Electronic Supporting Information

Hydrophobic functionalization of metal-organic framework as ammonia visual sensing material for high humidity

Yuxin Wang[a], Zhengxuan Song[a], Yutao Liu[a], Yang Chen[a], Jinping Li[a], Libo Li[a]*, Jia Yao[b]*

[a]College of Chemical Engineering and Technology, State Key Laboratory of Clean and Efficient Coal Utilization, Taiyuan University of Technology, Taiyuan 030024, China.

[b]Department of Gastroenterology, Shanxi Bethune Hospital, Shanxi Academy of Medical Sciences, Tongji Shanxi Hospital, Third Hospital of Shanxi Medical University, Taiyuan 030024, China

E-mail: lilibo@tyut.edu.cn; yaojia2006@163.com

Fig. S1 Digital images of static volumetric device.

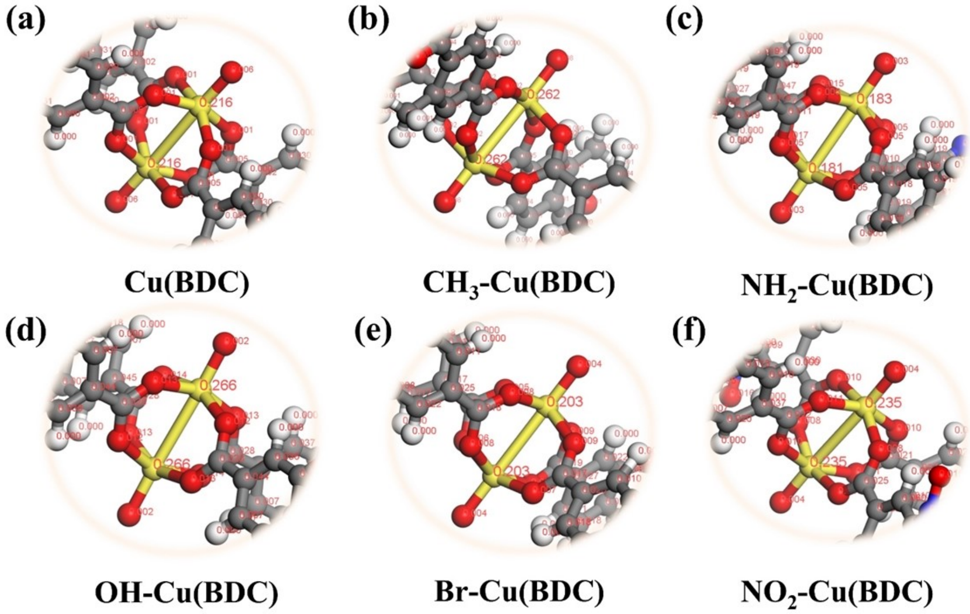

Fig. S2 Electrophilicity of Cu(BDC) and functionalized Cu(BDC).

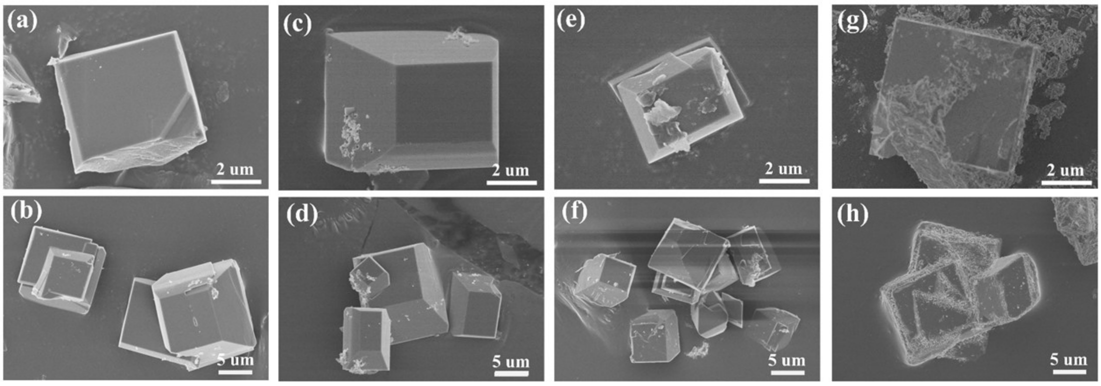

Fig. S3 SEM images of CH_3-Cu(BDC) (a-b), NH_3@CH_3-Cu(BDC) (c-d), activated CH_3-Cu(BDC) (e-f) and NH_3@CH_3-Cu(BDC) after 10 cycles (g-h).

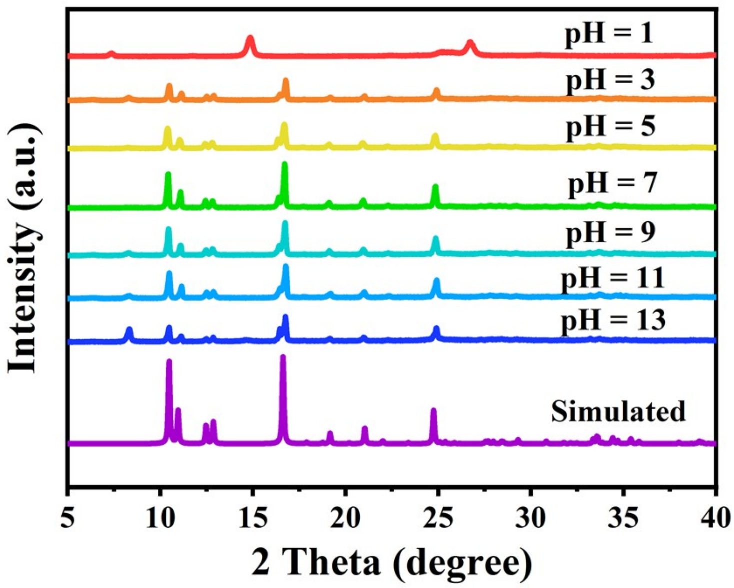

Fig. S4 PXRD profiles of CH_3-Cu(BDC) samples soaked in the aqueous solutions with pH = 1, 3, 5, 7, 9, 11, 13 solution for 24 h.

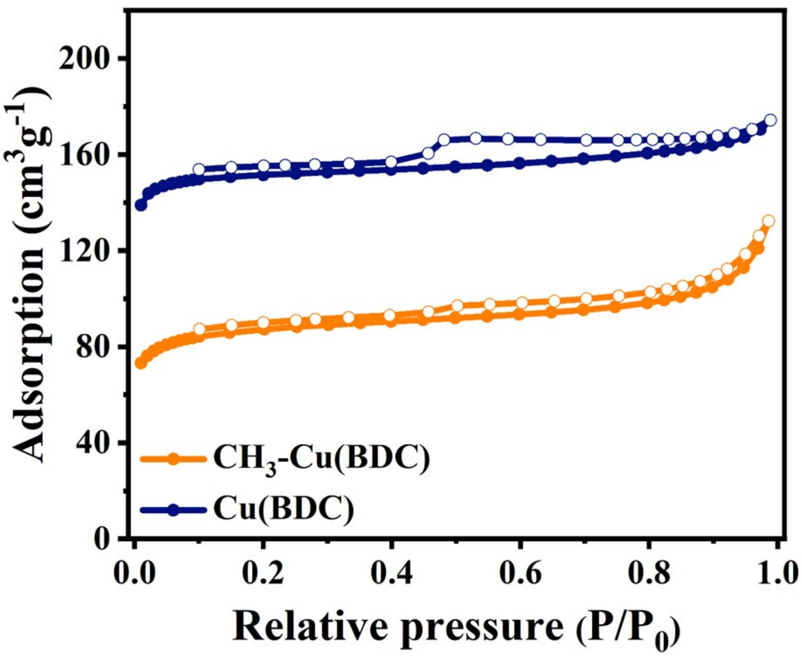

Fig. S5 N_2 sorption isotherms of CH_3-Cu(BDC) and Cu(BDC) at 77 K. The Brunauer-Emmett-Teller (BET) surface area was 339 m^2g^{-1}, there is decreased by 44% compared with Cu(BDC) (603 m^2g^{-1})

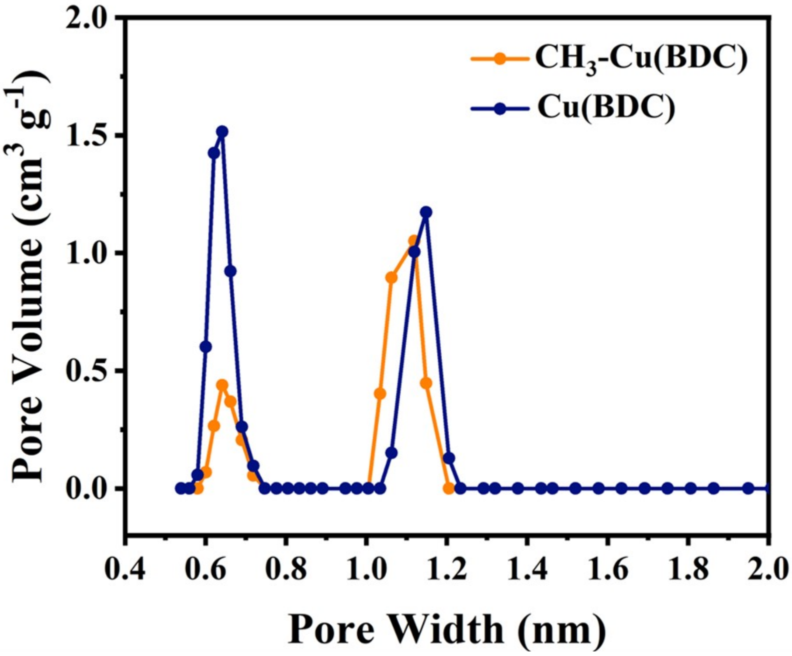

Fig. S6 The pore-size distribution of CH_3-Cu(BDC) and Cu(BDC).

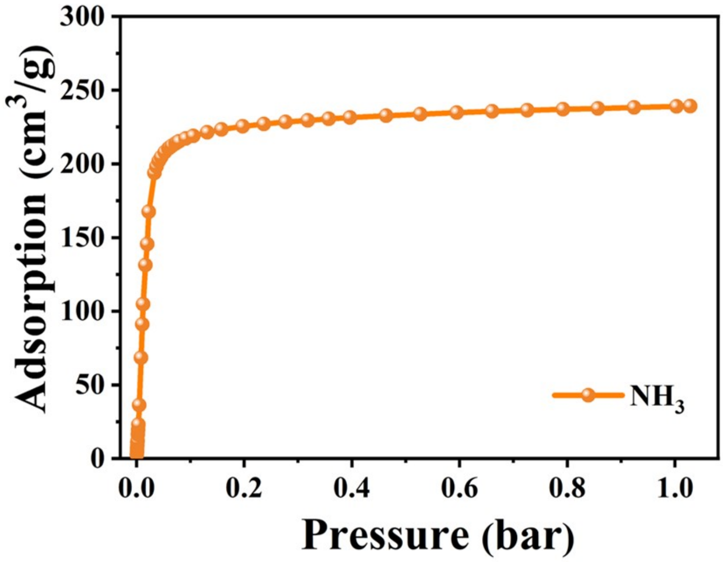

Fig. S7 Ammonia adsorption isotherm of CH_3-Cu(BDC).

Fig. S8 Digital images of CH_3-Cu(BDC) after exposed to 25, 50 and 75 ppm NH_3 for different times.

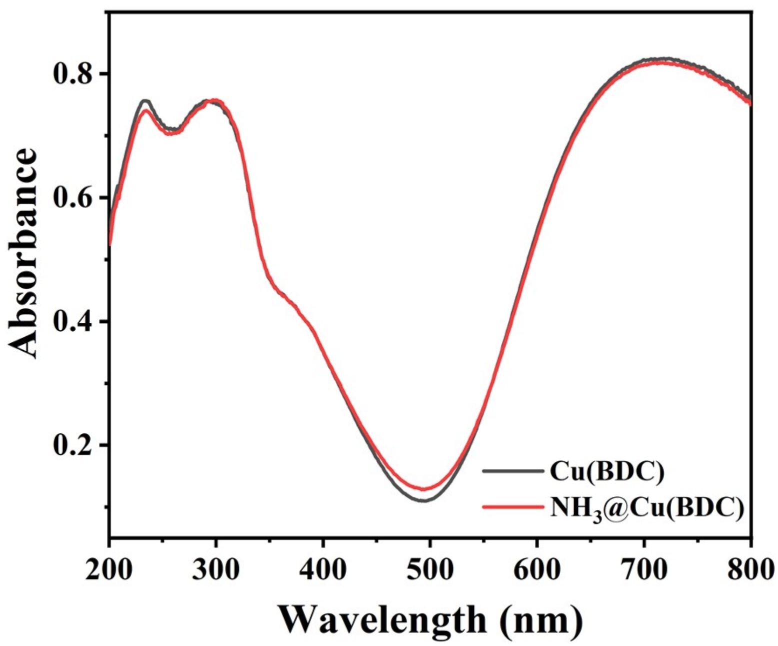

Fig. S9 UV-vis DRS of Cu(BDC) exposed to 50 ppm NH_3 for 25 min.

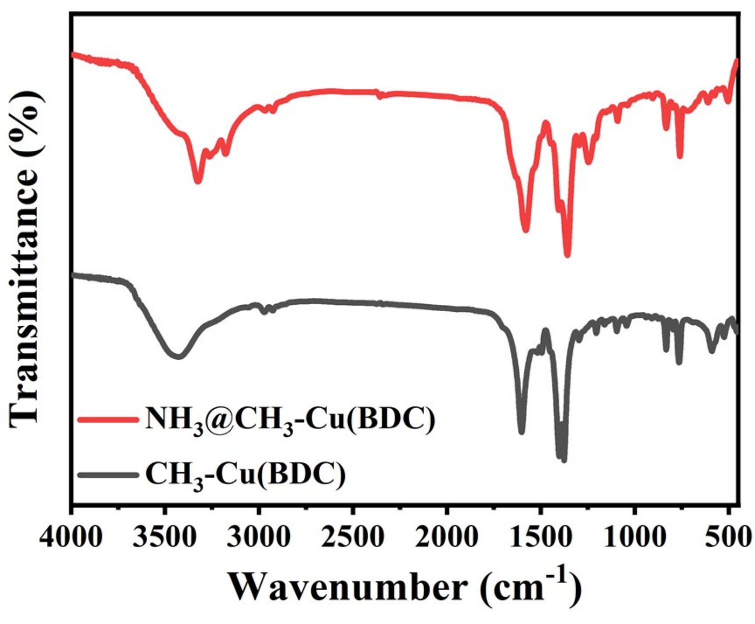

Fig. S10 FT-IR spectra of CH_3-Cu(BDC) and NH_3@CH_3-Cu(BDC).

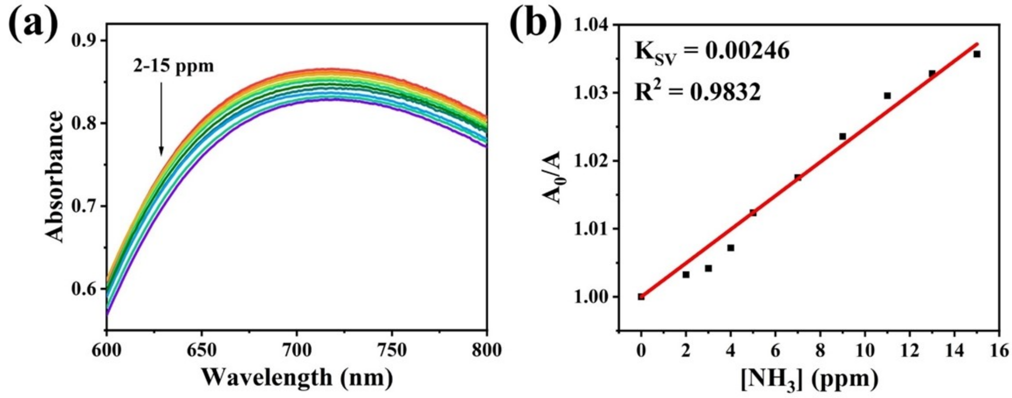

Fig. S11 (a) UV-Vis DRS of CH_3-Cu(BDC) after exposed to 2, 3, 4, 5, 7, 9, 11, 13 and 15 ppm ammonia. (b) Absorbance curve over ammonia levels.

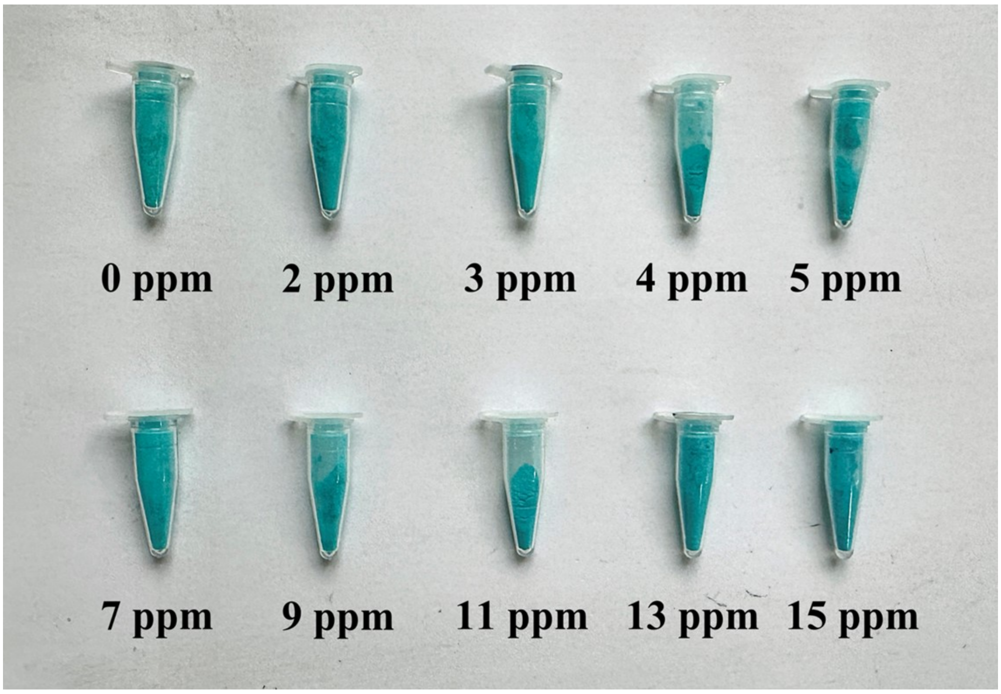

Fig. S12 Digital images of CH_3-Cu(BDC) after exposed to 2, 3, 4, 5, 7, 9, 11, 13 and 15 ppm ammonia.

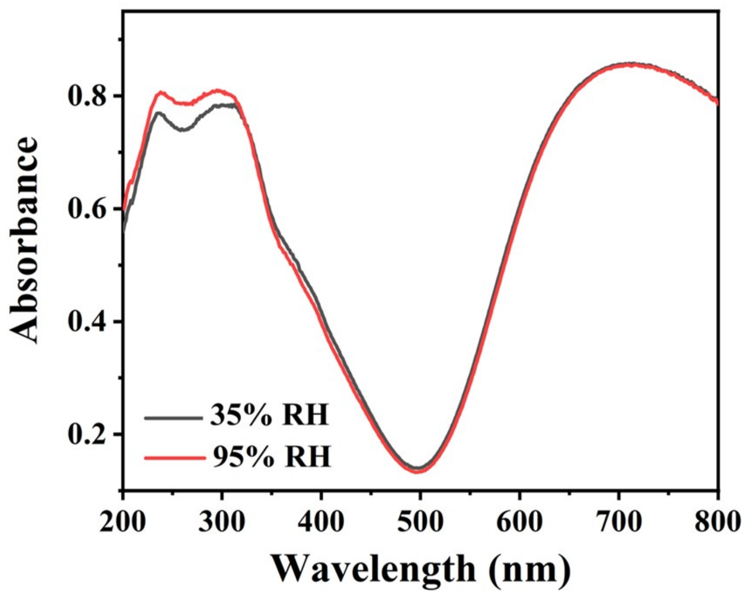

Fig. S13 UV-Vis DRS of CH_3-Cu(BDC) after exposed to different relative humidity.

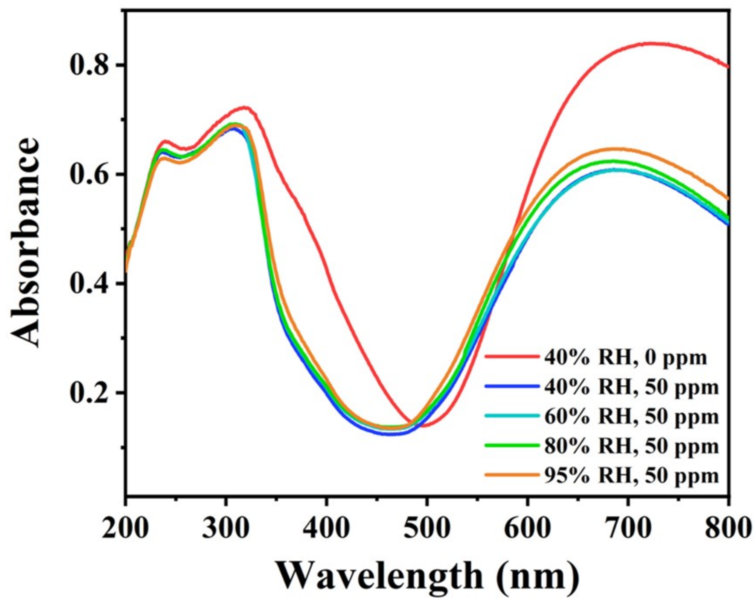

Fig. S14 UV-Vis DRS of CH_3-Cu(BDC) exposed to 50 ppm NH_3 with different relative humidity.

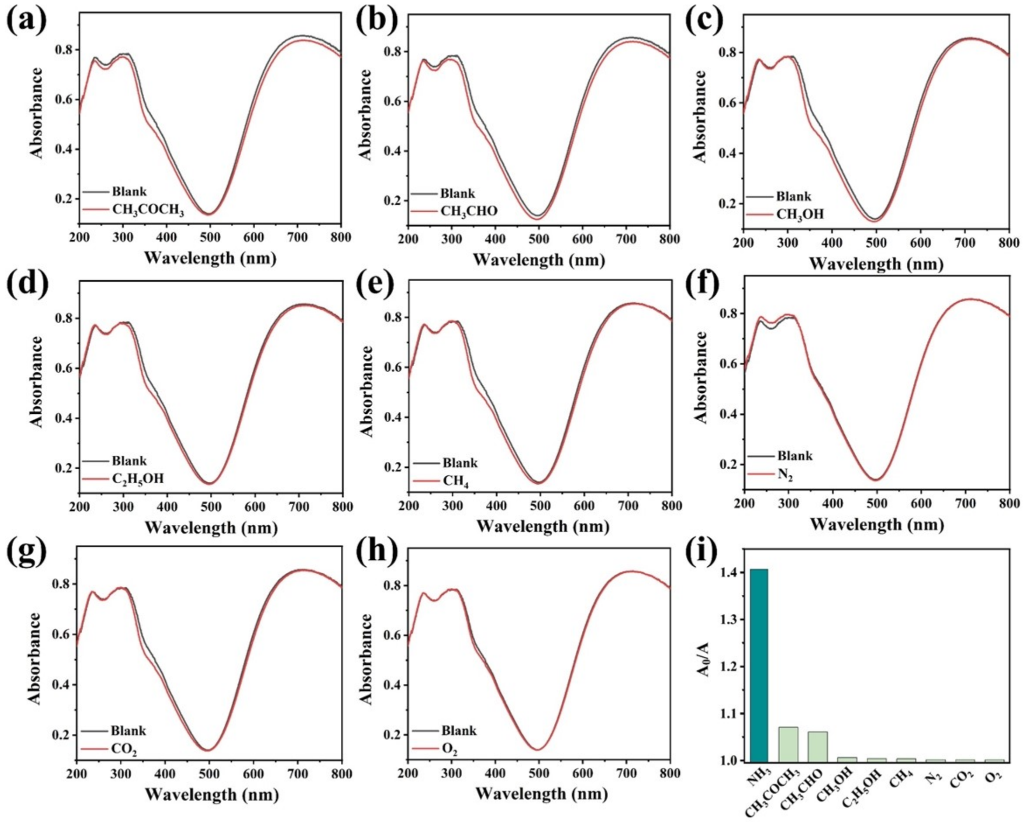

Fig. S15 Response of CH_3-Cu(BDC) against NH_3 and other exhaled air. The concentration of acetone, acetaldehyde, methanol and ethanol were 50 ppm, the rest of gases were high-purity.

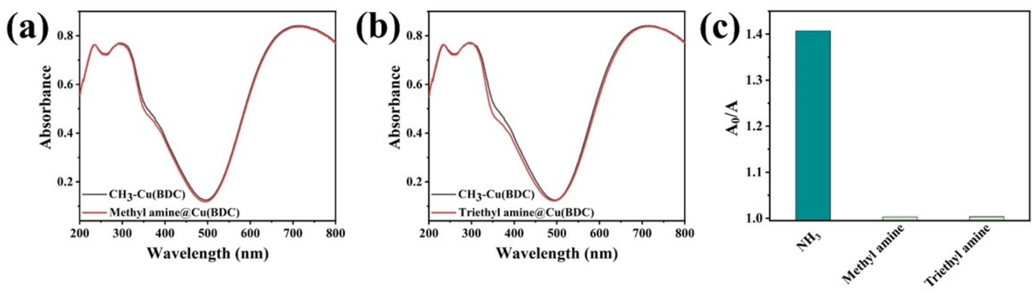

Fig. S16 (a-b) UV-Vis DRS of CH_3-Cu(BDC) exposed to 50 ppm methyl amine (a) and triethyl amine (b) atmosphere. (c) Response of CH_3-Cu(BDC) against NH_3 and bulkier amines.

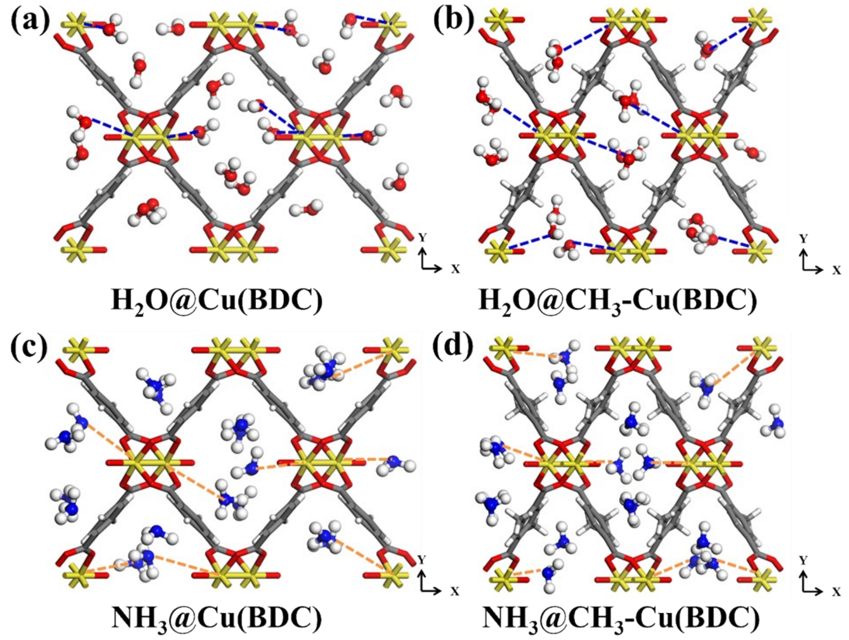

Fig. S17 GCMC simulations of H_2O and NH_3 adsorption sites in Cu(BDC) and CH_3-Cu(BDC).

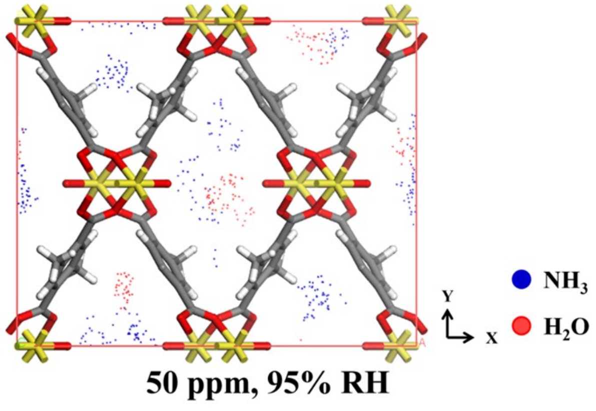

Fig. S18 GCMC simulations of the competitive adsorption between H_2O and NH_3 on CH_3-Cu(BDC) (50 ppm NH_3, 95 % RH).

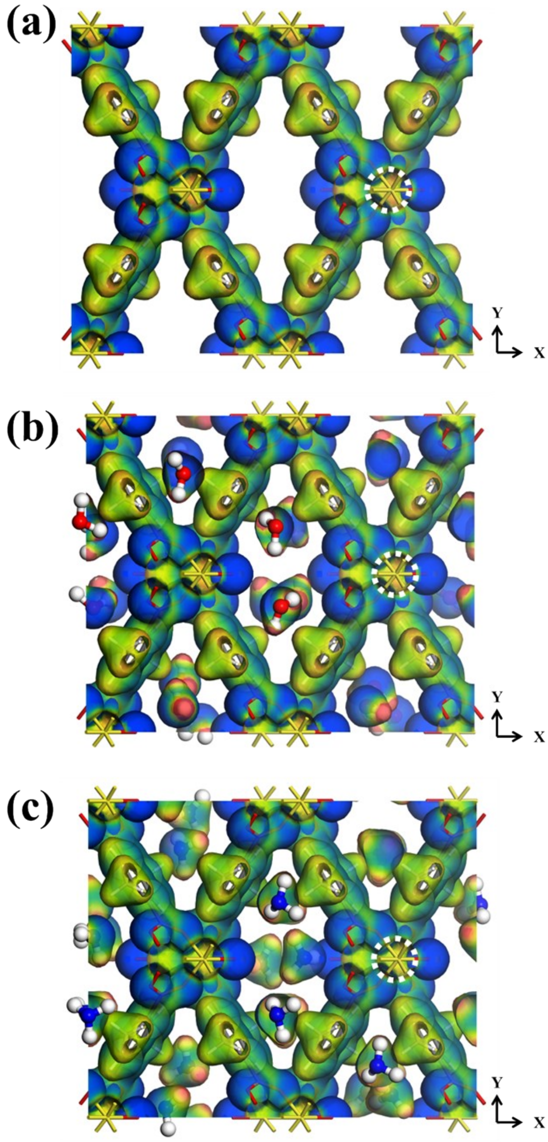

Fig. S19 Electrostatic potential patterns of (a) CH_3-Cu(BDC), (b) H_2O@CH_3-Cu(BDC) and NH_3@CH_3-Cu(BDC).

Items	Blood ammonia	Exhale ammonia	Abnormal
Reference value	10.0-47.0 umol L^{-1}	0.05-1.5 ppm	
Patient 1	48.3 umol L^{-1}	3.05 ppm	↑
Patient 2	50.0 umol L^{-1}	3.88 ppm	↑
Patient 3	50.1 umol L^{-1}	3.91 ppm	↑

Table S1 Compared of blood test and exhale test.

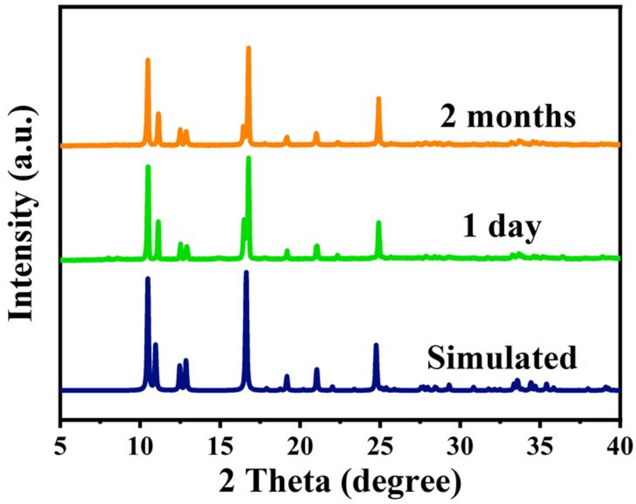

Fig. S20 PXRD patterns of CH_3-Cu-BTC for 1 day and 2 months in the atmospheric environment.

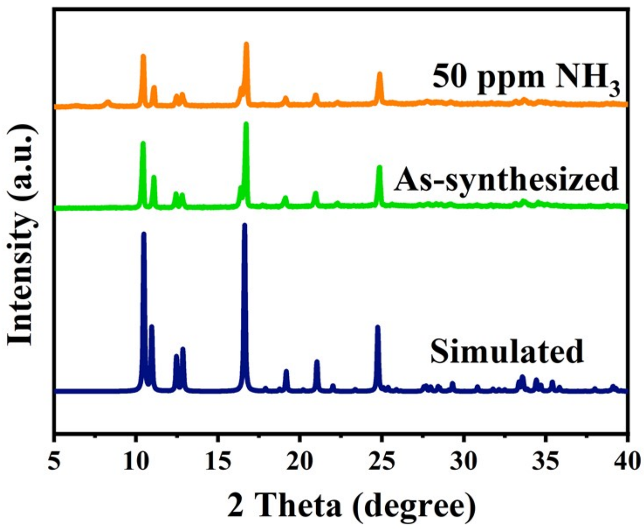

Fig. S21 PXRD patterns of CH_3-Cu-BTC and NH_3@CH_3-Cu(BDC).

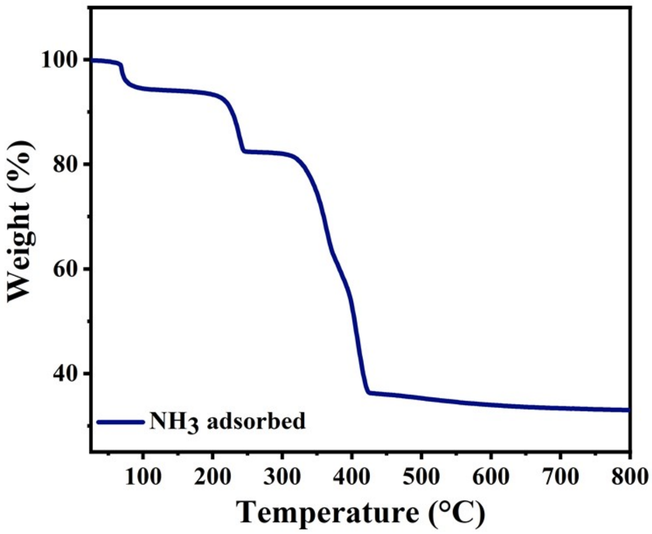

Fig. S22 TGA curves of $NH_3@CH_3$-Cu(BDC) under N_2 flow. The result show that the NH_3 in $NH_3@CH_3$-Cu(BDC) will be desorbed at 80 °C

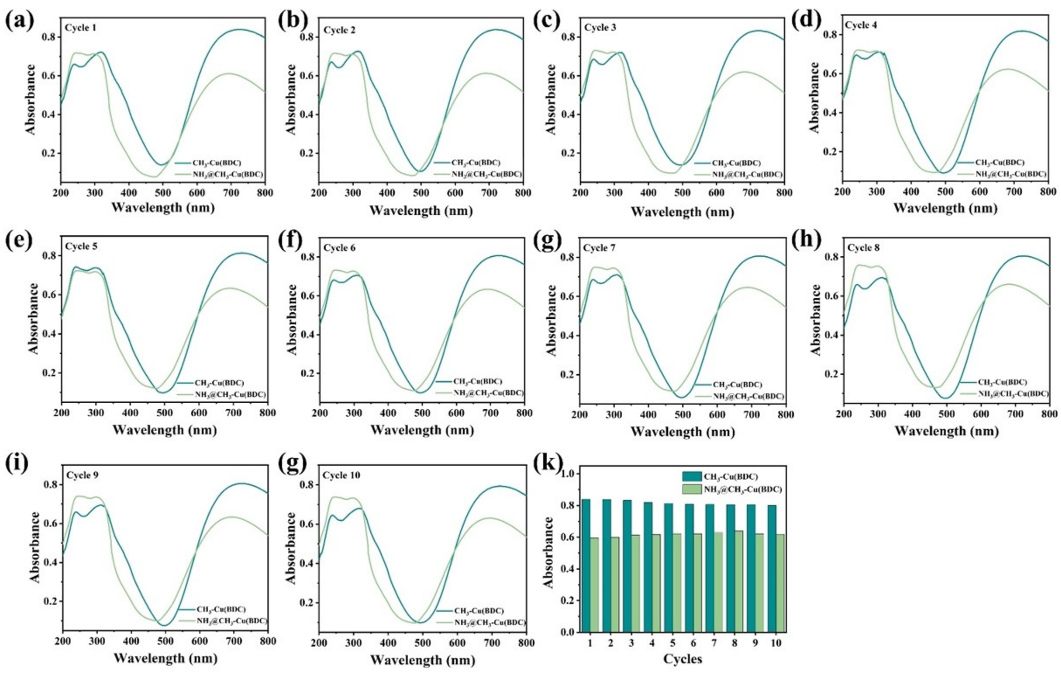

Fig. S23 Response to NH_3 (50 ppm) during 10 cycles of adsorption and desorption.