

Project report

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XAS studies on the copper environment in mesoporous copper incorporated MCM-41 materials.

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Previously, XAS have been used to determine the copper surroundings in the microporous material CuAPO-5.^{1,2} In this project, mesoporous structures being copper-incorporated have been studied, Cu-MCM-41 and Cu-SBA-15. As these materials have pore openings in a wide range, 20-300 Å,³ depending on synthesis conditions, they are interesting candidates for catalytic processes, for example in the conversion of biomass.⁴

A large number of transition metals have been substituted into the porous frameworks. As shown earlier,^{1,2} copper dislike tetrahedral environments, and require particular synthesis conditions to substitute for framework atoms. The XAS-results for Cu-MCM-41 and Cu-SBA-15 have shown that in these materials, copper is present as an extra-framework being oxidized to copper oxide upon calcination, rather than being sited framework. This is clearly seen from comparing the XANES and EXAFS spectra with the model compound, CuO (the spectra are shown by Nicholson and Nilsen¹), and also from refining the data (Figure 1 and Table 1).

Table 1: Comparison of multiplicities and distances for calcined Cu-Al-MCM-41 and CuO.

	calcined Cu-Al-MCM-41		CuO ⁵	
Bonding	N	r (Å)	N	r (Å)
Cu-O	4.1	1.95	4	1.96
Cu-O	—	—	2	2.78
Cu...Cu	8.3	2.93	8	2.90
Cu...Cu	2.1	3.13	2	3.08

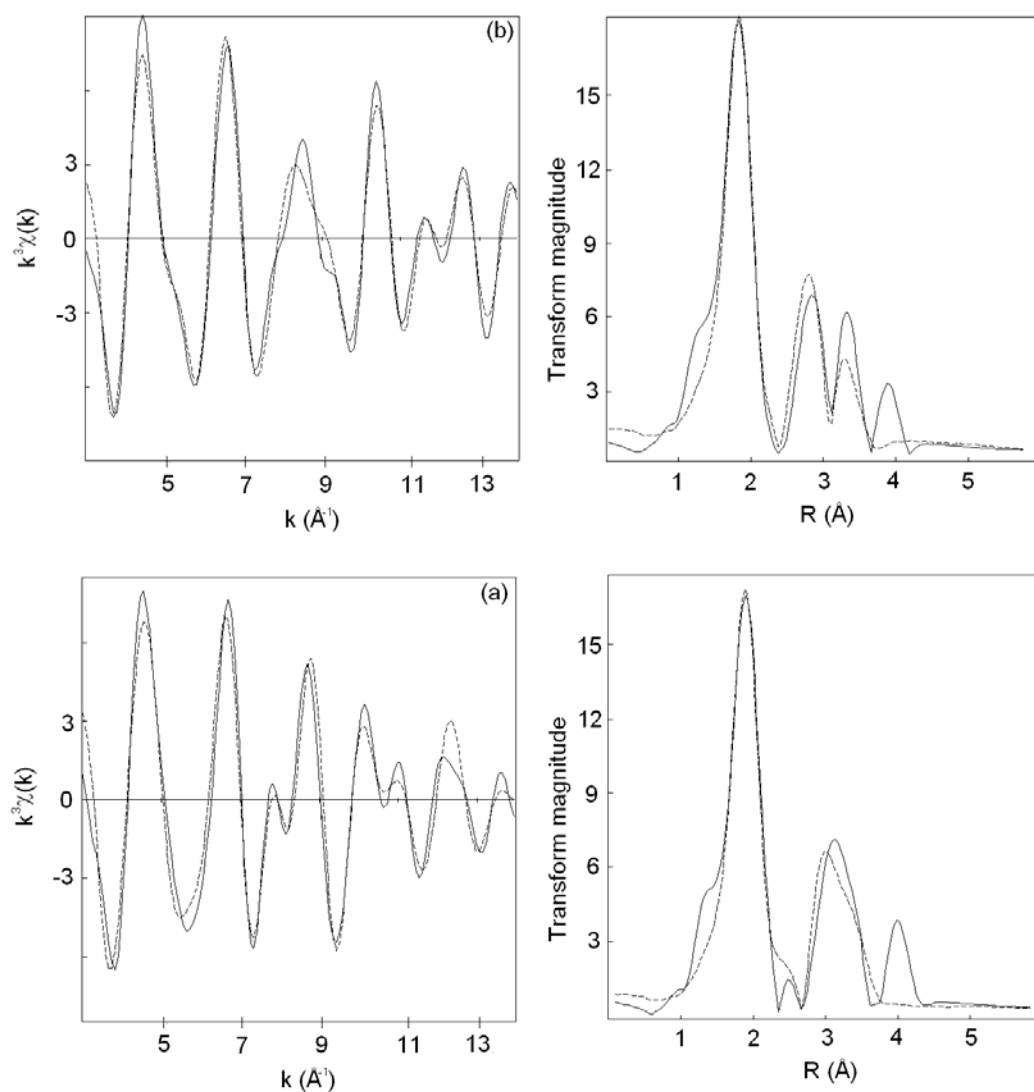


Figure 1 Experimental (—) and theoretical (---) Fourier filtered (1.0-25 Å) k^3 -weighted EXAFS and their Fourier transforms for Cu-Al-MCM-41, (a) as-synthesised sample and (b) calcined sample.

References

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