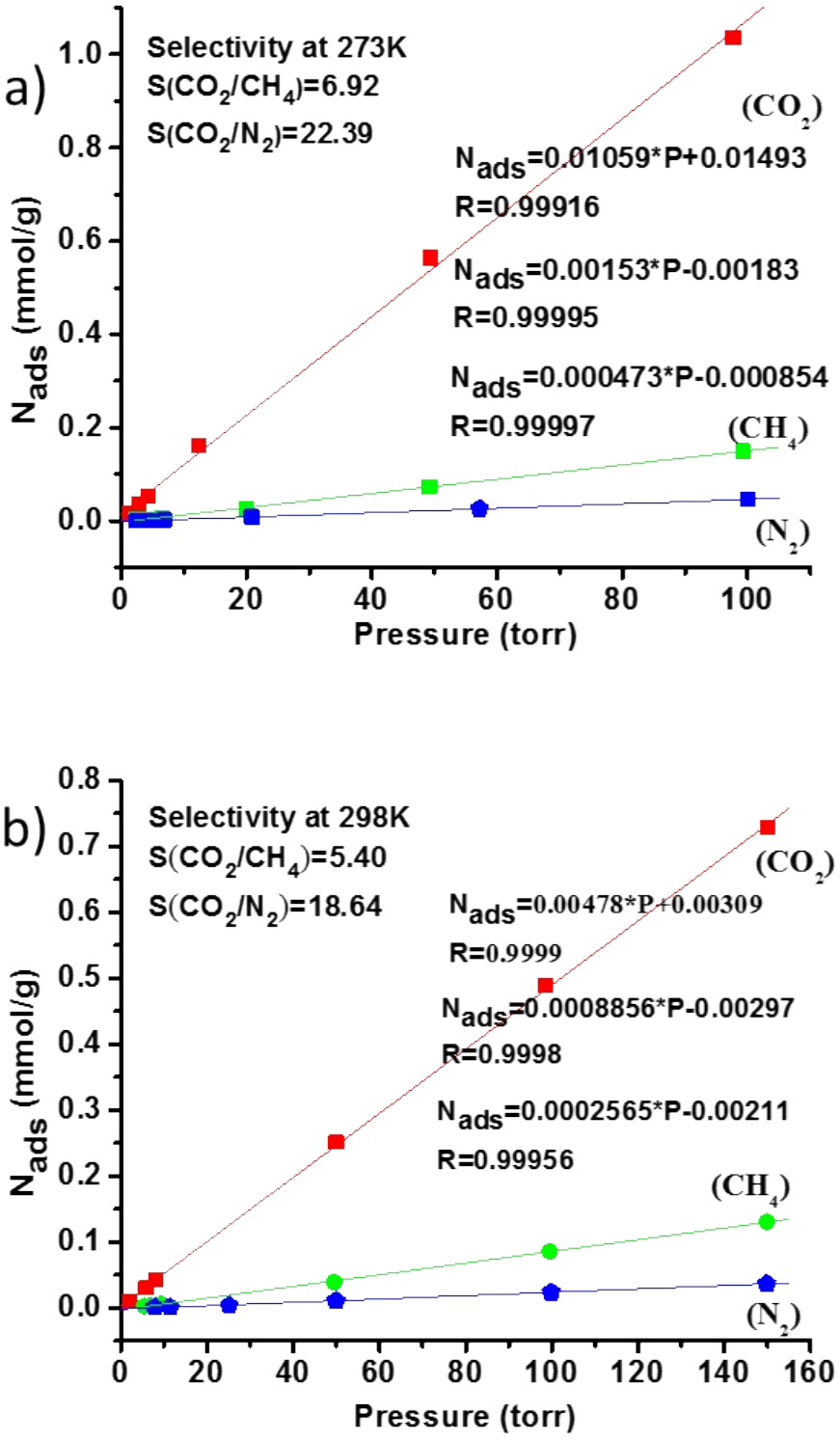

Fig. S10 The fitting initial slope for CO_2, CH_4 and N_2 isotherms for **HNUST-7** collected at 273 K and 298 K (N_{ads} = gases uptake; R = related coefficient).

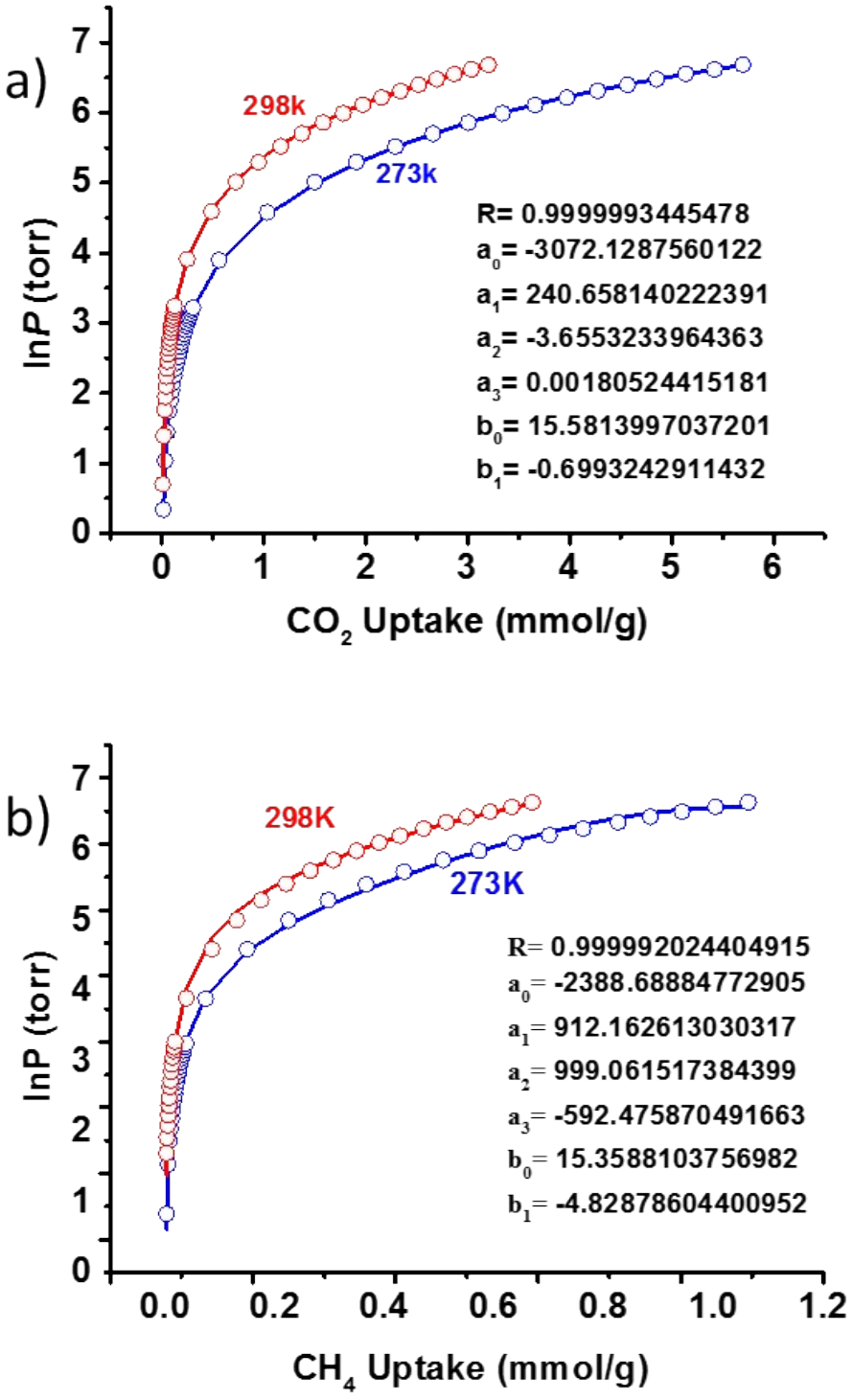

Fig. S11 Details of virial equation (symbols) fitting to the experimental CO_2 and CH_4 adsorption data (solid lines) for **HNUST-7** collected at 273 K (blue) and 298 K (red).

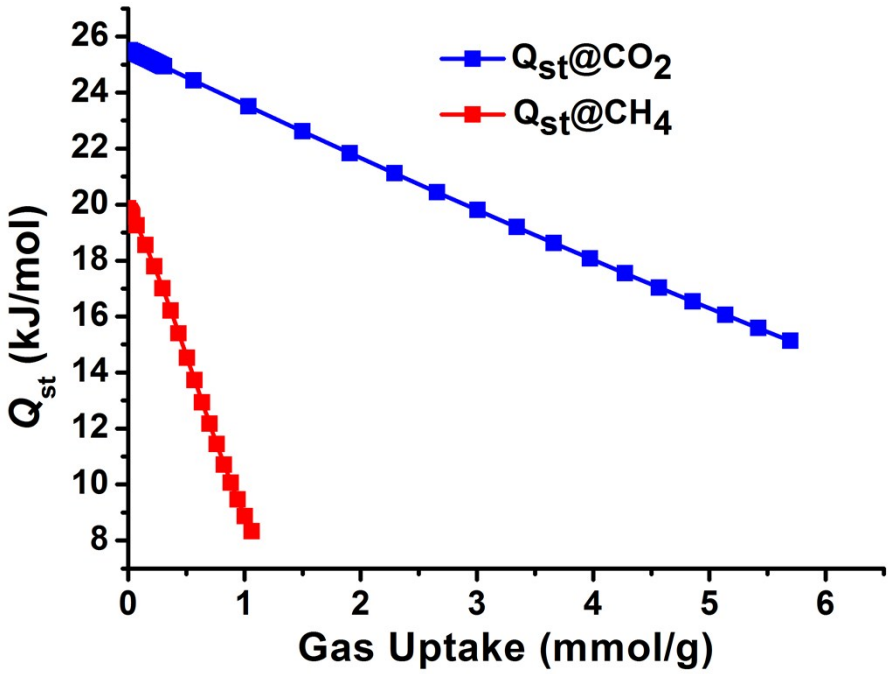

Fig. S12 The CO_2 and CH_4 isosteric adsorption enthalpies of **HNUST-7** calculated from the adsorptions at two different temperatures up to 1 bar (298 K and 273 K) through the Virial method.

Reference

[1]. (*a*) K. S. Walton and R. Q. Snurr, *J. Am. Chem. Soc.*, 2007, **129**, 8552; (*b*) J. Rouquerol, P. Llewellyn and F. Rouquerol, *Stud. Surf. Sci. Catal.*, 2007, **160**, 49.