

Supporting information for

The Synergistic Effect of Oxygen and Water on the Stability of the Isostructural Family of Metal- Organic Frameworks $[\text{Cr}_3(\text{BTC})_2]$ and $[\text{Cu}_3(\text{BTC})_2]$

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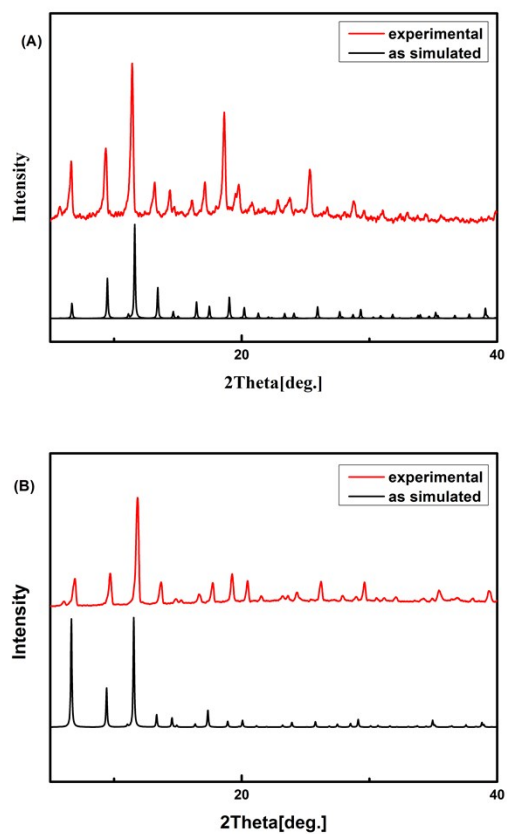


Figure S1. Powder X-ray diffraction patterns of samples and simulations of $\text{Cr}_3(\text{BTC})_2$ (A) and $\text{Cu}_3(\text{BTC})_2$ (B)

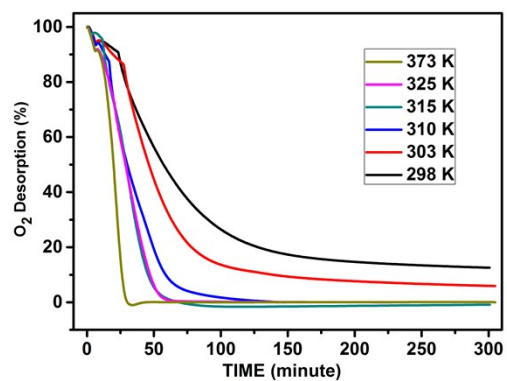


Figure S2. O_2 desorption curve of $\text{Cr}_3(\text{BTC})_2$ at different temperature

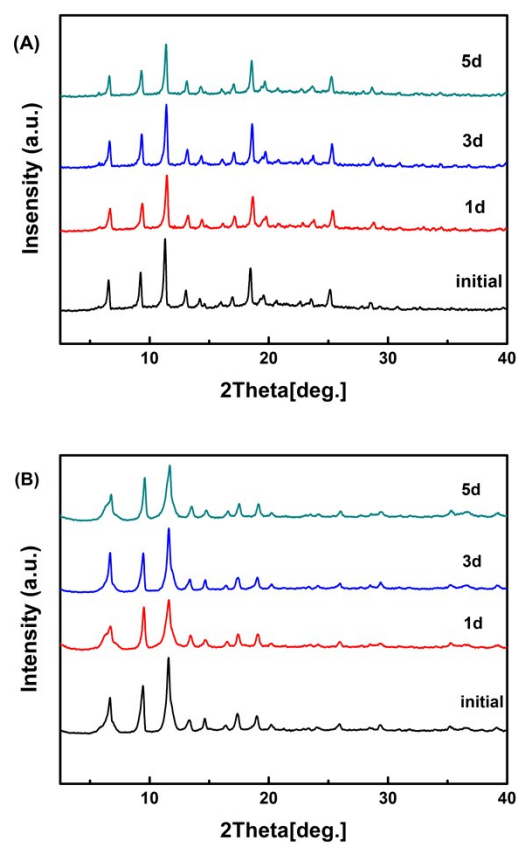


Figure S3. PXRD patterns of the $\text{Cr}_3(\text{BTC})_2$ (A) and $\text{Cu}_3(\text{BTC})_2$ (B) exposure under oxygen atmosphere for different time

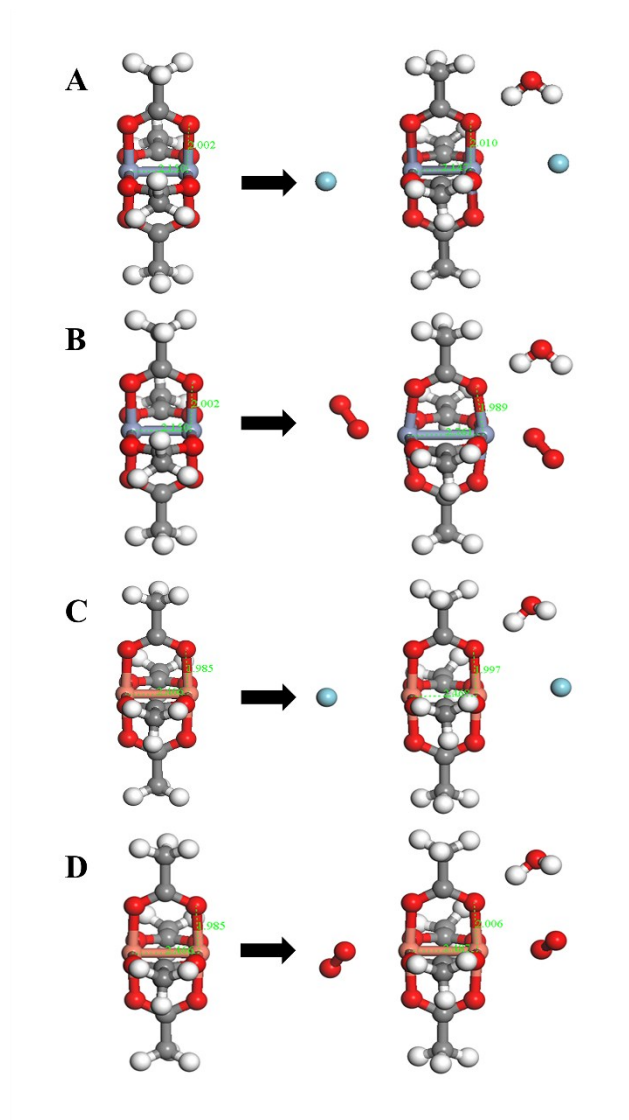


Figure S4. The changes in the bond length in $\text{Cr}_3(\text{BTC})_2$ and $\text{Cu}_3(\text{BTC})_2$ under the different environments (A. $\text{Cr}_3(\text{BTC})_2$ under a H_2O environment; B. $\text{Cr}_3(\text{BTC})_2$ in a mixed O_2 - H_2O environment; C. $\text{Cu}_3(\text{BTC})_2$ under a H_2O environment and D. $\text{Cu}_3(\text{BTC})_2$ under a mixed O_2 - H_2O environment).

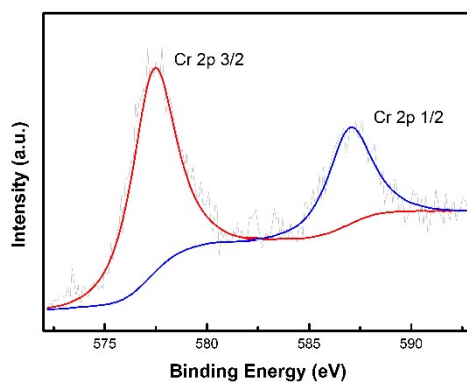


Figure S5. XPS spectrum of Cr in $\text{Cr}_3(\text{BTC})_2$ after exposing under oxygen-water atmosphere

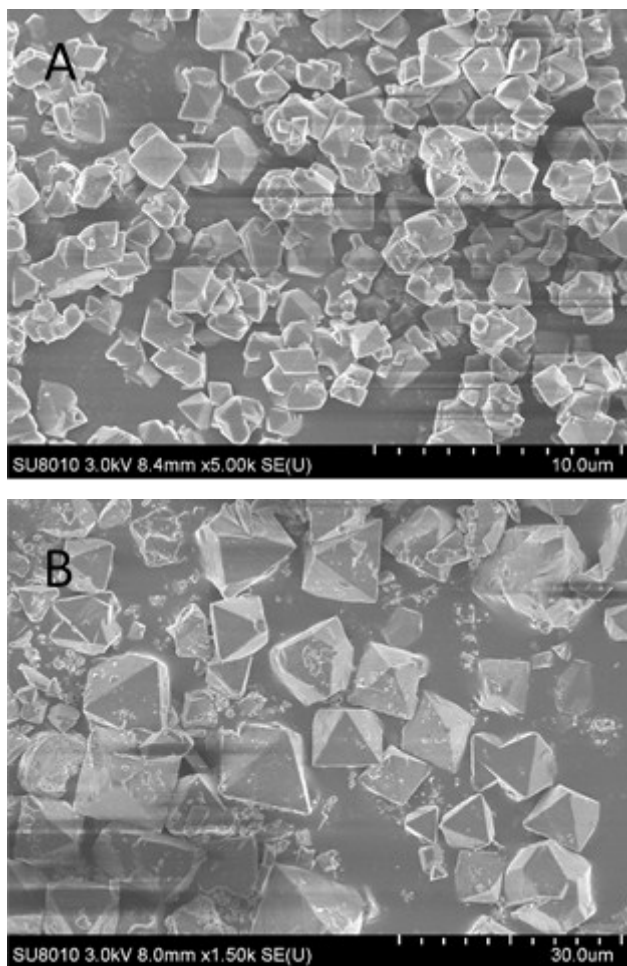


Figure S6 SEM images of $\text{Cr}_3(\text{BTC})_2$ (A) and $\text{Cu}_3(\text{BTC})_2$ (B)

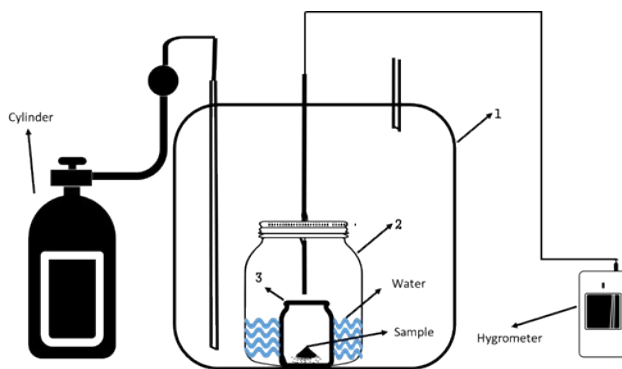


Figure S7. Schematic diagram of stability test

The NO.1 container is filled with the required gas. Some water is placed in container No. 2 and is in a closed state. The sample is the No. 3 container. According to the measurement results, the humidity of the No. 2 container can be guaranteed at 90% -95% RH. Thus, the sample can be in a certain gas and certain relative humidity environment.

Table S1. Comparison of key parameters in oxygen adsorption test of $\text{Cr}_3(\text{BTC})_2$

	Activation temperature	Test temperature	Maximum pressure	Oxygen adsorption capacity
Literature ¹	433 K	298 K	1 bar	11 wt%
Our work	393 K	298 K	1 bar	14 wt%

Table S2. Comparison of key parameters in water adsorption test of $\text{Cr}_3(\text{BTC})_2$

	Activation temperature	Test temperature	Relative humidity	Water adsorption capacity	Surface area (m^2/g)
Literature ²	393 K	298 K	80% RH	420 cm^3/g	1400
Our work	393 K	298 K	80% RH	355 cm^3/g	1067

Table S3. Comparison of key parameters in N₂ adsorption test of Cr₃(BTC)₂

	Activation temperature	Activation time	Test temperature	Maximum pressure (P/P ₀)	Surface area (m ² /g)
Literature ¹	433 K	48 h	77 K	1	2040 (langmuir)
Our work	393 K	16 h	77 K	1	1403 (BET)

Table S4. Comparison of key parameters in N₂ adsorption test of Cu₃(BTC)₂ under water environment

	Activation temperature	Test temperature	Maximum pressure (P/P ₀)	Surface area(m ² /g)		
				initial	After water	loss
Literature ³	423 K	77 K	1	1270	945	26%
Literature ⁴	/	77 K	1	1340	647	48%
Our work	393 K	77 K	1	1067	922	13%

References

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