

Bimetallic Ag-Cu-trimesate metal-organic framework for hydrogen sulfide removal

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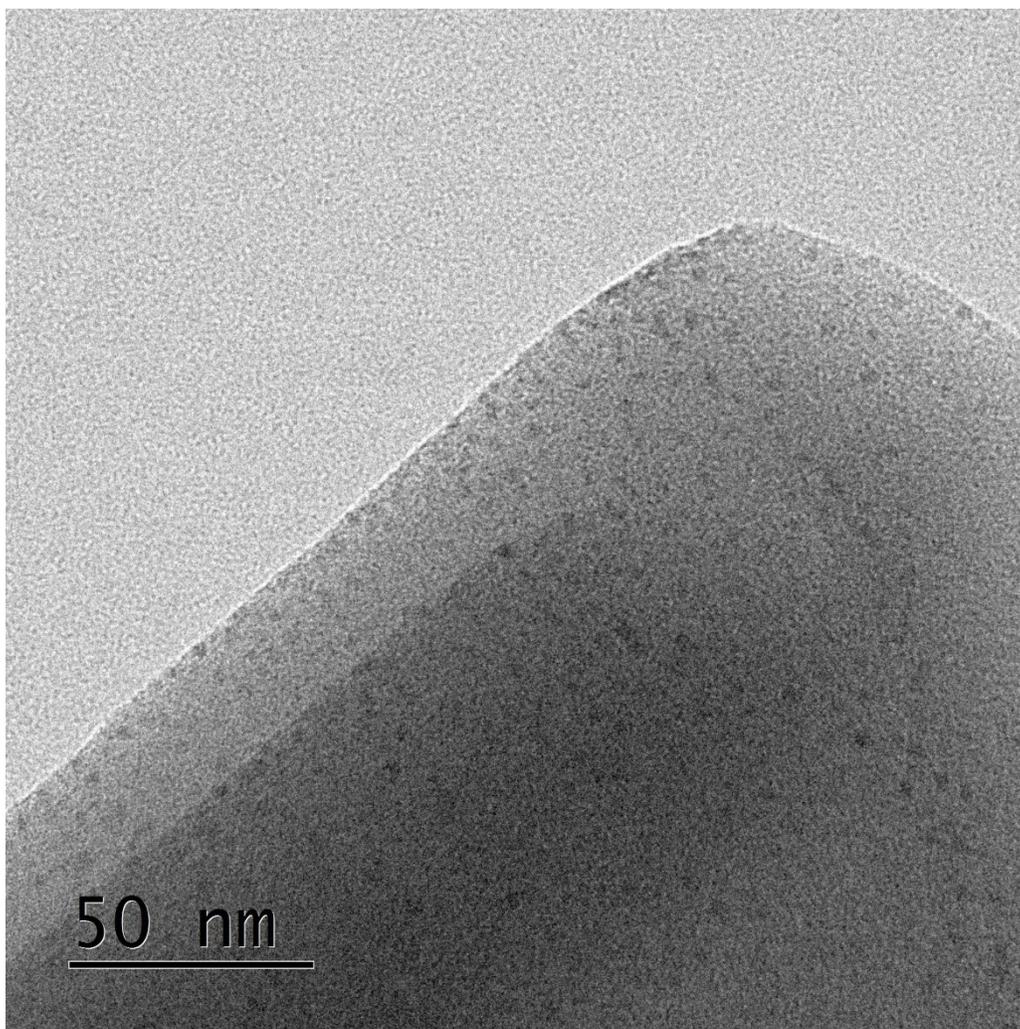


Fig. S1. HR-TEM image of Ag-Cu-MOF.

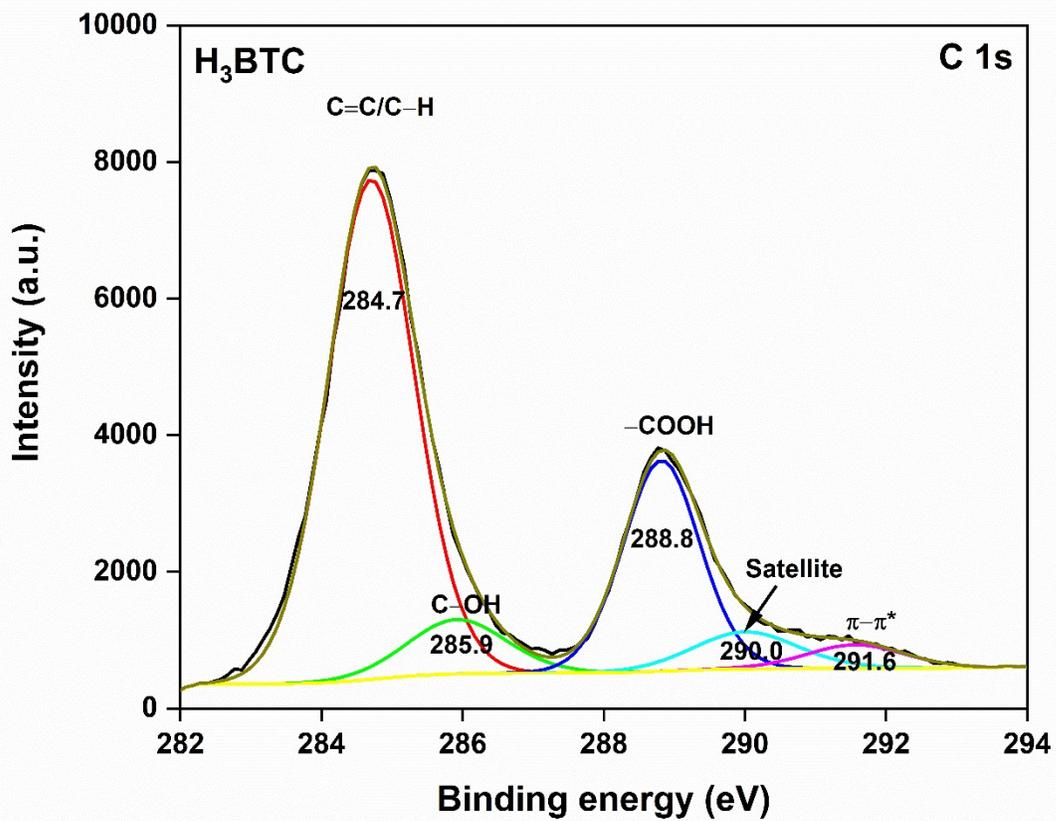


Fig. S2. HRXPS C 1s spectrum of H₃BTC ligand.

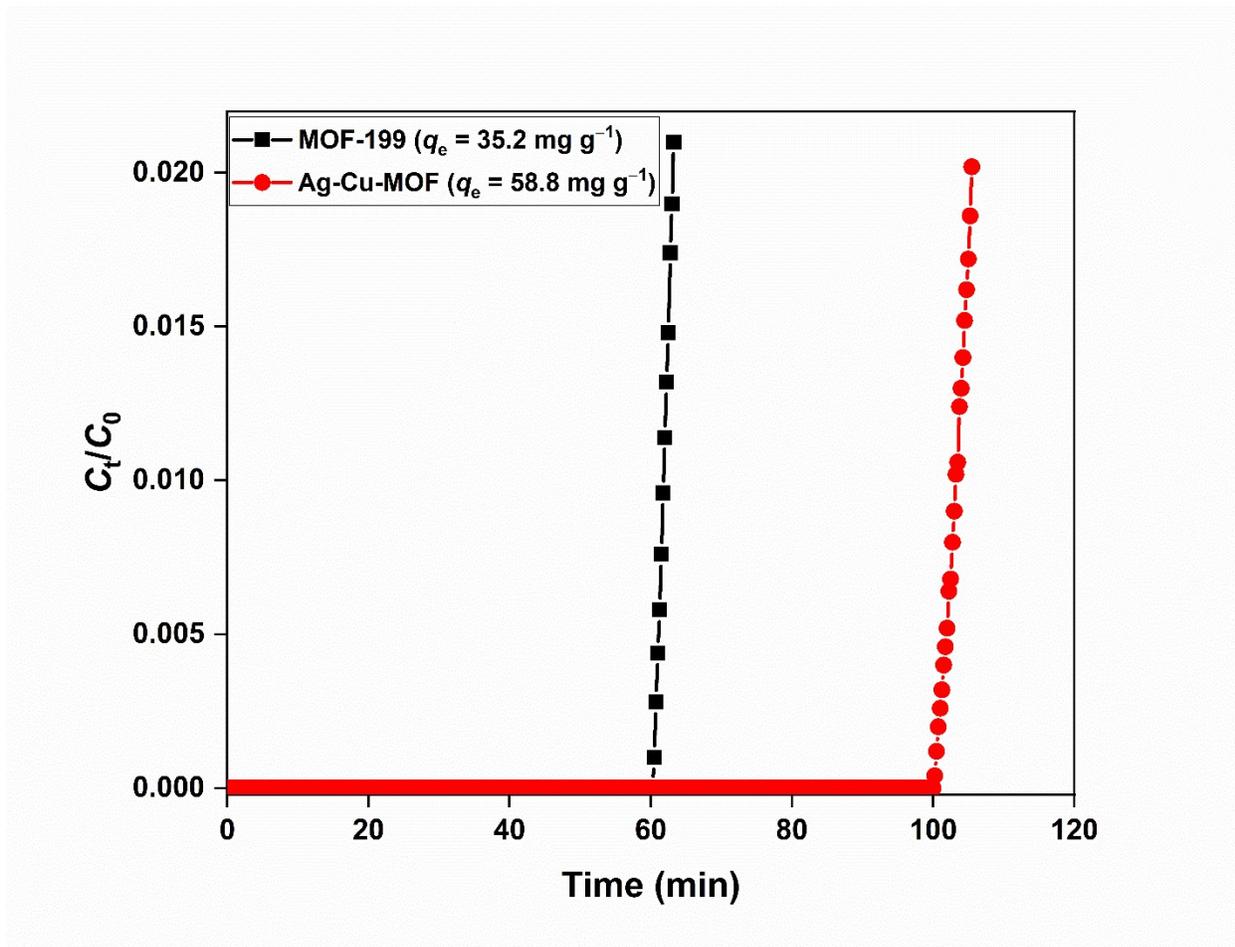


Fig. S3. H₂S breakthrough curves of MOF-199 and Ag-Cu-MOF. Experimental conditions:

[MOF] = 0.25 g, flow rate = 0.2 L min⁻¹, BTP = 2%.

The MOF-199 studied in this work was fabricated using the same method without silver nitrate salt.

Table S1. Curve fitting parameters for C 1s spectra of MOF and H₃BTC ligand.

Samples	Assignment	E_B (eV)	FWHM (eV)	At. %
Ag-Cu-MOF	C1s _{C=C/C-H}	284.7	1.4	53.5
	C1s _{C=O}	286.1	1.6	20.0
	C1s _{O-C=O}	288.5	1.6	19.8
	C1s _{satellite}	290.0	1.9	6.7
H₃BTC	C1s _{C=C/C-H}	284.7	1.4	61.1
	C1s _{C-OH}	285.9	1.6	7.6
	C1s _{O-C=O}	288.8	1.3	22.7
	C1s _{Satellite}	290.0	1.7	5.4
	C1s _{Satellite}	291.6	1.6	3.2

Table S2. Curve fitting parameters for O 1s, N 1s, Cu 2p, and Ag 3d spectra of Ag-Cu-MOF.

Curve	Assignment	E_B (eV)	FWHM (eV)	At. %
O 1s	O-Ag/O-Cu	531.2	1.4	19.8
	O-C=O	531.9	1.6	40.7
	Water	533.1	1.8	39.6
N 1s	NO_3^-	407.1	1.7	100
Cu 2p	Cu 2p _{3/2} Cu ⁺	932.2	1.7	10.1
	Cu 2p _{3/2} Cu ²⁺	934.6	2.3	89.9
	Satellite Cu ²⁺	939.7	4.0	-
	Satellite Cu ²⁺	943.8	3.5	-
Ag 3d	Ag 3d _{5/2} Ag ⁺	368.0	1.3	72.8
	Ag 3d _{5/2} Ag ⁰	369.3	1.6	27.2

Table S3. Curve fitting parameters for Cu 2p, S 2p, and Ag 3d spectra of spent and regenerated MOF.

Curve	Assignment	E_B (eV)	FWHM (eV)	At. %
Spent MOF/ Cu 2p	Cu 2p _{3/2} Cu ⁺	932.1	1.7	17.3
	Cu 2p _{3/2} Cu ²⁺	934.5	2.2	77
	Satellite Cu ²⁺	938.8	4.0	-
	Satellite Cu ²⁺	943.5	3.5	-
Reg. MOF/ Cu 2p	Cu 2p _{3/2} Cu ⁺	932.4	1.4	13.9
	Cu 2p _{3/2} Cu ²⁺	934.7	2.3	86.1

	Satellite Cu^{2+}	939.2	4.0	-
	Satellite Cu^{2+}	943.8	3.5	-
Spent MOF/ Ag 3d	Ag 3d $_{5/2} \text{Ag}^+$	368.2	1.6	22.3
	Ag 3d $_{5/2} \text{Ag}^0$	370.1	2.1	77.7
Reg. MOF/ Ag 3d	Ag 3d $_{5/2} \text{Ag}^+$	368.4	1.4	69.1
	Ag 3d $_{5/2} \text{Ag}^0$	369.4	1.8	30.9
Spent MOF/ S 2p $_{3/2}$	S $^{2-}$	162.1	1.6	17.4
	SO $_4^{2-}$	169.0	1.7	58.2
	HSO $_4^-$	170.8	1.9	24.4
Reg. MOF/ S 2p $_{3/2}$	S $^{2-}$	162.9	1.6	20.2
	SO $_4^{2-}$	168.9	1.7	59.4
	HSO $_4^-$	171.0	1.9	20.4