# Metal-Organic Frameworks(MOFs) Composite Materials for Photocatalytic $CO_2$ Reduction under Visible Light

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## Synthesis

**Preparation of 2,4,6-tris (2-(pyridin-4-yl)vinyl)-1,3,5-triazine**

Weighing 0.560 g (10 mmol) of KOH and dissolve in 20 mL of methanol, then add 0.749 g (7 mmol) of 4-pyridinecarboxaldehyde in 10 mL of methanol, stir with a magnet and heat to reflux, the solution is very brightly yellow. 0.246 g (2 mmol) trimethyl-s-triazine and 0.680 g KOH dissolved in 25 mL of methanol were added dropwise at a rate of 5 seconds per drop. During the addition, the color of the solution gradually changed from light yellow to dark purple. After the addition, the reaction has continued for 1 h, and then the temperature was lowered to room temperature. The resulting solution was suction filtered, and then washed twice with methanol. After drying, 0.585 g of white powder was obtained with a yield of 75%. 1H-NMR (600 MHz, DMSO), δ (TMS, ppm): 8.69 (d, 6H, J = 5.4 Hz), 8.29 (d, 3H, J =16.2 Hz), 7.81 (d, 6H, J = 5.4 Hz), 7.54 (d, 3H, J = 16.2 Hz).

**Preparation of g-$C_3N_4$**

5 g of melamine was poured into a semi-closed crucible and heated in a muffle furnace at 520 °C for 6 hours with temperature rate of 9 °C/ min. The color of obtained sample was yellow.[1]

**Water absorption test of MOF**

We dried MOF at 100℃ for 12 h, then transferred to special vacuum flask, and added an appropriate amount of distilled water, pumped to vacuum, the system was stable for 2 h, then transferred MOF material to the synchronous thermal analyzer quickly to test its quality changes.

## Characterization and measurement

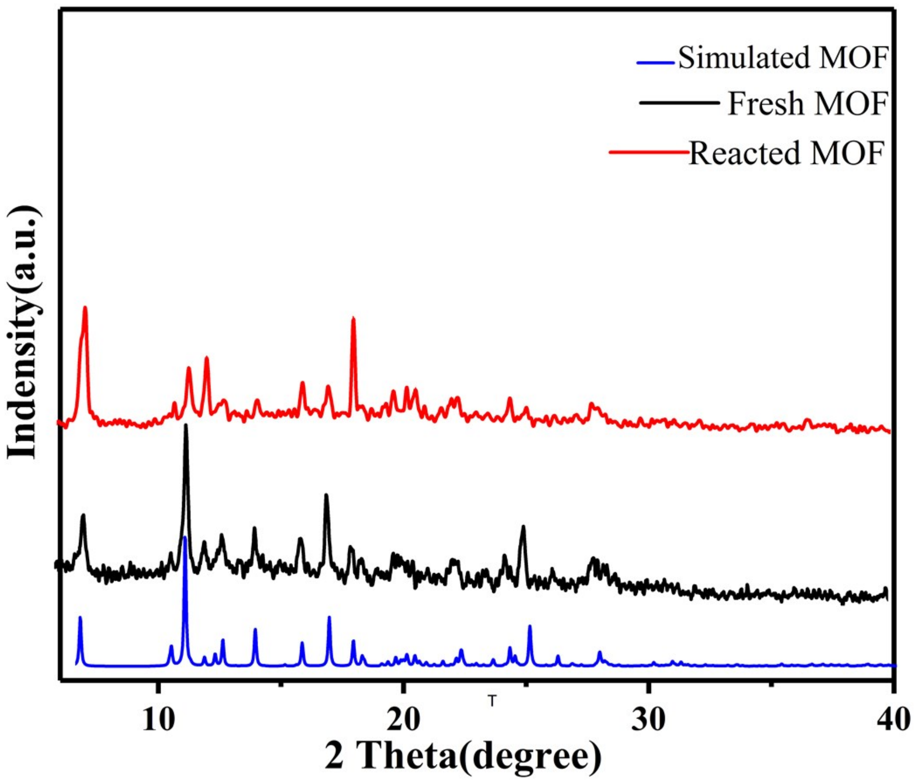


Figure S1 The XRD patterns of simulated MOF, fresh MOF.and reacted MOF in composite condition without g-$C_3N_4$.

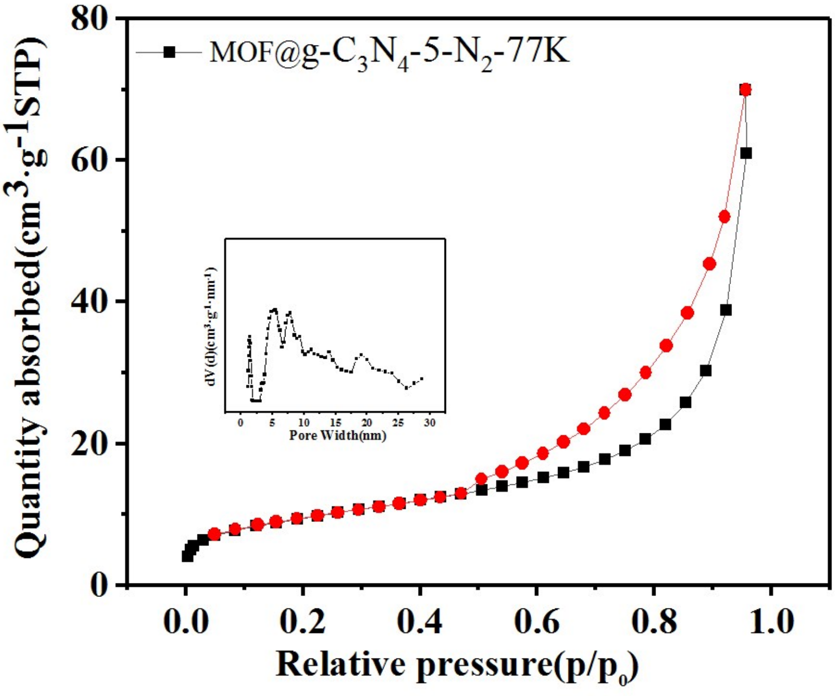


Figure S2 $N_2$ adsorption and pore size distribution of TPVT-MOFs@g-$C_3N_4$-5.

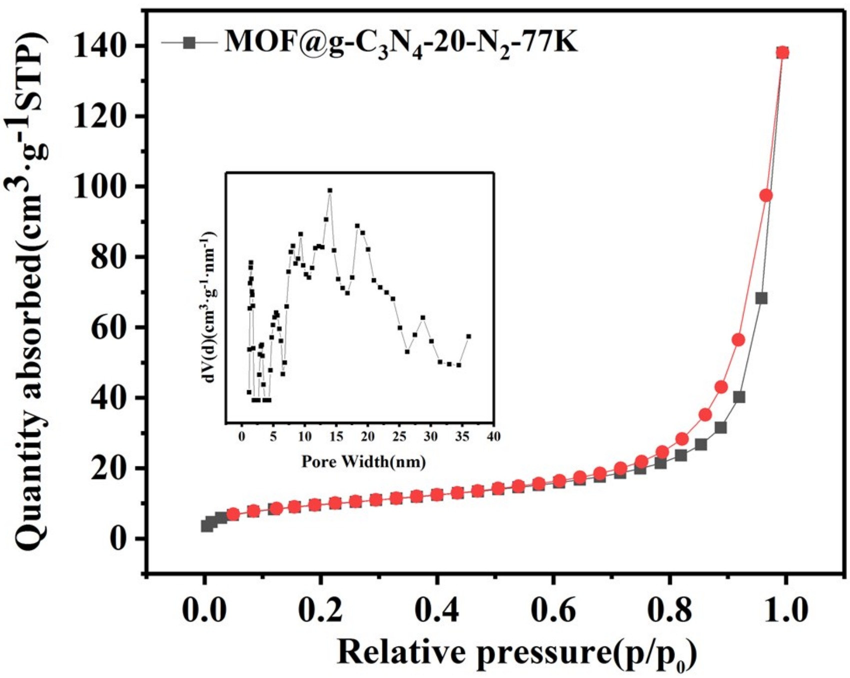


Figure S3 $N_2$ adsorption and pore size distribution of TPVT-MOFs@g-$C_3N_4$-20.

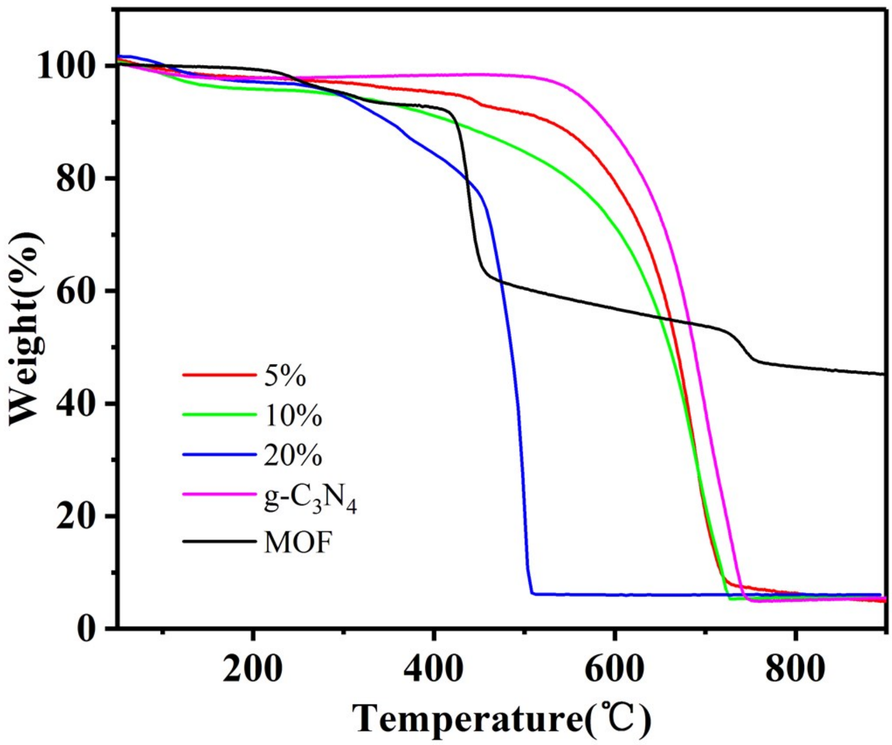


Figure S4 TGA curves of $g-C_3N_4$, TPVT-MOFs and TPVT-MOFs@$g-C_3N_4$.

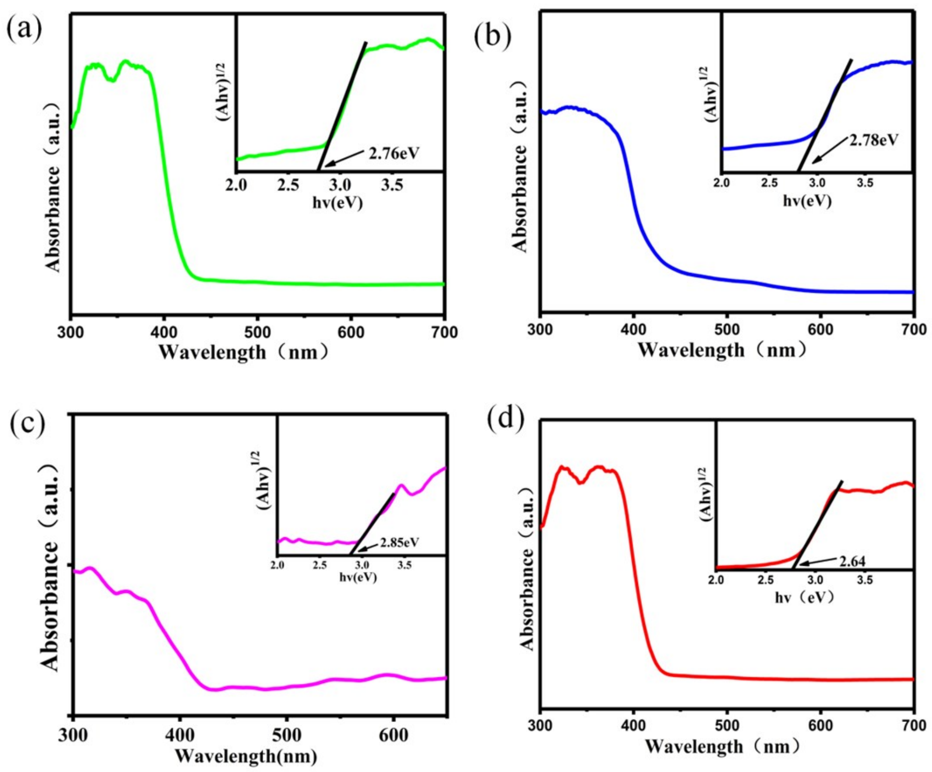


Figure S5 UV-visible spectra of (a)TPVT-MOFs@$g-C_3N_4$-5(b)TPVT-MOFs@$g-C_3N_4$-10(c)TPVT-MOFs@$g-C_3N_4$-20(d)$g-C_3N_4$.

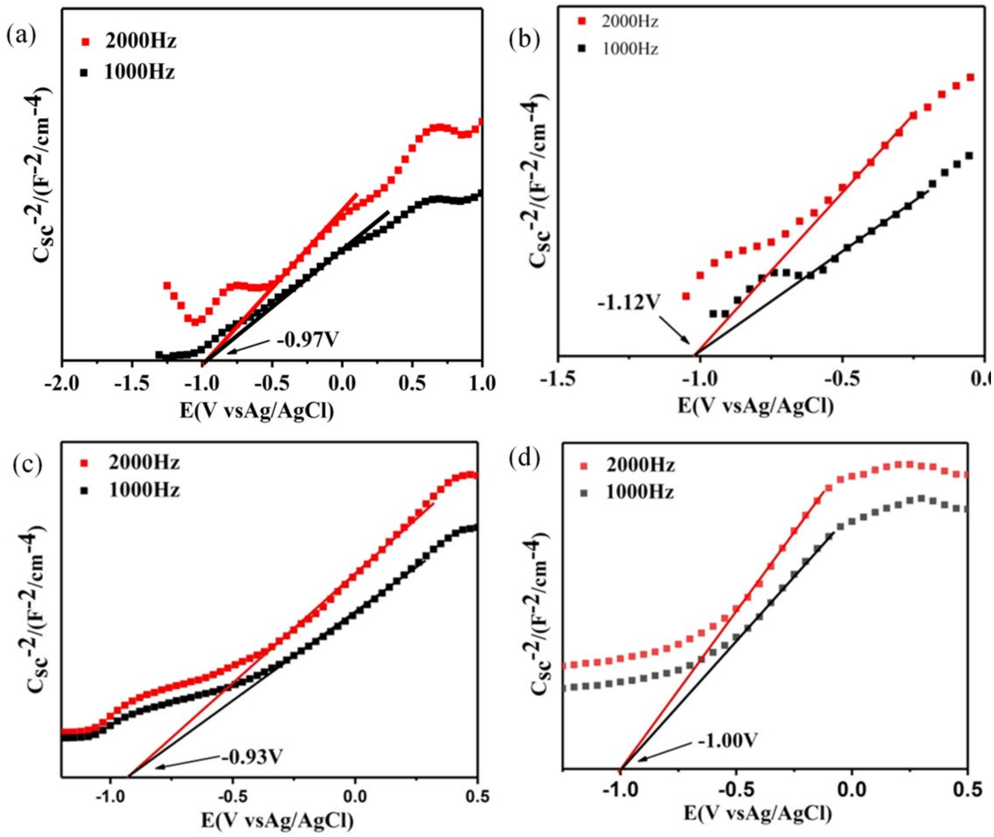


Figure S6 Mott-Schottky measurements of (a)TPVT-MOFs@g-$C_3N_4$-5 (b)TPVT-MOFs@g-$C_3N_4$-10 (c)TPVT-MOFs@g-$C_3N_4$-20 (d)g-$C_3N_4$.

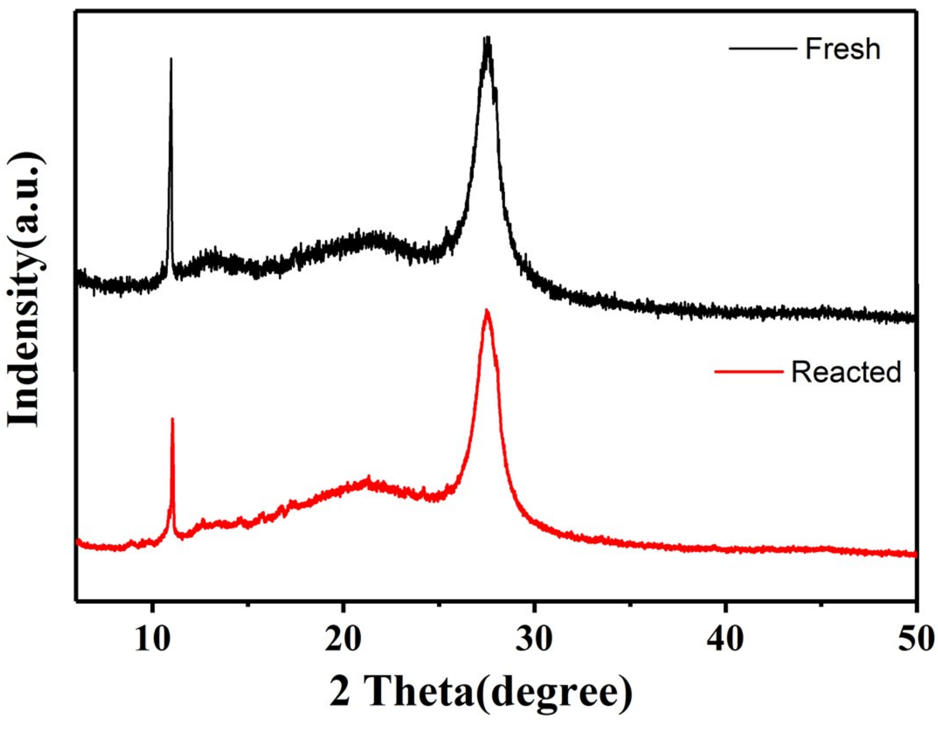


Figure S7 The XRD patterns of (a)fresh and (b)reacted TPVT-MOFs@g-$C_3N_4$-10.

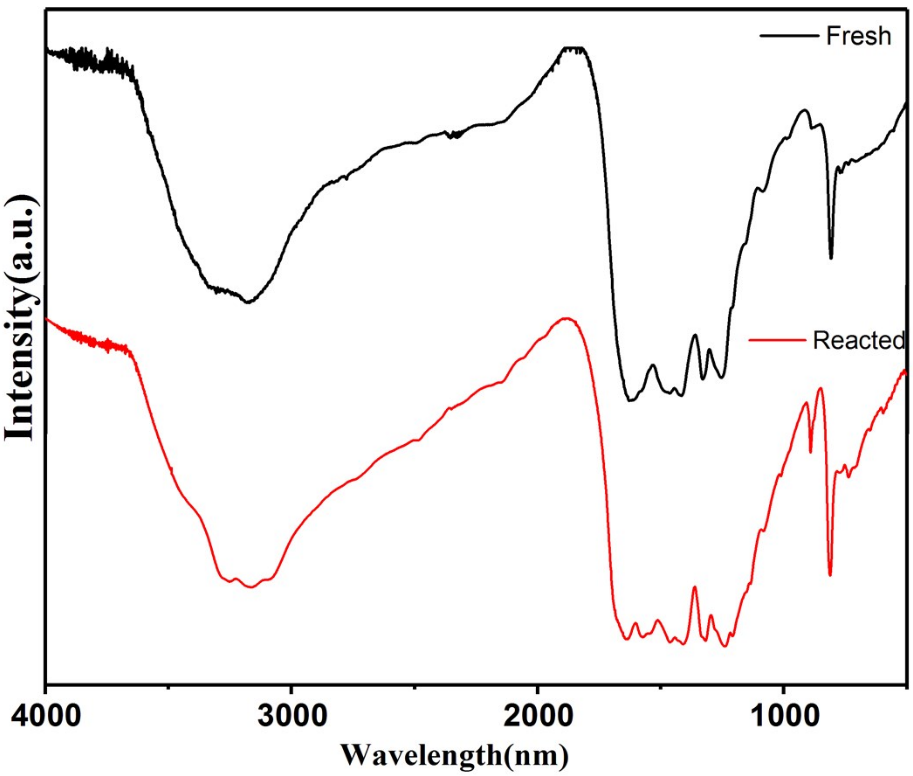


Figure S8 The FT-IR spectra of (a)fresh and (b)reacted TPVT-MOFs@g-$C_3N_4$-10.

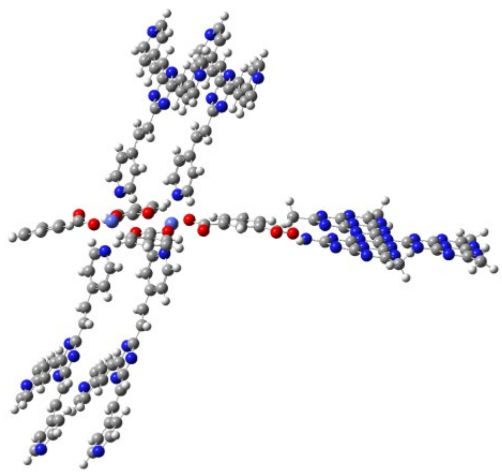

Figure S9 Computational model for TVPT-MOFs@g-$C_3N_4$. Carbon(grey), Nitrogen(blue), Hydrogen(white), Oxygen(red) .

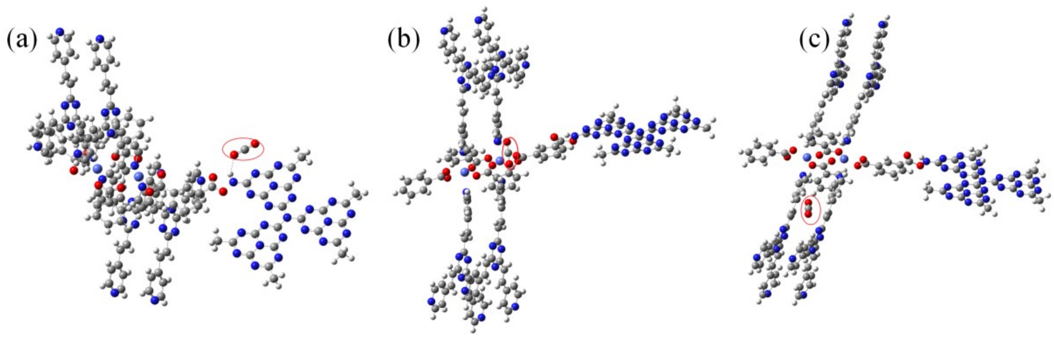


Figure S10 Geometry optimization of $CO_2$ adsorption energy of TPVT-MOFs@g-$C_3N_4$-10 (a)$CO_2$-a (b)$CO_2$-b (c)$CO_2$-c.

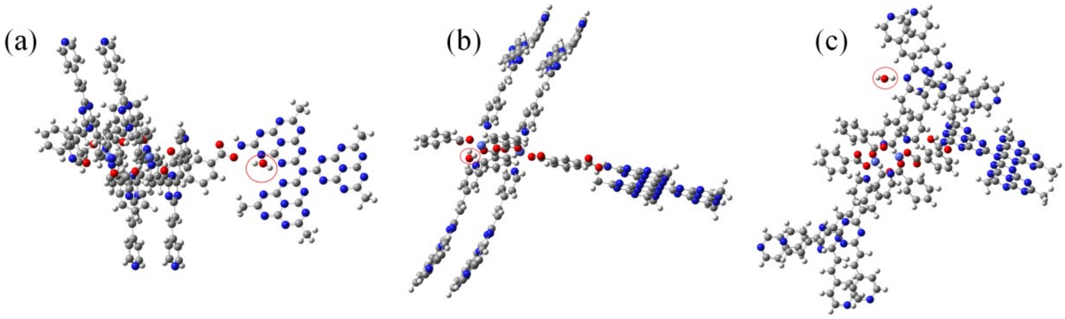


Figure S11 Geometry optimization of $H_2O$ adsorption energy of TPVT-MOFs@g-$C_3N_4$-10 (a)$H_2O$-a (b)$H_2O$-b (c)$H_2O$-c.

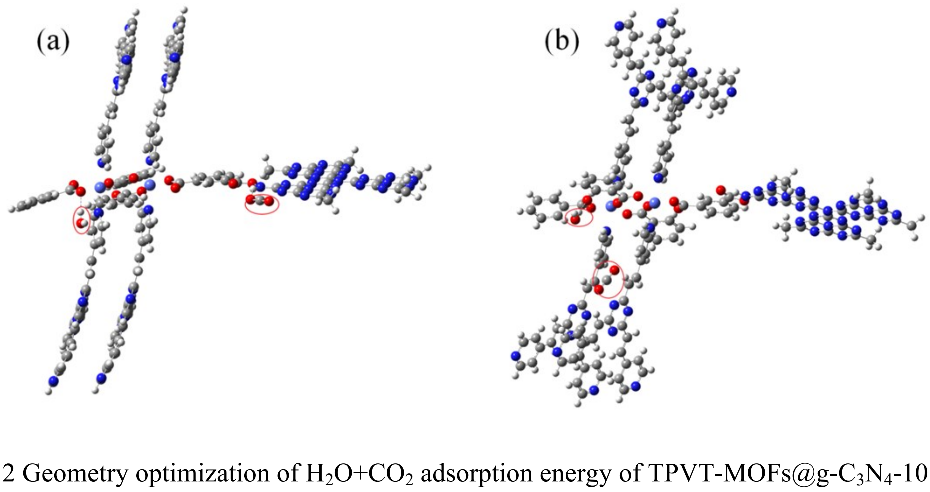


Figure S12 Geometry optimization of $H_2O$+$CO_2$ adsorption energy of TPVT-MOFs@g-$C_3N_4$-10 (a)$H_2O$+$CO_2$-a (b)$H_2O$+$CO_2$-b.

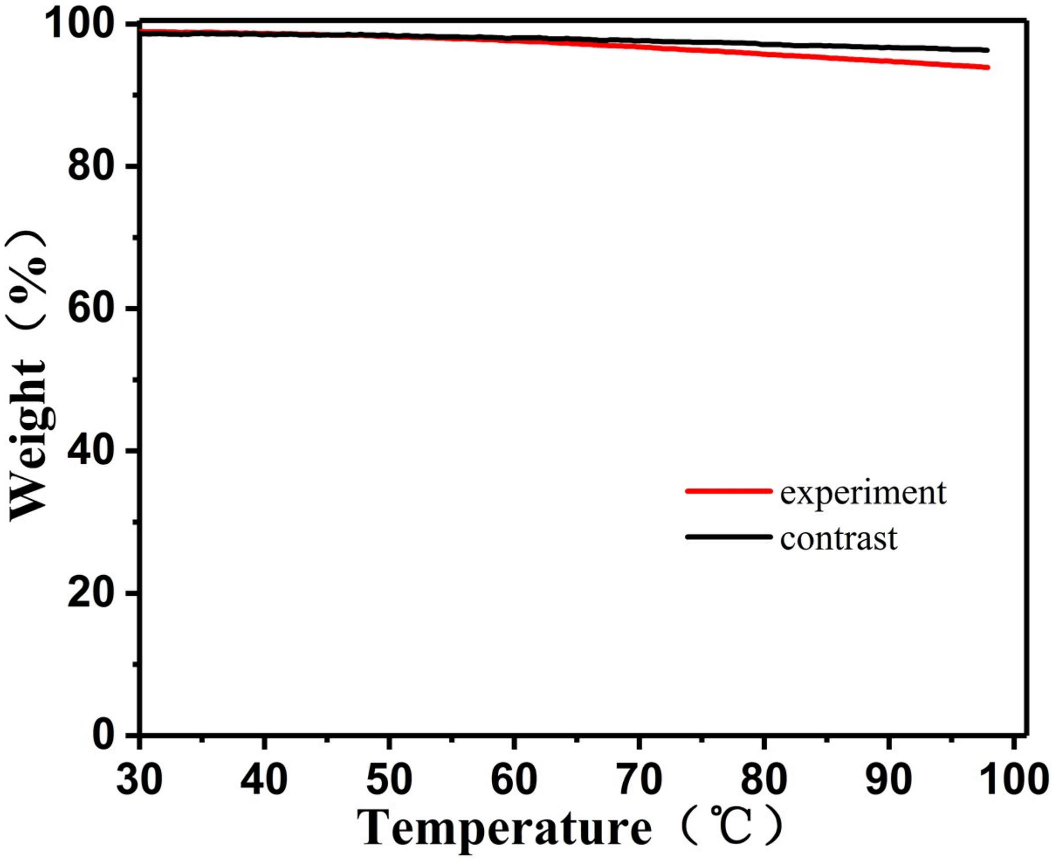


Figure S13 TGA of MOF with $H_2O$ and pure MOF.

## Notes and references


[1] Shekardasht M B , Givianrad M H , Gharbani P , et al. Diamond and Related Materials, 2020, **109**,108008.