

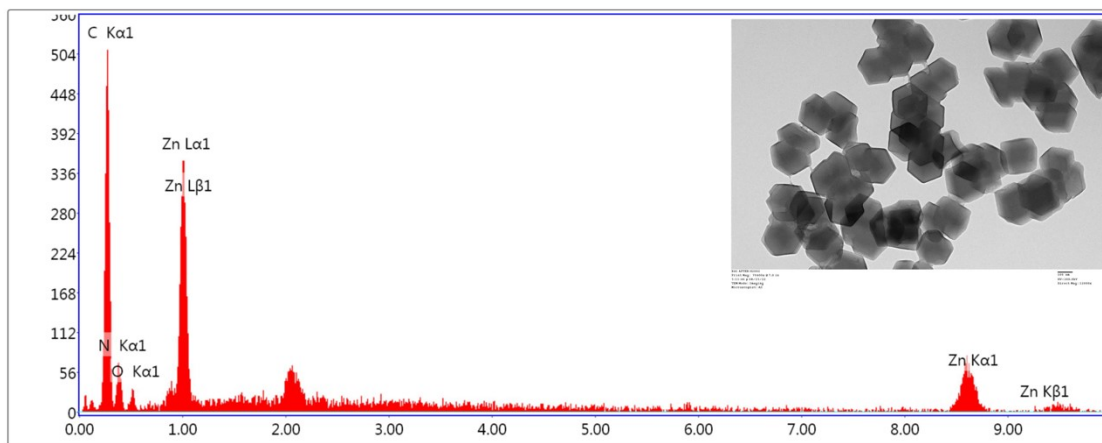
Supplementary Information

Room temperature hydrogen storage enhancement in copper-doped zeolitic imidazolate frameworks with trioctylamine

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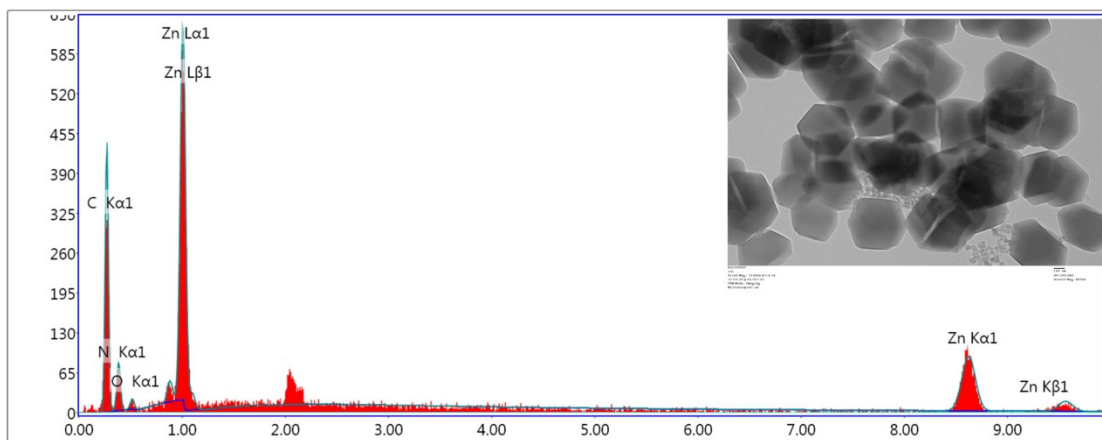
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Lsec: 30.0 0 Cnts 0.000 keV Det: Octane Prime Det

Figure S1 EDX spectrum of ZIF-8.



Lsec: 30.0 0 Cnts 0.000 keV Det: Octane Prime Det

Figure S2 EDX spectrum of ZIF-8-T.

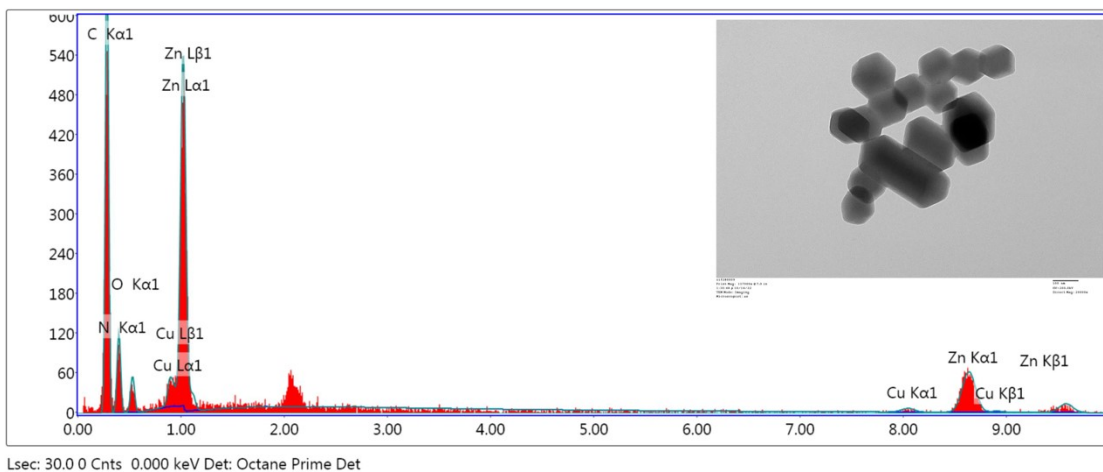


Figure S3 EDX spectrum of CuZIF-8.

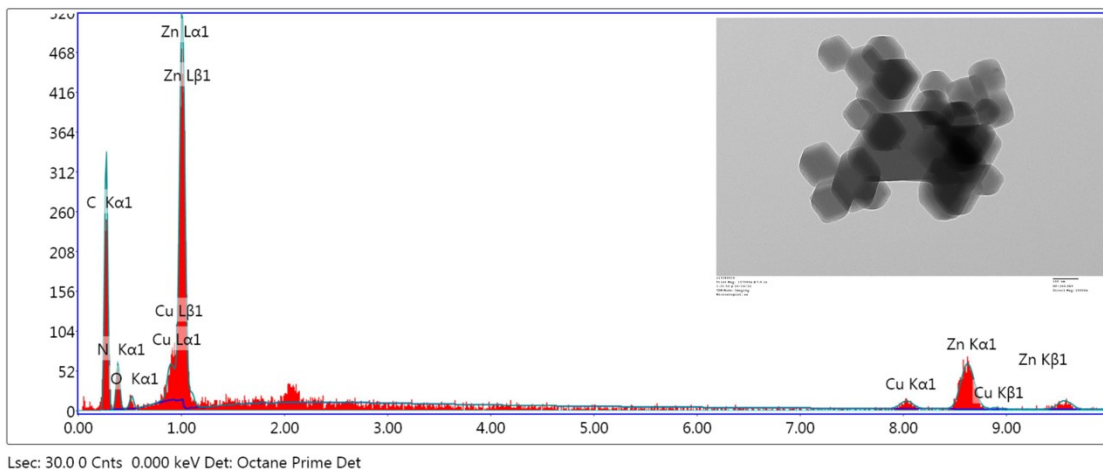


Figure S4 EDX spectrum of CuZIF-8-T.

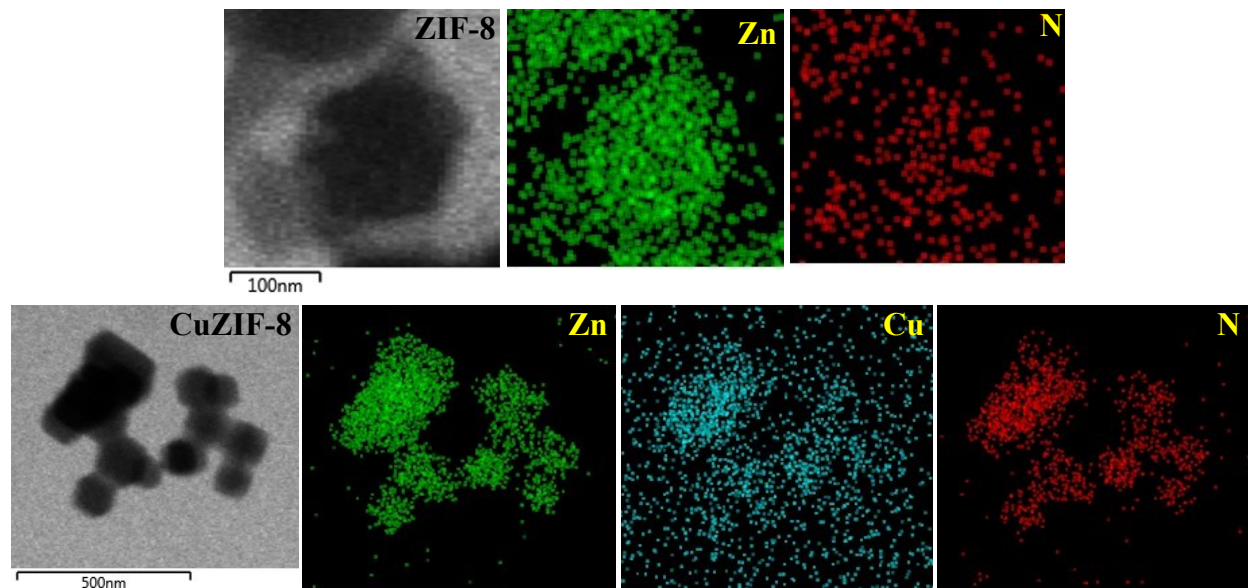


Figure S5 Elemental mapping of ZIF-8 and CuZIF-8 from TEM/EDX.

Table S1 Particle size and product yield of all four materials.

Samples	Particle size range (nm)	Average particle size (nm)	Product yield (%)
ZIF-8	100 – 320	252	90.21
ZIF-8-T	100 – 558	474	93.40
CuZIF-8	100 – 186	159	86.78
CuZIF-8-T	100 – 275	152	89.74

Table S2 Elemental composition of the adsorbents from XPS survey spectra.

Samples	C1s	N1s	O1s	Zn2p	Cu2p
ZIF-8	66.4	20.7	6.6	6.3	-
ZIF-8-T	65.6	21.4	5.7	7.3	-
CuZIF-8	68.5	17.1	7.7	5.6	1.1
CuZIF-8-T	68.1	22.4	2.4	6.1	1

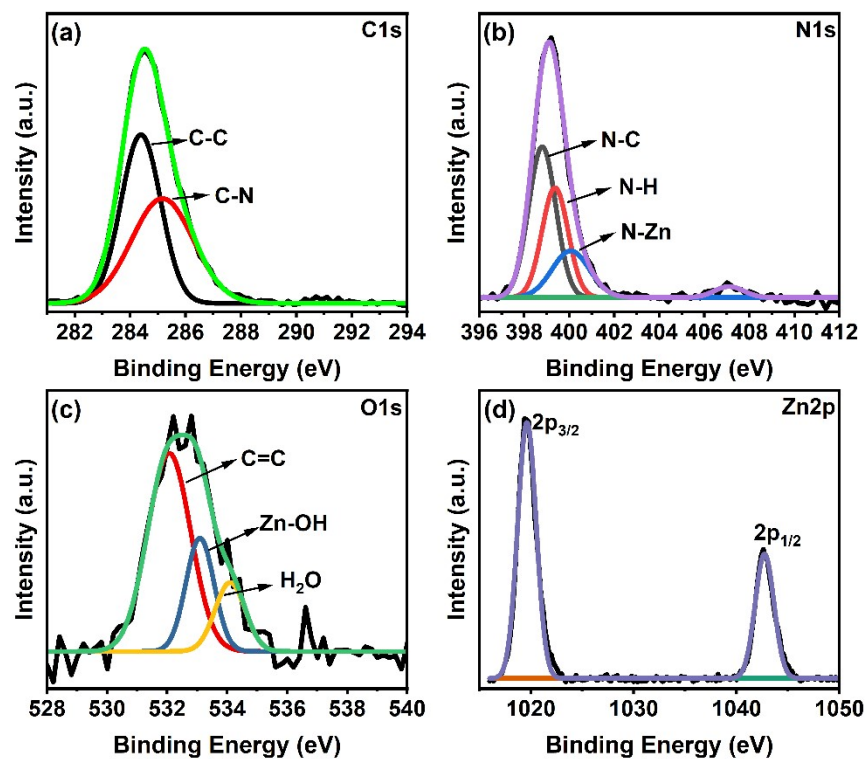


Figure S6 Deconvoluted high-resolution XPS spectra of ZIF-8.

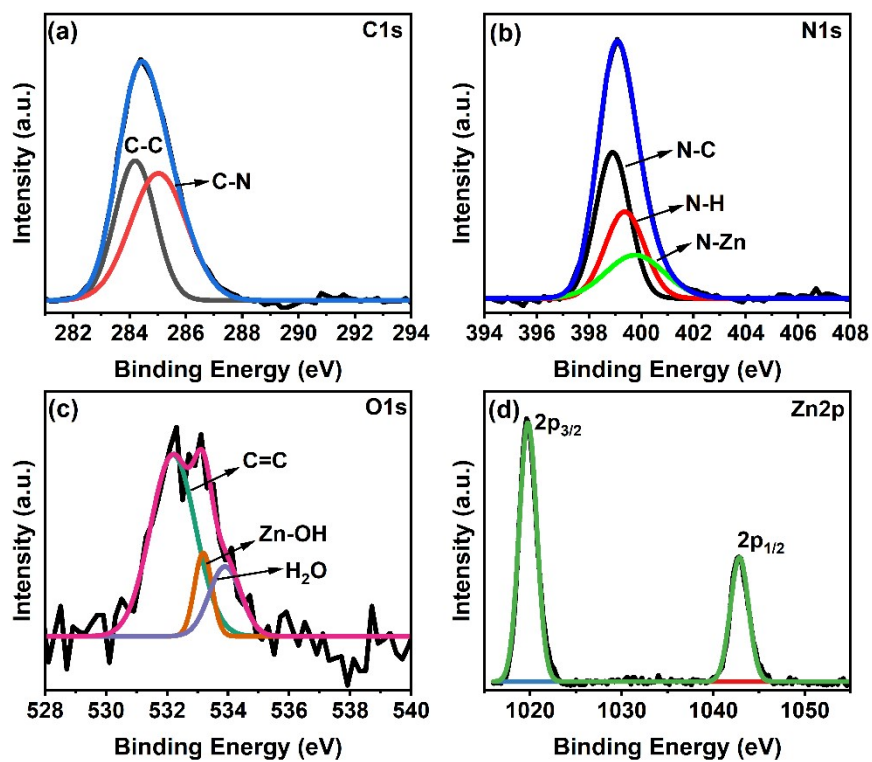


Figure S7 Deconvoluted high-resolution XPS spectra of ZIF-8-T.

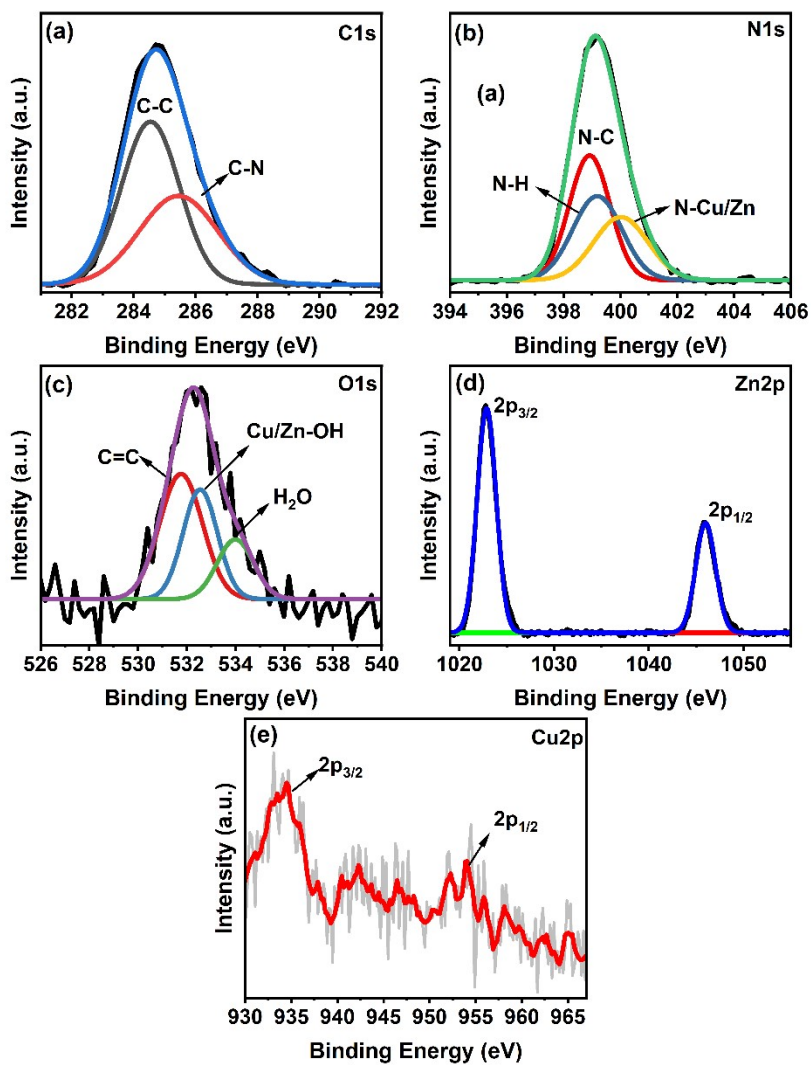


Figure S8 Deconvoluted high-resolution XPS spectra of CuZIF-8.

Table S3 Fitting results of deconvoluted high-resolution XPS spectra given in at. %, with binding energy mentioned in parenthesis.

Samples	C1s			N1s				O1s		
	C-C	C-N	$\pi-\pi^*$	N-C	N-H	N-Zn or N-Cu	Extra N	C=C	Zn-OH or Cu-OH	H ₂ O
ZIF-8	50.9 (284.3)	49.1 (285.1)	-	45.4 (398.8)	31.8 (399.4)	19.3 (400.1)	3.6 (407.1)	61.9 (532.1)	23.0 (533.0)	15.1 (534.1)
ZIF-8-T	44.1 (284.2)	55.9 (285.0)	-	45.7 (398.9)	31.3 (399.3)	23.0 (399.8)	-	69.0 (532.2)	12.3 (533.1)	18.8 (533.9)
CuZIF-8	57.6 (284.5)	42.4 (285.4)	-	44.2 (398.9)	34.6 (399.2)	21.2 (400.0)	-	47.4 (531.8)	33.3 (532.5)	19.2 (533.9)
CuZIF-8-T	48.4 (284.6)	48.7 (285.3)	2.9 (291.6)	57.3 (399.0)	17.2 (399.5)	25.5 (400.5)	-	17.6 (531.3)	36.0 (532.3)	46.5 (533.1)

Table S4 Fitting results of deconvoluted high-resolution XPS spectra of Zn2p. The values are in at. %, with binding energy mentioned in parenthesis.

Sample	Zn2p	
	Zn2p3/2	Zn2p1/2
ZIF-8	66.9 (1019.6)	33.1 (1042.7)
ZIF-8-T	66.7 (1019.7)	33.3 (1042.8)
CuZIF-8	66.3 (1022.9)	33.7 (1045.9)
CuZIF-8-T	67.2 (1022.8)	32.8 (1045.9)

Table S5 TGA and DTG results of the synthesized materials.

Samples	Temperature (°C)			Yield (wt.%)
	Onset	Inflection	Endpoint	
ZIF-8	432.2	466.1	530.0	34.8
ZIF-8-T	437.3	485.4	575.9	33.4
CuZIF-8	442.1	488.2	617.9	34.2
CuZIF-8-T	423	536.6	564.4	34.9

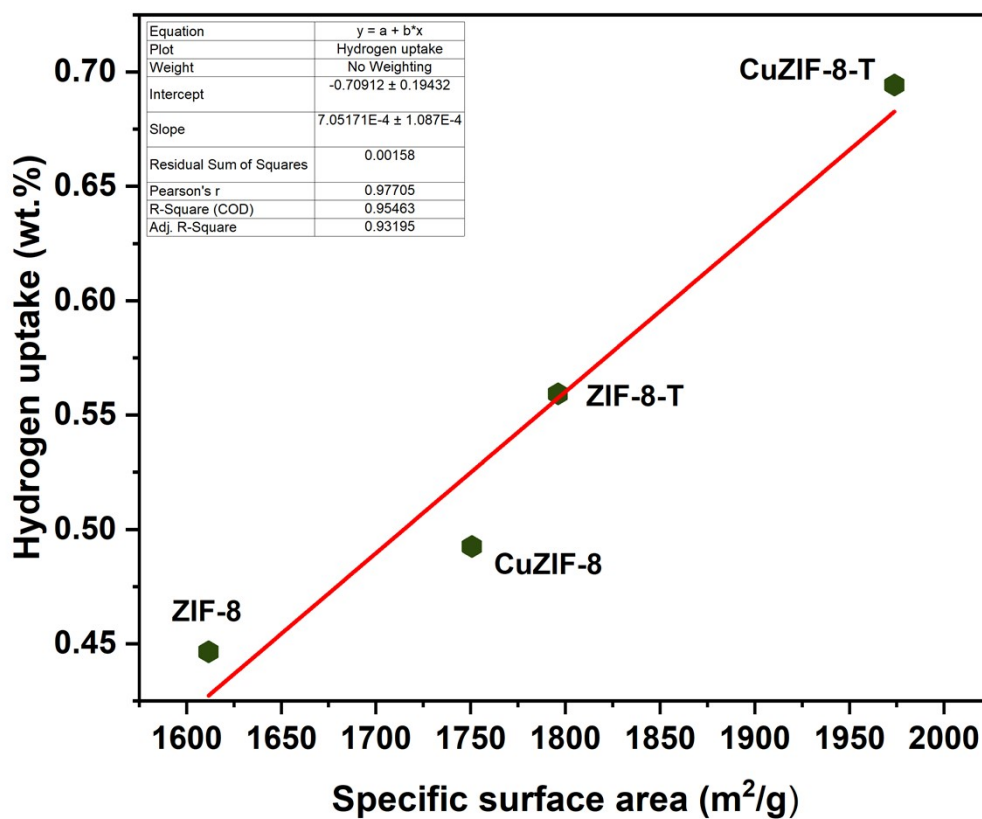


Figure S9 Linear trend between hydrogen uptake and specific surface area for the four samples.