Supplementary Information

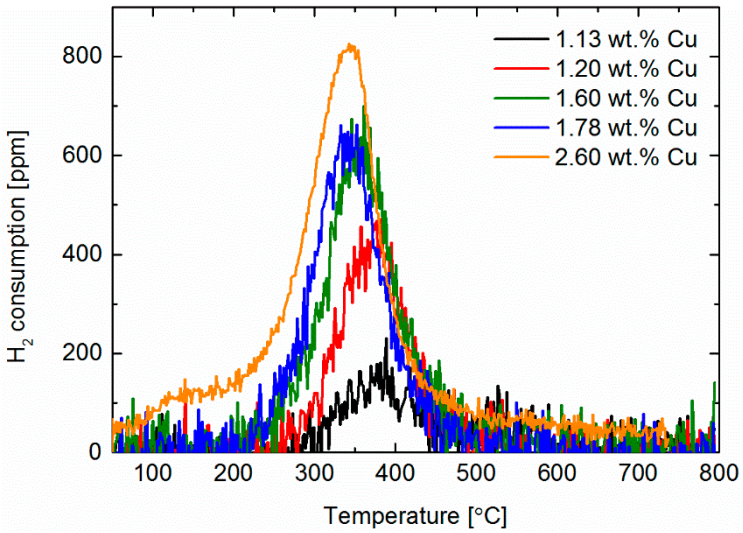
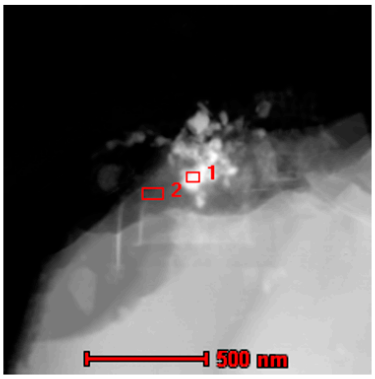
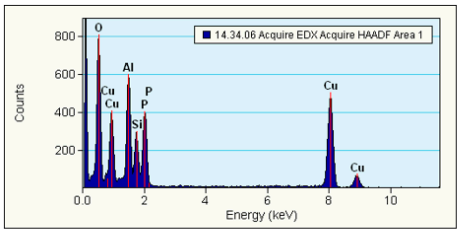


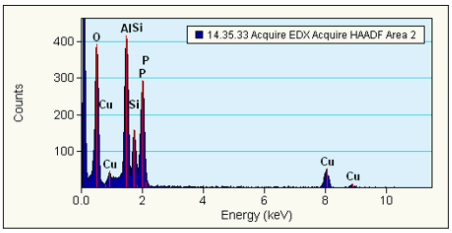
Figure S1. H_2 consumption during H_2-TPR. Feed: 0.3% H_2 in Ar. TPR performed from 50 to 800◦C with a heating rate of 10 ˚C/min.



There is a marked difference in the Cu signal between region 1 and 2. Region 1 clearly contains a high concentration of Cu.



Spectrum from region 1



Spectrum from region 2

Figure S2. TEM/EDS results of 2.60 wt.% Cu Cu/SAPO-34.

	Copper-exchanged SAPO-34					Parent SAPO-34		
Molarity $Cu(NO_3)_2$ solution (M)	Cu (wt.%)	Al (wt.%)	P (wt.%)	Si (wt.%)	Level of ion exchange (%)	Al (wt.%)	P (wt.%)	Si (wt.%)
	H-SAPO-34	16.10	11.90	4.89		17.20	12.40	5.10
0.05	1.13	15.90	11.60	4.71	21.2	19.40	14.20	5.98
0.2	1.20	16.00	11.50	4.72	22.4	19.40	14.20	5.98
0.4	1.60	16.30	11.90	4.78	29.6	17.20	12.40	5.10
0.6	1.78	18.00	13.30	5.26	29.8	17.80	12.70	5.43
0.8	2.60	19.60	16.30	5.86	39.1	n.m. [a]	n.m. [a]	n.m. [a]

Table S1. Elementary composition of the catalysts synthesised in this study, as determined by ICP-SMFS. a – not measured

In aluminosilicate zeolites, the level of copper ion exchange is calculated as 2 Cu (mol/g) / Al (mol/g) x 100%. However, this is not applicable to SAPO-34, because the number of negative framework charges to be compensated by the Cu ions does not depend on the number of Al atoms in the framework. SAPO-34 is generally viewed as arising from two possible isomorphic substitutions in a hypothetical AlPO4 lattice: 1) One Si substituted for one P (a negative charge results), and 2) two Si substituted for Al+P (an electrostatically neutral mechanism, since 3+5=2x4) [1]. If one assumes that one Si atom substitutes one P, then only mechanism 1 occurred [2, 3]. Thus there will be an exchange site for every Si atom in the framework [1]. The level of ion exchange may therefore be calculated as 2 Cu (mol/g) / Si (mol/g) x 100%, which equals 100% when ion exchange is complete (i.e., 2 Cu per Si). Over-exchanged SAPO-34 catalysts will have ion exchange levels above 100%. The levels of ion exchange thus calculated are shown in Table S1 and range between 21.2 and 39.1%, which means that none of the samples are over-exchanged. Note however that the validity of these exchange levels depends on the validity of the assumed substitution mechanism, which would need to be proven by identification of different Si species by ^{29}Si NMR.

References

1. Weitkamp, J.; Puppe, L., *Catalysis and Zeolites*. Softcover reprint of the hardcover 1st edition 1999 ed.; Springer-Verlag Berlin Heidelberg New York: 1999.
2. Wang, J.; Yu, T.; Wang, X.; Qi, G.; Xue, J.; Shen, M.; Li, W., The influence of silicon on the catalytic properties of Cu/SAPO-34 for NOx reduction by ammonia-SCR. *Applied Catalysis B: Environmental* **2012,** 127, (0), 137-147.
3. Xu, L.; Du, A.; Wei, Y.; Wang, Y.; Yu, Z.; He, Y.; Zhang, X.; Liu, Z., Synthesis of SAPO-34 with only Si(4Al) species: Effect of Si contents on Si incorporation mechanism and Si coordination environment of SAPO-34. *Microporous and Mesoporous Materials* **2008,** 115, (3), 332-337.