

Supplementary Data to

A Colloidal ZnO@Cu Nanocatalyst for Methanol Synthesis

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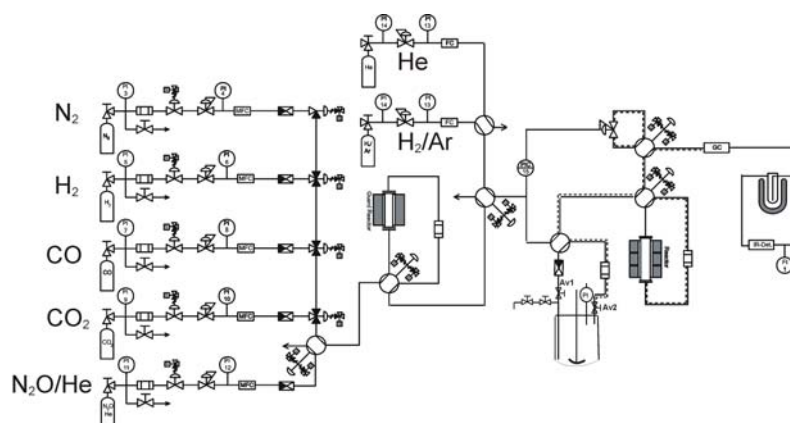
EXAFS

Table S1: Fitting parameters of Cu and ZnO@Cu colloids referring to Figure 2 of the main text. The k^2 weighted EXAFS were modelled between $k = 3.5$ and $k = 12.90$. For structural parameters FEFF files were used of Cu, CuO, Cu₂O (Cu-edge), Zn, ZnO (Zn-edge). All structural parameters were verified using the respective reference compounds.

Sample	Shell	C.N.	r (Å)	σ (10^{-3}Å^{-1})	E ₀	R-factor
Cu - As is	Cu-Cu	9.7 ± 0.6	2.542 ± 0.004	11.2 ± 0.5	0.6	5.8
Cu - Air 1x	Cu-O	0.6 ± 0.2	1.88 ± 0.03	7.0 ± 3.0	6.2	5.7
	Cu-Cu	5.1 ± 0.4	2.545 ± 0.004	11.5 ± 0.7	0.5	
Cu - Air 2x	Cu-O	0.7 ± 0.1	1.89 ± 0.03	4.9 ± 2.2	9.5	7.9
	Cu-Cu	3.7 ± 0.4	2.542 ± 0.006	10.5 ± 0.8	0.7	
Cu@ZnO - As is	Cu-Cu	8.6 ± 0.5	2.512 ± 0.005	14.2 ± 0.7	4.9	5.6
Cu@ZnO - Air 1x	Cu-O	0.7 ± 0.1	1.89 ± 0.03	5.9 ± 3.7	9.7	6.4
	Cu-Cu	6.6 ± 0.4	2.515 ± 0.005	14.2 ± 0.8	5.0	
Cu@ZnO - Air 2x	Cu-O	0.6 ± 0.1	1.83 ± 0.02	1.0 ± 0.0	11.1	10.0
	Cu-O	0.7 ± 0.2	1.97 ± 0.03	2.2 ± 2.9	12.1	
	Cu-Cu	2.7 ± 0.4	2.50 ± 0.01	12.1 ± 1.4	-0.1	
Cu@ZnO - As is	Zn-O	3.4 ± 0.1	1.990 ± 0.004	9.7 ± 0.7	10.0	8.7
Cu@ZnO - Air 1x	Zn-O	3.7 ± 0.1	1.98 ± 0.003	8.8 ± 0.6	8.8	6.4
Cu@ZnO - Air 2x	Zn-O	4.0 ± 0.1	1.98 ± 0.003	8.2 ± 0.6	9.3	6.4

Catalytic Tests

The colloid synthesis was scaled up and the freshly synthesised samples were diluted in 200 ml squalane and brought to the reactor under inert conditions. The experimental set-up according to Scheme S1 below used in these investigations consists of a 450 ml stainless steel reactor made by Parr Instruments. The autoclave was equipped with a magnetic stirrer with two four-blade impellers. The solution was mixed vigorously to ensure complete mixing of the liquid phase, uniform distribution of the catalyst, and high mass and heat transfer rates. The temperature of the reactor was controlled by a combination of an electric heating mantle and a cooling coil in the liquid phase. The pressure was controlled by a back-pressure regulator. The gas phase was analyzed with a gas chromatograph equipped with a Porapak and a Molecular sieve column. The complete online analysis time of one run is 22 minutes. The catalytic tests were run for a period of 3 h over several days up to two weeks without noticeable changes.



Scheme S1

Transmission electron microscopy

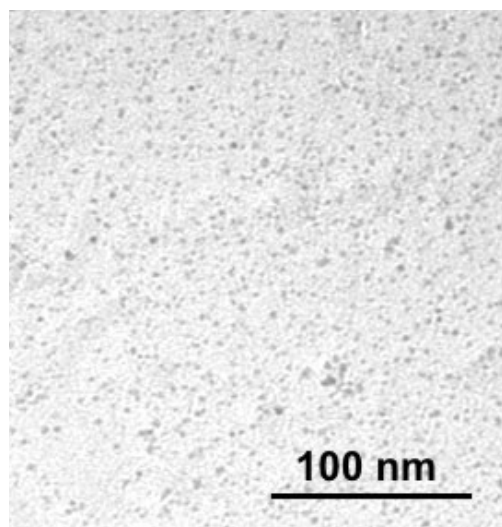


Figure S2: TEM image of ZnO@Cu (25:75) colloids, particle diameter 1-3 nm.