Supplementary Materials for

Synergistic binding sites in a hybrid ultramicroporous material for one-step ethylene purification from ternary C$_2$ hydrocarbon mixtures

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Table S1. EXAFS fitting parameters at the Cu K-edge for CuTiF<sub>6</sub>-TPPY samples
($\xi^2=0.75, 0.86$)

| Sample  | Shell  | $N^a$ | $R(\text{Å})^b$ | $\sigma^2 \times 10^3 (\text{Å}^2)$ | $\Delta E_0 (\text{eV})^d$ | $R$ factor |
|---------|--------|-------|-----------------|----------------------------------|-----------------|------------|
| Cu foil | Cu-Cu  | 12*   | 2.54±0.01       | 8.9±0.3                          | 4.5±0.5         | 0.002      |
|         | Cu-N   | 4.2±1.1| 1.95±0.02       | 4.4±2.4                          | 8.3±2.9         |            |
|         | Cu-C   | 4.3±1.4| 2.94±0.03       | 7.2±5.2                          | 7.0±4.4         | 0.009      |
| CuPc    | Cu-F   | 3.8±1.4| 1.91±0.01       | 2.8±0.8                          | 2.6±1.6         | 0.012      |
| CuF<sub>2</sub> | Cu-F | 3.8±1.4| 1.91±0.01       | 2.8±0.8                          | 2.6±1.6         | 0.012      |
| Cu1     | Cu-N   | 5.8±0.8| 1.97±0.01       | 4.5±1.3                          | -4.0±6.6        | 0.003      |
| Cu2     | Cu-N   | 4*    | 1.92±0.04       | 18.1±5.0                         | -5.6±10.5       | 0.017      |
|         | Cu-F   | 2*    | 1.92±0.04       | 2.2±1.0                          | -6.5±12.5       |            |

$^a$N: coordination numbers; $^b$R: bond distance; $^c\sigma^2$: Debye-Waller factors; $^d\Delta E_0$: the inner potential correction. $R$ factor: goodness of fit.

In EXAFS fitting, the adjacent coordination elements in the periodic table are difficult to be precisely distinguished, as well as the Cu-N and Cu-F paths. For this reason, Cu is firstly only considered as one M-N shell, and the obtained results showed that the coordination number is close to 6. On this basis, Cu-F was introduced to limit the coordination number, the result of Cu2 and expected Cu-N<sub>4</sub>F<sub>2</sub> was fitted. As shown in Table S1, the fitting parameters for the Cu-N<sub>4</sub>F<sub>2</sub> coordination environment are reasonable.
Fig. S1. The wavelet transform (WT) plots. The WT plots for (a) Cu foil, (b) CuPc, (c) CuF₂, and (d) CuTiF₆-TPPY.
**Structure simulation**

The structure model of CuTiF$_6$-TPPY was generated, based on the coordination mode by XAS data, using the Materials Studio suite of programs. The unit cell structures (e.g., cell parameters and atomic positions) of CuTiF$_6$-TPPY were calculated using the Forcite and Castep module. The Rietveld refinement, a software package for crystal determination from the XRD pattern, was performed to optimize the lattice parameters iteratively until the wRp value converges. The pseudo-Voigt profile function was used for whole profile fitting and Berrar–Baldinozzi function was used for asymmetry correction during the refinement processes. Line broadening from crystallite size and lattice strain were both considered.

![PXRD Rietveld refinement](image)

**Fig. S2. PXRD Rietveld refinement.** Rietveld refinement plot for CuTiF$_6$-TPPY.
Fig. S3. PXRD patterns. PXRD patterns of simulated, as-synthesized, and activated CuTiF$_6$-TPPY.

Fig. S4. PXRD patterns after treatments. PXRD patterns of CuTiF$_6$-TPPY after treatment in different solvents for one week.
Fig. S5. Sample synthesis with different Cu salts and their C$_2$H$_2$ adsorption isotherms. (a) XRD patterns and (b) C$_2$H$_2$ isotherms at 298 K of CuTiF$_6$-TPPY using different Cu salts.

Fig. S6. XPS wide survey. XPS wide spectra of CuTiF$_6$-TPPY.
**Table S2. Lattice parameters of the modeled structure of CuTiF$_6$TPPY.**

| Unit cell parameters | CuTiF$_6$TPPY |
|----------------------|---------------|
| Formula              | C$_{40}$H$_{26}$N$_8$F$_6$TiCu |
| Formula weight       | 843.42        |
| Crystal system       | Orthorhombic  |
| Space group          | P222          |
| a (Å)                | 13.85785      |
| b (Å)                | 13.78813      |
| c (Å)                | 8.23169       |
| α (°)                | 90            |
| β (°)                | 90            |
| γ (°)                | 90            |
| V (Å$^3$)            | 1572.86       |
| Z                    | 1             |
| D$_{calc}$ (g cm$^{-3}$) | 0.8912    |
| Rp $^a$              | 0.0213        |
| R$_{wp}$ $^b$        | 0.0326        |
| GOF                  | 1.06          |

$^a R_p = \frac{\sum |cY_{\text{Sim}}(2\theta) - I_{\text{exp}}(2\theta) + Y_{\text{back}}(2\theta))/|I_{\text{exp}}(2\theta)|.}$

$^b R_{wp} = \left\{ \frac{w_p[cY_{\text{Sim}}(2\theta) - I_{\text{exp}}(2\theta) + Y_{\text{back}}(2\theta)]^2/\sum w_p[I_{\text{exp}}(2\theta)]^2 \right\}^{1/2},$ and $w_p = 1/I_{\text{exp}}(2\theta).$

**Table S3. The elemental analysis for CuTiF$_6$-TPPY**

| CuTiF$_6$-TPPY | Cu  | Ti  | Si  | F   | C   | N   | H   |
|----------------|-----|-----|-----|-----|-----|-----|-----|
| Theoretical value | 7.64 | 5.73 | /   | 13.5 | 56.9 | 13.3 | 3.08 |
| ICP-OES (wt%)        | 9.07 | 7.06 | /   | /   | /   | /   | /   |
| Element analysis (wt%) | / | /   | /   | /   | /   | 53.9 | 11.3 | 3.95 |
| XPS                | 3.02 | 2.00 | /   | 8.61 | 73.59 | 12.78 | /   |
Table S4. Fractional atomic coordinates for the unit cell of CuTiF$_6$-TPPY (P222 model obtained from the Rietveld refinement, $R_p = 0.0213$ $R_{wp} = 0.0326$).

|   | a= 13.85785 | b = 13.78813 | c = 8.23169 |
|---|--------------|--------------|--------------|
|   | alpha = 90.000 | beta = 90.000 | gamma = 90.000 |
| C | 0.4511        | 0.8092       | 0.4986       |
| C | 0.4213        | 0.7081       | 0.5001       |
| C | 0.3239        | 0.6783       | 0.4991       |
| C | 0.2479        | 0.7541       | 0.4992       |
| C | 0.2417        | 0.8223       | 0.6270       |
| C | 0.1695        | 0.8921       | 0.6241       |
| N | 0.1040        | 0.8960       | 0.5005       |
| C | 0.1087        | 0.8309       | 0.3763       |
| C | 0.1794        | 0.7596       | 0.3721       |
| H | 0.4034        | 0.8716       | 0.4954       |
| H | 0.2924        | 0.8206       | 0.7299       |
| H | 0.1613        | 0.9450       | 0.7231       |
| H | 0.0556        | 0.8386       | 0.2777       |
| H | 0.1815        | 0.7092       | 0.2687       |
| F | -0.0963       | 0.9033       | 0.9998       |
| C | 0.1934        | 0.5496       | 0.5006       |
| C | 0.2914        | 0.5819       | 0.4989       |
| H | 0.1313        | 0.5971       | 0.5027       |
| N | 0.5000        | 0.6476       | 0.5000       |
| N | 0.3482        | 0.5000       | 0.5000       |
| H | 0.4223        | 0.5000       | 0.5000       |
| Cu | 0.0000       | 1.0000       | 0.5000       |
| Ti | 0.0000       | 1.0000       | 1.0000       |
| F | 0.0000       | 1.0000       | 0.7662       |
**Fig. S7. Crystal coordination mode.** The coordination mode of Cu, TiF$_6^{2-}$, and TPPY.

**Fig. S8. The interactions and rotations of TPPY.** (a) The hydrogen bond formed between TiF$_6^{2-}$ pillars and pyridine rings, (b) the rotation angle of pyridine rings in CuTiF$_6$-TPPY.
Fig. S9. Pore structures of CuTiF$_6$-TPPY. (a) 3D structures showing uniform one-dimensional channels and (b) the pore aperture sectional drawing in the $x, y$ plane of CuTiF$_6$-TPPY.

Fig. S10. Pore structures of SIFSIX-1-Cu. (a) 3D structures showing uniform one-dimensional channels and (b) the pore aperture sectional drawing in the $x, y$ plane of SIFSIX-1-Cu.
**Fig. S11. TGA curves.** TGA curve of the as-synthesized CuTiF₆-TPPY.

**Fig. S12. BET calculation plot.** BET calculation plot for CuTiF₆-TPPY based on its corresponding N₂ adsorption isotherm at 77 K.
Fig. S13. N$_2$ adsorption isotherms at 77 K. N$_2$ adsorption isotherms of CuTiF$_6$-TPPY at 77 K after treating in different conditions.
Isotherm fitting

The pure-component isotherms of $C_2H_2$, $C_2H_4$ and $C_2H_6$ were fitted using single-site Langmuir-Freundlich model for full range of pressure (0~1 bar).

$$q = q_{sat} \frac{bp^v}{1 + bp^v}$$

Here, $p$ is the pressure of the bulk gas at equilibrium with the adsorbed phase (bar), $q$ is the adsorbed amount per mass of adsorbent (mmol g$^{-1}$), $q_{sat}$ is the saturation capacities (mmol g$^{-1}$), $b$ is the affinity coefficient (bar$^{-1}$), and $v$ represent the deviation from an ideal homogeneous surface.

Table S5. Single-site Langmuir-Freundlich parameters of different gases on CuTiF$_6$-TPPY.

| Gas | T    | $q_{sat}$ | $b$   | $v$   |
|-----|------|-----------|-------|-------|
|     | K    | mol kg$^{-1}$ | bar$^{-1}$ | dimensionless |
| $C_2H_2$ | 273  | 4.63989 | 8.23274 | 0.70065 |
|       | 288  | 4.16236 | 9.63506 | 0.85908 |
|       | 298  | 3.98252 | 7.03971 | 0.85311 |
|       | 273  | 3.61553 | 5.28016 | 0.82235 |
| $C_2H_4$ | 288  | 3.43124 | 4.44434 | 0.92472 |
|       | 298  | 3.27381 | 2.73929 | 0.86244 |
|       | 273  | 4.06598 | 8.00487 | 0.7914  |
| $C_2H_6$ | 288  | 4.13356 | 4.05425 | 0.74243 |
|       | 298  | 3.58502 | 3.49011 | 0.77377 |
**Fig. S14.** C2 adsorption isotherms for CuTiF$_6$-TPPY at 273 and 288 K. The C$_2$H$_2$, C$_2$H$_4$, and C$_2$H$_6$ adsorption isotherms on CuTiF$_6$-TPPY at (a) 273 K and (b) 288 K.

**Fig. S15.** C2 adsorption isotherms and IAST plot for SIFSIX-1-Cu. (a) C$_2$H$_2$, C$_2$H$_4$, and C$_2$H$_6$ adsorption isotherms on SIFSIX-1-Cu at 298 K, and (b) IAST selectivity of SIFSIX-1-Cu at different binary mixture compositions at 298 K.
Fig. S16. Breakthrough curves for SIFSIX-1-Cu. The breakthrough curve of (a) C_2H_2/C_2H_6/C_2H_4 (1/9/90, v/v/v) and (b) C_2H_6/C_2H_4 (10/90, v/v) for SIFSIX-1-Cu (0.8 g) with a flow rate of 2.5 mL/min at 298 K.

Fig. S17. The Langmuir-Freundlich fittings of C2 isotherms. The corresponding Langmuir-Freundlich fittings of C_2H_2, C_2H_4, and C_2H_6 adsorption isotherms on CuTiF_6-TPPY at different temperatures.
IAST calculations

The selectivity of the preferential adsorption of component 1 over component 2 in a mixture containing 1 and 2 can be formally defined as:

\[ S = \frac{x_1 / y_1}{x_2 / y_2} \]

In the above equation, \( x_1 \) and \( y_1 \) (\( x_2 \) and \( y_2 \)) are the molar fractions of component 1 (component 2) in the adsorbed and bulk phases, respectively. We calculated the values of \( x_1 \) and \( x_2 \) using the Ideal Adsorbed Solution Theory (IAST) of Myers and Prausnitz.

Fig. S18. IAST selectivity plots. IAST selectivity of CuTiF\(_6\)-TPPY at different binary mixture compositions and temperatures.
Isosteric heat of adsorption

The isosteric heat of C$_2$H$_2$, C$_2$H$_4$, and C$_2$H$_6$ adsorption, $Q_{st}$, defined as

$$Q_{st} = RT^2 \left( \frac{\partial \ln P}{\partial T} \right)_q$$

determined using the pure component isotherm fits using the Clausius-Clapeyron equation. Where $Q_{st}$ (kJ/mol) is the isosteric heat of adsorption, $T$ (K) is the temperature, $P$ (bar) is the pressure, $R$ is the gas constant, and $q$ (mmol/g) is the adsorbed amount.

![Graph showing isosteric adsorption heats](image)

**Fig. S19.** C2 adsorption heats. C$_2$H$_2$, C$_2$H$_4$, and C$_2$H$_6$ isosteric adsorption heats on CuTiF$_6$-TPPY.
**Fig. S20. Breakthrough apparatus.** Representation of the column breakthrough experiment.

**Fig. S21. Breakthrough curve for CuTiF₆-TPPP.** The breakthrough curve of C₂H₂/C₂H₆/C₂H₄ (1/9/90, v/v/v) for CuTiF₆-TPPP with the flow rates of 5.0 mL/min at 298 K.
Fig. S22. Breakthrough curve for CuTiF$_6$-TPPY. The breakthrough curve of C$_2$H$_6$/C$_2$H$_4$ (50/50, v/v) for CuTiF$_6$-TPPY at the flow rate of 8.0 mL/min at 298 K.

Fig. S23. Desorption curves for CuTiF$_6$-TPPY. The signals of desorbed C$_2$H$_6$ and C$_2$H$_4$ for CuTiF$_6$-TPPY (1.8 g) during the regeneration process under a He flow rate of 20 mL/min at 298 K.
Fig. S24. Desorption curves for CuTiF₆-TPPY. The signals of desorbed C₂H₆ and C₂H₄ during the regeneration process from the adsorption column of CuTiF₆-TPPY (1.3 g).

Fig. S25. Adsorption and desorption kinetics of C₂H₄ and C₂H₆. (a) Time-dependent gas uptake profiles of CuTiF₆-TPPY at pressures up to 1000 mbar with a raising rate of 100 mbar min⁻¹ and kept for 60 min to reach full adsorption equilibriums and (b) desorption rate profiles for C₂H₄ and C₂H₆ on CuTiF₆-TPPY (from 100 to 0 mbar) at 298 K.
**Fig. S26. Distribution density and binding sites for $\text{C}_2\text{H}_4$.** (a) Computational simulations for the density distribution of $\text{C}_2\text{H}_4$ on CuTiF$_6$-TPPY at 100 kPa and 298 K, (b) (c) $\text{C}_2\text{H}_4$ binding sites in CuTiF$_6$-TPPY. The closest contacts between framework atoms and the gas molecules are defined by the distances (in Å) and the distances include the van der Waals radius. (Framework: C, grey-80%; H, white; N, blue; F, cyan; Cu, pink; Ti, silvery, Gas: C, orange; H, white).

**Fig. S27. C2 distribution densities.** Computational simulations for the distribution density of (a) $\text{C}_2\text{H}_2$, (b) $\text{C}_2\text{H}_6$, and (c) $\text{C}_2\text{H}_4$ on CuTiF$_6$-TPPY at 100 kPa and 298 K.
**Fig. S28. In-situ IR spectrum.** In-situ IR spectrum of activated CuTiF$_6$-TPPY sample exposed to C$_2$H$_2$, C$_2$H$_4$, or C$_2$H$_6$.

The three characteristic bands of $\nu$(−CH), $\beta$-(CH), and δ(−CH) for C$_2$ gases were detected, indicating the adsorption of all C$_2$ gases in CuTiF$_6$-TPPY. The interactions between C$_2$ gases and TiF$_6^{2−}$ anion in CuTiF$_6$-TPPY cannot be directly characterized by IR spectroscopy because the vibrations of TiF$_6^{2−}$ occur below 650 cm$^{-1}$ that beyond the detection range of the infrared MCT-A detector. Nevertheless, some evidence for the interactions between gas molecules and TiF$_6^{2−}$ anions were observed, because TiF$_6^{2−}$ anions have strong electronegativity and can form strong hydrogen bonding with C$_2$ hydrocarbons.

As for C$_2$H$_2$ adsorption, the stretching band $\nu$(−CH) of adsorbed C$_2$H$_2$ appeared at a lower frequency of ~2950 cm$^{-1}$ besides the frequency at ~3260 cm$^{-1}$, which was induced by the formation of hydrogen bonding between C$_2$H$_2$ and TiF$_6^{2−}$ anions. The asymmetrical C≡C stretching band appears at a lower frequency of ~1950 cm$^{-1}$ rather than 2100~2140 cm$^{-1}$ also confirmed the formation of hydrogen bonding between C$_2$H$_2$ and TiF$_6^{2−}$ anions (56). For C$_2$H$_6$ adsorption, the stretching band $\nu$(−CH) of adsorbed C$_2$H$_6$ appeared at the lower frequency of 2800~3075 cm$^{-1}$ implies the interactions between C$_2$H$_6$ and TiF$_6^{2−}$ anions. The stretching bands of $\beta$-(CH) and δ(−CH) of adsorbed C$_2$H$_6$ were detected without frequency shifts, indicating that C$_2$H$_6$ also interacted with the aromatic skeleton of CuTiF$_6$-TPPY. As for C$_2$H$_4$, the δ(−CH) bending vibration bands appeared at ~1010 cm$^{-1}$ and ~950 cm$^{-1}$ belong to the absorption of...
peak of RCH=CH$_2$ (57,58), no other interaction can be observed.

Fig. S29. Time-dependent In-situ IR spectra. In-situ IR spectra showing adsorbed (a) C$_2$H$_2$, (b) C$_2$H$_6$, and (c) C$_2$H$_4$ in CuTiF$_6$-TPPY with different exposure times.

To check the dependence of these spectral changes on the loading amount of guest molecules inside MOFs, time-dependent in-situ IR spectra with C2 gas-loadings were conducted. As shown in Fig. S29, the characteristic absorption peaks of C$_2$H$_2$ ($\nu$(-CH) and asymmetrical C≡C stretching) and C$_2$H$_6$ ($\nu$(-CH)) appeared at 3 min. In contrast, the stretching bands of adsorbed C$_2$H$_4$ were detected at 10 min. These results indicated that C$_2$H$_2$ and C$_2$H$_6$ can be adsorbed in a stronger and faster manner than C$_2$H$_4$ by CuTiF$_6$-TPPY.
Fig. S30. Reproducibility of synthesis process. Images of different batches and blended mixtures of CuTiF$_6$-TPPY samples.

To verify the reproducibility of CuTiF$_6$-TPPY and its separation performances, we have parallelly synthesized ten batches of CuTiF$_6$-TPPY and measured their adsorptive separation performances. Due to the extremely time-consuming process for evaluating individual adsorption isotherms of 10-batch samples, we have blended samples 1-3 as labeled as “Mixture-1”, samples 4-6 as “Mixture-2”, and samples 7-10 as “Mixture-3” (Fig. S30).
Fig. S31. Structure and adsorption properties of blended samples. (a) XRD patterns and adsorption isotherms of (b) C$_2$H$_2$, (c) C$_2$H$_4$, and (d) C$_2$H$_6$ on blended samples.

Fig. S32. Breakthrough curves for blended samples. The breakthrough curves of (a) C$_2$H$_2$/C$_2$H$_6$/C$_2$H$_4$ (1/9/90, v/v/v) and (b) C$_2$H$_6$/C$_2$H$_4$ (10/90, v/v) for CuTiF$_6$-TPPY (1.3 g) with a flow rate of 5.0 mL/min.
Table S6. Comparison of the equilibrium adsorption capacity and selectivity of the selected C$_2$H$_6$-selective MOFs at 298 K and 1 bar.

| Adsorbents         | Adsorption uptake (mmol/g) | $Q_a$ (kJ/mol) at zero coverage | IAST Selectivity | Reference |
|--------------------|-----------------------------|---------------------------------|------------------|-----------|
|                    | $C_2H_6$ | $C_2H_4$ | $C_2H_6$ | $C_2H_4$ |                |
| UiO-66-ADC         | 1.7      | 1.8      | 36.0    | 36.0    | 1.8            | (43)      |
| MAF-49             | 1.7      | 1.7      | 56.7    | 45.5    | 2.7            | (42)      |
| ZIF-7              | 1.9      | 1.9      | 27.4    | 24.6    | 1.8            | (44)      |
| Cu(Qc)$_2$         | 1.9      | 0.8      | 28.1    | 25.2    | 3.5            | (35)      |
| ZIF-69             | 2.2      | 1.8      | 25.5    | 22.9    | 1.7            | (45)      |
| PAF-302            | 3.1      | 2.2      | 33.9    | 33.9    | 1.4            | (46)      |
| ZIF-8              | 3.2      | 2.0      | 21.5    | 16.0    | 2.0            | (47)      |
| PCN-245            | 3.3      | 2.4      | 23.0    | 20.5    | 1.8            | (48)      |
| Fe$_2$(O$_2$)(dobdc) | 3.3      | 2.7      | 66.8    | 37.6    | 4.4            | (33)      |
| MIL-142A           | 3.8      | 2.9      | 27.3    | 26.1    | 1.5            | (49)      |
| In-soc-MOF-1       | 4.0      | 3.7      | 28.4    | 25.2    | 1.4            | (50)      |
| IRMOF-8            | 4.1      | 3.1      | 52.7    | 49.8    | 1.8            | (51)      |
| MUF-15             | 4.7      | 4.2      | 29.2    | 28.2    | 2.0            | (34)      |
| Ni2-a              | 4.8      | 4.6      | 33.5    | 31.7    | 1.4            | (32)      |
| Ni(bdc)(ted)$_{0.5}$ | 5.0      | 3.4      | 21.5    | 18.4    | 2.0            | (53)      |
| PCN-250            | 5.2      | 4.2      | 23.6    | 21.1    | 1.9            | (54)      |
| Ni1-a              | 6.6      | 6.0      | 33.6    | 32.2    | 1.5            | (52)      |
| Zn-atz-IPA         | 1.76     | 1.75     | 45.8    | 40      | 2.0            | (55)      |
| CuTiF$_6$-TPPY     | 2.82     | 2.42     | 34.2    | 29.6    | 2.12           | This work |
Table S7. Comparison of the equilibrium adsorption capacity of the selected C$_2$H$_2$ and C$_2$H$_6$ simultaneous adsorption MOFs at 298 K and 1 bar.

| Adsorbents   | Adsorption uptake (mmol/g) | Uptake ratio (298 K 1 bar) | IAST Selectivity | Reference |
|--------------|-----------------------------|-----------------------------|-------------------|-----------|
|              | C$_2$H$_2$ | C$_2$H$_6$ | C$_2$H$_4$ | C$_2$H$_2$/C$_2$H$_4$ | C$_2$H$_2$/C$_2$H$_6$ (50/50) | C$_2$H$_6$/C$_2$H$_4$ (50/50) |
| ZJNU-7       | 5.04   | 4.13    | 3.80    | 1.33 | 1.09   | 1.68   | 1.56   | (25) |
| ZJNU-115     | 4.73   | 4.20    | 3.75    | 1.26 | 1.12   | 2.05   | 1.56   | (24) |
| NPU-1        | 5.10   | 4.50    | 4.20    | 1.21 | 1.07   | 1.4    | 1.32   | (20) |
| NPU-2        | 3.99   | 4.42    | 3.42    | 1.17 | 1.29   | 1.25   | 1.52   | (20) |
| NPU-3        | 2.19   | 3.33    | 2.19    | 1.0  | 1.52   | 1.32   | 3.21   | (20) |
| TJT-100      | 4.46   | 3.70    | 3.44    | 1.3  | 1.08   | 1.8    | 1.2    | (5)  |
| Azole-Th-1   | 3.51   | 4.42    | 3.56    | 0.99 | 1.24   | 1.09   | 1.46   | (21) |
| NUM-9a (313 K) | 1.98  | 2.06    | 1.79    | 1.11 | 1.15   | 1.50   | 1.62   | (23) |
| MOF-525      | 2.65   | 2.71    | 2.11    | 1.26 | 1.28   | 1.45   | 1.22   | (22) |
| MOF-525(Co)  | 2.62   | 2.22    | 1.92    | 1.36 | 1.16   | 1.95   | 1.1    | (22) |
| UPC-612      | 3.01   | 3.57    | 2.79    | 1.08 | 1.28   | 1.08   | 1.4    | (22) |
| UPC-613      | 2.83   | 2.55    | 2.30    | 1.23 | 1.11   | 1.39   | 1.48   | (22) |
| MIL-125      | 7.05   | 4.83    | 3.98    | 1.77 | 1.21   | 2.32   | 1.21   | (27) |
| NH$_2$-MIL-125 | 7.82 | 4.69    | 4.41    | 1.78 | 1.06   | 3.75   | 1.18   | (27) |
| ZSTU-2       | 3.11   | 2.73    | 2.35    | 1.32 | 1.16   | 2.36   | 1.62   | (27) |
| CuTiF$_6$-TPPY | 3.62  | 2.82    | 2.42    | 1.50 | 1.17   | 5.47   | 2.12   | This work |
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