SUPPORTING INFORMATION

Copper Oxide as Efficient Catalyst for Oxidative Dehydrogenation of Alcohols with Air

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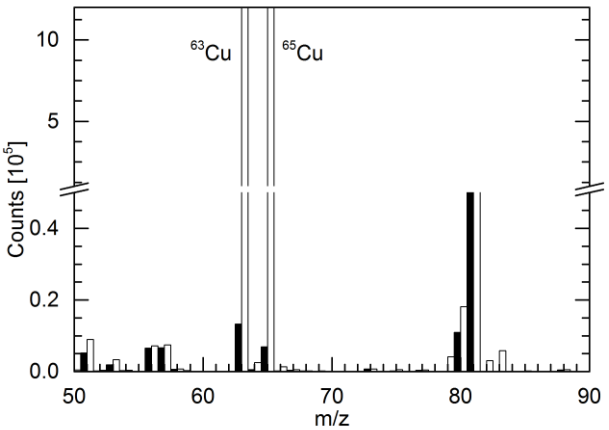
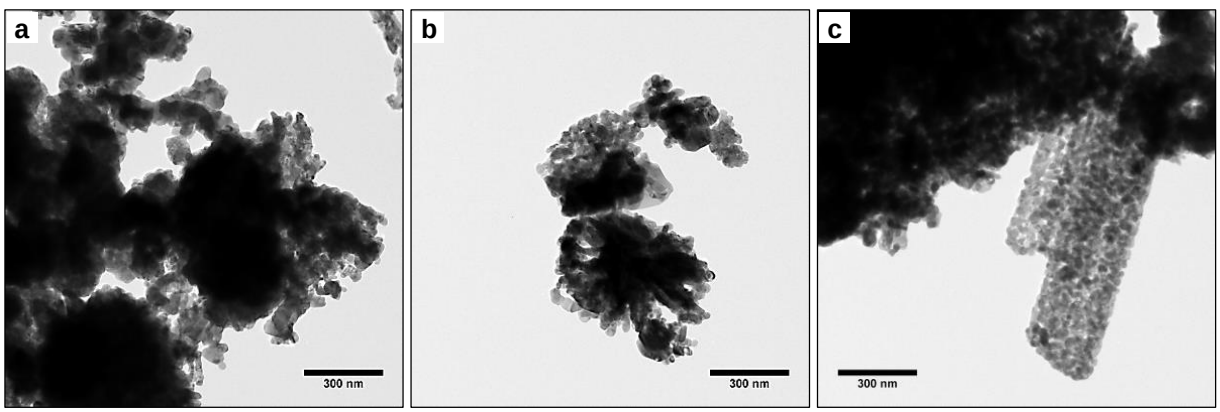
Inductively coupled plasma mass spectrometry (ICP-MS)



SI Fig. 1. ICP-MS of dissolved CAPS-CuO (white) and filtered solution after reaction for 24 h with CAPS-CuO catalyst (black).

Transmission electron microscopy

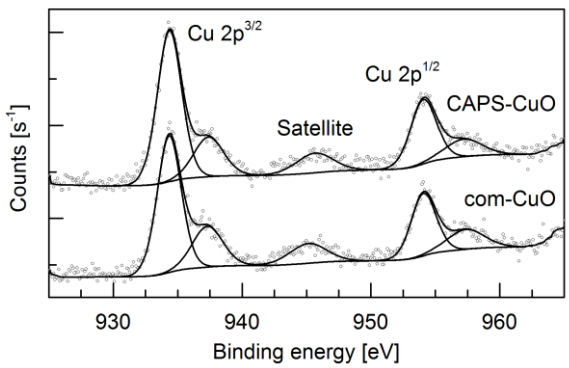


SI Fig. 2. TEM micrographs of as-received commercial CuO (com-CuO).

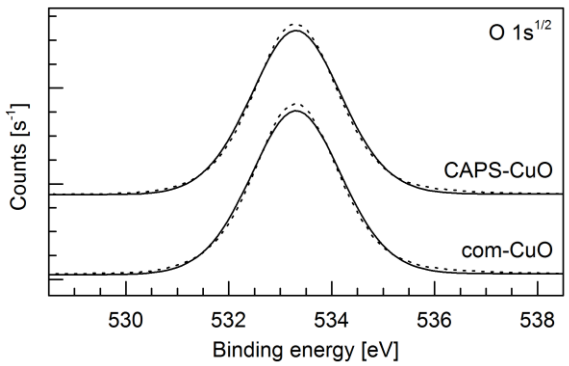
SI Table 1. Observed lattice spacings derived from the FFTs shown in Fig. 3 compared with calculated values.

	CAPS-CuO				MES-CuO		
	(hkl)	d_{obs}	d_{cal}		(hkl)	d_{obs}	d_{cal}
Fig. 3b	(020)	1.70 Å	1.71 Å	Fig. 3f	$(3\bar{1}1)$	1.33 Å	1.30 Å
	(200)	2.31 Å	2.31 Å		$(31\bar{1})$	1.42 Å	1.41 Å
	(110)	2.73 Å	2.75 Å		$(0\bar{2}2)$	1.45 Å	1.42 Å
	$(\bar{1}10)$	2.78 Å	2.75 Å		(200)	2.33	2.31 Å
Fig. 3d	(020)	1.72 Å	1.71 Å	Fig. 3h	$(1\bar{1}1)$	2.35	2.32 Å
	(200)	2.33 Å	2.31 Å		$(11\bar{1})$	2.56 Å	2.52 Å
	(110)	2.73 Å	2.75 Å		$(3\bar{1}1)$	1.33 Å	1.30 Å
	$(\bar{1}10)$	2.80 Å	2.75 Å		(200)	2.30 Å	2.31 Å

X-ray photoelectron spectroscopy (XPS)

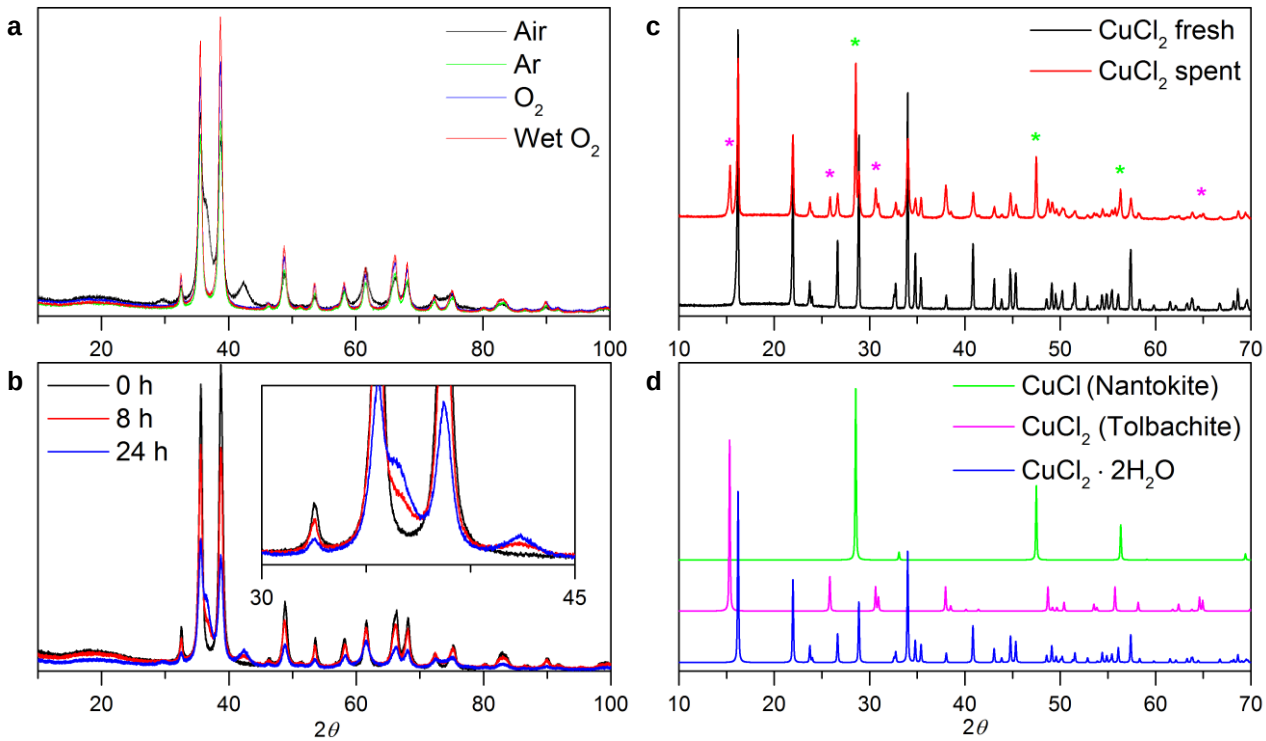


SI Fig. 3. XPS at the Cu 2p transition of CAPS-CuO (top) and MES-CuO (bottom).



SI Fig. 4. XPS at the O1s transition of CAPS-CuO (top) and com-CuO (bottom).

X-ray powder diffraction (XRD)



SI Fig. 5. XRD patterns of CAPS-CuO (a) after 24 h reaction in different atmospheres and (b) at different times during reaction. Inset in (b) shows a magnified view of the predominant Cu_2O peaks at 36.5° and 42.4°, respectively. The XRD patterns in (c) show the structural changes of $CuCl_2$ when used as catalyst. Reference patterns in (d) support that both dehydration and significant reduction to CuCl occurs.

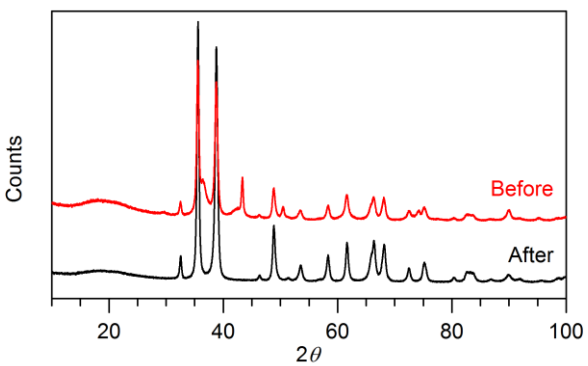
Rietveld refinement parameters

The crystal structures of fresh and spent CAPS-CuO and MES-CuO were refined by WINPOW (a local variation of LHMP). The Rietveld refinement for anatacamite was carried out by refining in a 2θ range from 20° (fresh) and 10° (spent) to 100° in steps of 0.02°. No atomic coordinates were refined. A Voigt profile function and a Chebyshev background polynomial were applied in all refinements. Crystallographic data and refinement summary are given in SI Table 2 and the refined patterns are shown in Fig. 1.

SI Table 2. Crystallographic data and refinement summary for the as-synthesized and spent CuO catalysts.

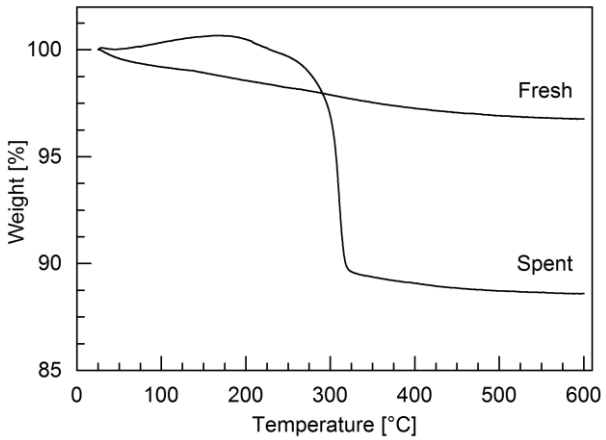
Sample	CAPS-CuO (Fresh)	MES-CuO (Fresh)	CAPS-CuO (Spent)			MES-CuO (Spent)		
Formula	CuO	CuO	CuO	Cu_2O	Cu	CuO	Cu_2O	Cu
Formula mass (g/mol)	79.55	79.55	79.55	143.1	63.55	79.55	143.1	63.55
Crystal system	Monoclinic	Monoclinic	Monoclinic	Cubic	Cubic	Monoclinic	Cubic	Cubic
Space group	C 1 c 1	C 1 c 1	C 1 c 1	P n -3 m Z	F m -3 m	C 1 c 1	P n -3 m Z	F m -3 m
***a* (Å)**	4.6817(2)	4.6833(2)	4.6930(4)	4.2596(3)	3.5938(1)	4.730(2)	4.2631(2)	3.6151(1)
***b* (Å)**	3.4175(2)	3.4170(2)	3.4260(3)	4.2596(3)	3.5938(1)	3.415(1)	4.2631(2)	3.6151(1)
***c* (Å)**	5.1317(3)	5.1302(3)	5.1240(5)	4.2596(3)	3.5938(1)	5.022(2)	4.2631(2)	3.6151(1)
***α* (°)**	90	90	90	90	90	90	90	90
***β* (°)**	99.266(2)	99.275(2)	99.332(5)	90	90	99.39(2)	90	90
***γ* (°)**	90	90	90	90	90	90	90	90
***V* (Å^3)**	81.04(1)	81.03(1)	81.29(2)	77.29(2)	46.42(5)	80.04(9)	77.48(1)	47.245(5)
Z	4	4	4	2	4	4	2	4
***ρ* (g/cm^3)**	6.519	6.520	6.498	6.148	9.092	6.600	6.133	8.933
Voigt particle size (Å)	175(0)	188(1)	-	-	-	-	-	-
Composition (wt%)			77.6(3)	21.1(1)	1.29(4)	6.8(1)	77.6(3)	15.60(8)
No. of parameters	12	12		27			24	
***R_{wp}* (%)**	2.49	2.81		4.93			5.50	
χ^2	0.35	0.48		2.30			2.82	
***R_p* (%)**	1.80	2.08		3.50			4.14	
No. of Bragg reflections	46	46	46	12	5	42	12	5
***R_B* (%)**	1.25	1.51	2.49	1.54	0.83	1.54	1.70	1.79

XRD of spent and regenerated CAPS-CuO



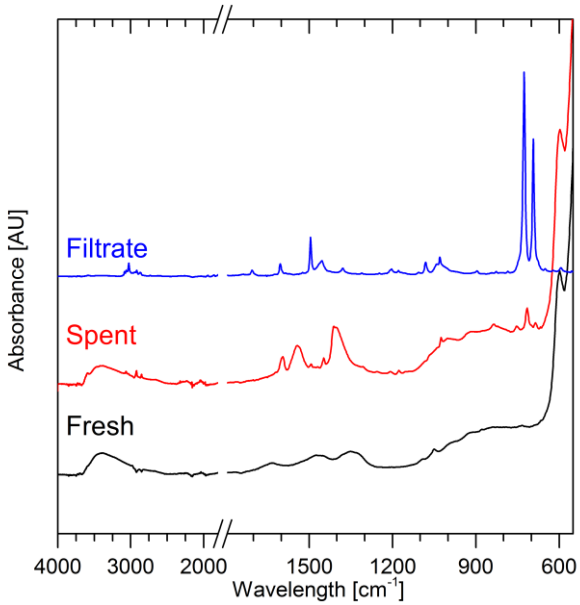
SI Fig. 6. XRD of CAPS-CuO before and after the thermal treatment.

Thermogravimetric analysis (TGA)



SI Fig. 7. TGA of fresh and spent CAPS-CuO with a heating rate of 10 °C/min.

Attenuated total reflectance Fourier transformed infrared spectroscopy (ATR-FTIR)



SI Fig. 8. ATR-FTIR spectra of fresh CAPS-CuO (black), spent CAPS-CuO after fourth reaction run without regeneration (red) and the reaction filtrate (blue).