Supporting Information for

Structure of Copper sites in Zeolites Examined by Fourier and Wavelet Transform Analysis of EXAFS

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Computational Details

All ground-state total energy calculations in this work have been performed with the all-electron full-potential DFT code FHI-aims (*S1, S2*) within the periodic boundary conditions model. Electronic exchange and correlation was treated on the hybrid functional level with the PBE0 functional (*S3*). All geometry optimization were done with the "tier2" atom-centered basis set using "tight" settings for numerical integrations. Tkatchenko-Scheffler dispersion correction (*S4*) has been used to account for the van der Waals energies arising from the attraction between induced dipoles formed due to charge fluctuations in the interacting species. Mordenite geometries reported herein correspond to the locally optimized configurations. Faujasite geometries correspond to locally optimized configurations under the assumption that the copper oxide cluster inside of the pore exhibits the C_{2v} symmetry, consistent with the experimentally observed bond lengths distribution.

Mordenite centers correspond to the periodic model of the mordenite structure, having 8- and 12-ring channels running parallel to the *c* axis, which are intersected by sinusoidal 8-ring channels that run parallel to the *b* axis. These form side pockets that connect the 12-ring channel with the 8-ring channel. There are two 12-ring and two 8-ring channels per unit cell of mordenite. Two symmetrically located aluminium atoms per 8-ring channel have been assumed, which corresponds to the Si/Al ratio of 11.

Faujasite centers correspond to the periodic model, composed of sodalite cages with diameter of 6.6 Å connected to supercages having a diameter of 12.4 Å. These two units are interconnected by hexagonal prisms whose opening is of 2.3 Å. These supercages are linked together by a 12MR ring with diameter of 7.4 Å, forming the porous accessible network.

Wavelet transform details

For the continuous wavelet transform of EXAFS data Morlet mother function was used:

$$\psi(x) = 1/\sqrt[4]{\pi}\cos(x\pi\sqrt{2/\log(2)})\exp(-\frac{x^2}{2}),$$

which corresponds to the frequency $\omega = \pi\sqrt{2/\log(2)}$ and bandwidth $\sigma^2 = 1$. The used frequency in close to the frequencies of backscattered waves making the resolution in k-space of WT better.

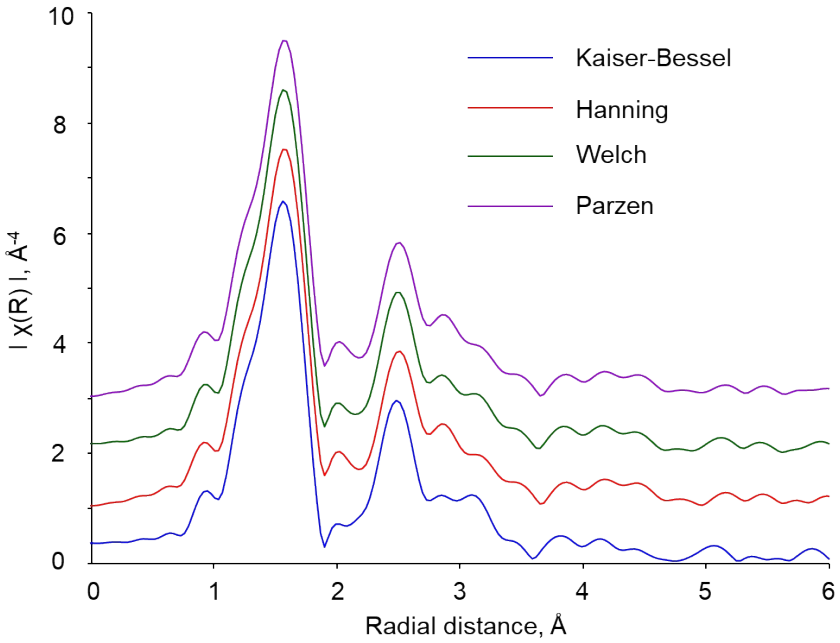

Fig. S1. Results of the Fourier transform of the k^3-weighted EXAFS spectrum of Cu(2.7)FAU(15) with different apodization window functions. It shows the splitting observed for the second coordination sphere is not a function of applied apodization.

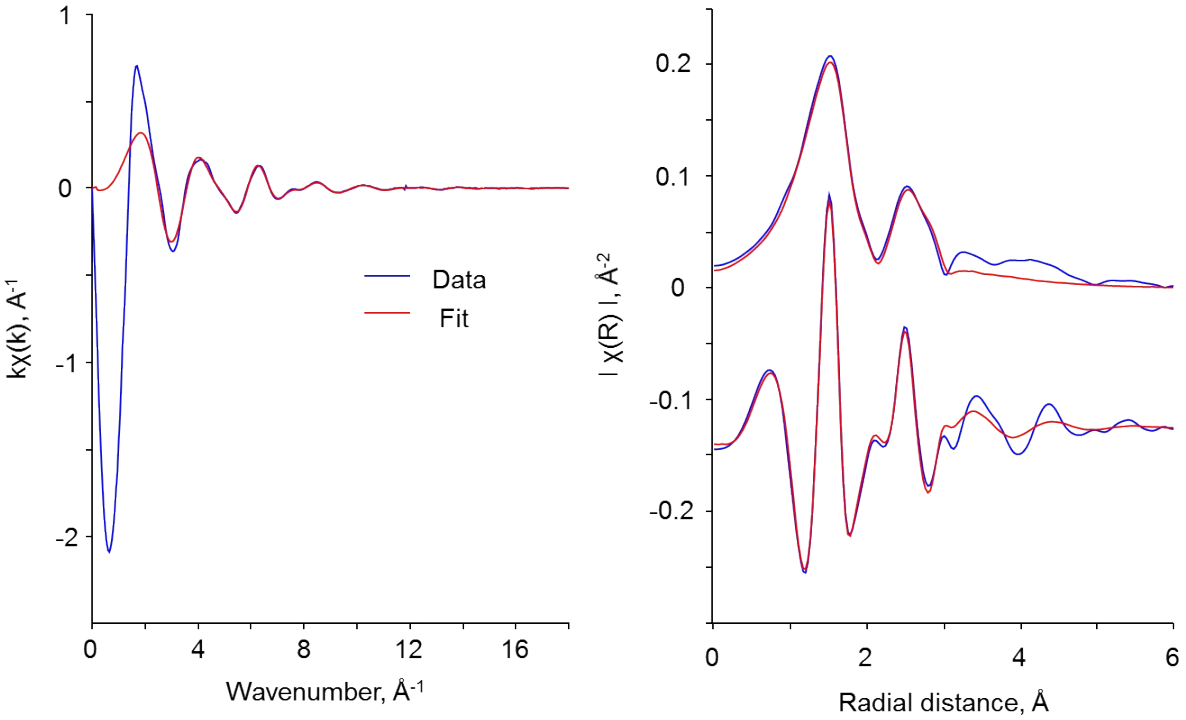

Fig. S2. Results of the fitting of k^3-weighted FT EXAFS spectrum of Cu(3.4)MOR(10), displayed with k^1-weightening. Left part corresponds to the fitted k-space and right part shows R-space magnitudes and real part of FT. The fit was performed in R-space, in the range of 1.0–3.0 Å, employing the k-range of 3.0–16.0 $Å^{-1}$ for the FT. The absence of additional peaks in k^1 data indicated the negligible contribution of multiple scattering pathways to the EXAFS spectrum.

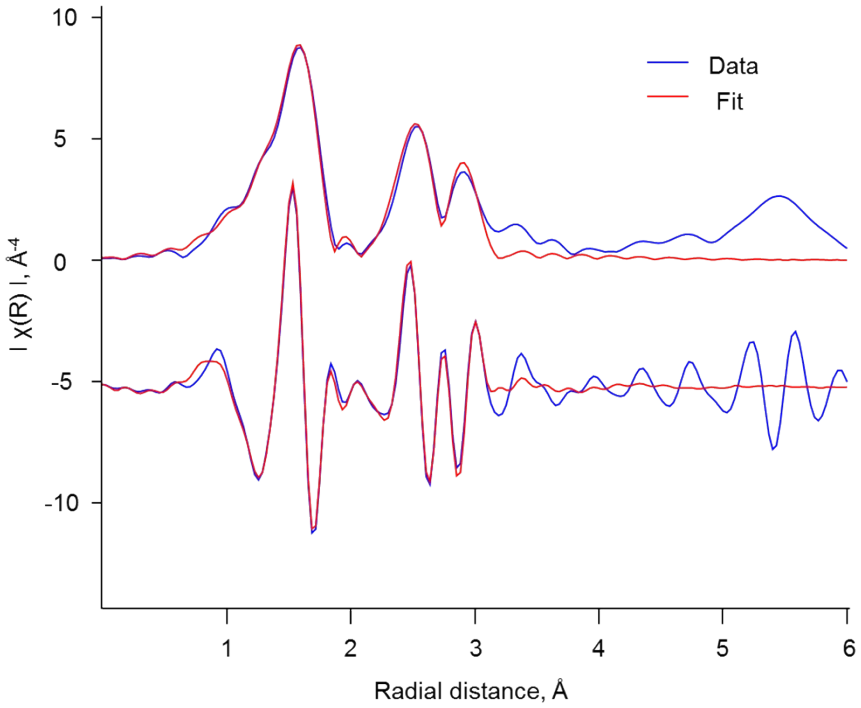

Fig. S3. Results of the fitting of k^3-weighted FT EXAFS spectrum of CuO standard. The fit was performed in R-space, in the range of 1.0–3.3 Å, employing the k-range of 3.0–16.4 $Å^{-1}$ for the FT. Five main single scattering paths extracted from tenorite crystallographic structure were used for the fitting. The details of the fit are given in Table S1. The obtained data points to the negligible contribution of multiple scattering paths in the range of 1.0–3.3 Å.

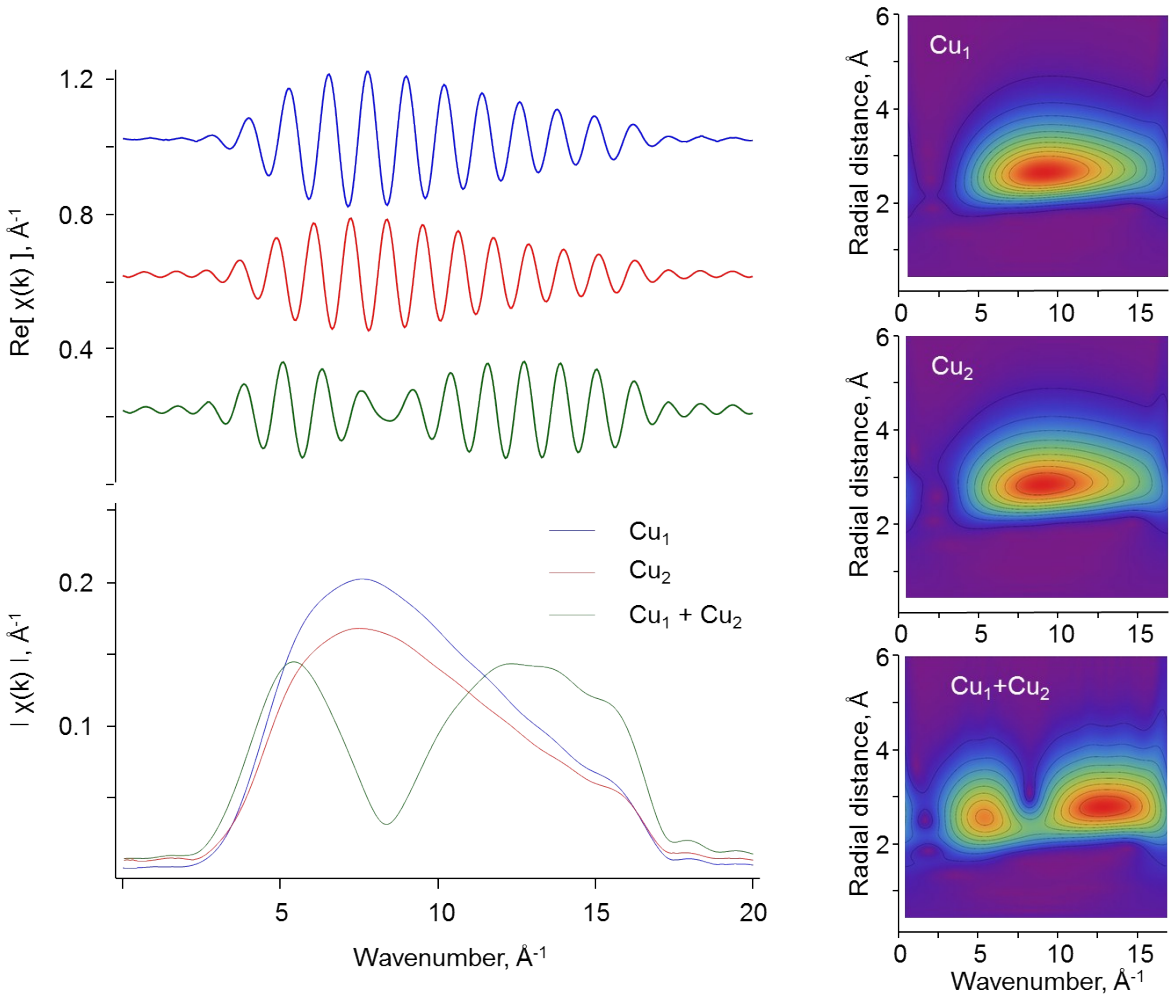

Fig. S4. Real parts of backscattering waves, their wavelet transforms and corresponding amplitudes obtained by simulation of scattering paths from copper atoms in copper (II) oxide, remoted by 2.88 and 3.07 A from the absorber.

For the atoms of a particular nature, having a low to moderate Z number, there is a single main maximum on the curve describing backscattering factor dependence on k value. This is indeed the case for the isolated atoms. However, in case, multiple non-equivalent atoms of similar nature are located at similar distances, the addition of backscattered waves can lead to destructive interference, which results in the appearance of several maxima on the corresponding magnitude curve.

As an example, the magnitude of the wave, obtained by a combination of two backscattering waves from copper atoms in copper oxide is shown. It is clear, that those two atoms individually have magnitudes with one maximum. However, the sum of these waves results in beating and the appearance of two maxima on the magnitude curve and, respectively, in the WT counterplots.

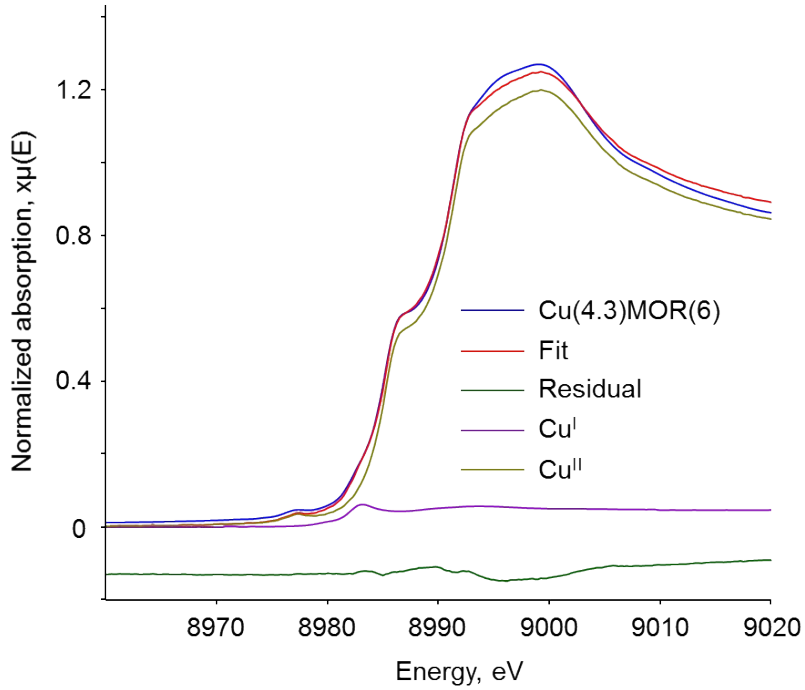

Fig. S5. Results of linear combination fitting analysis of XANES spectrum for the Cu(4.3)MOR(6), using two standards obtained by the treatment: i) in oxygen at 773K and ii) in methane at 773K for 1h. It returns the Cu^{I} concentration of 3.4%.

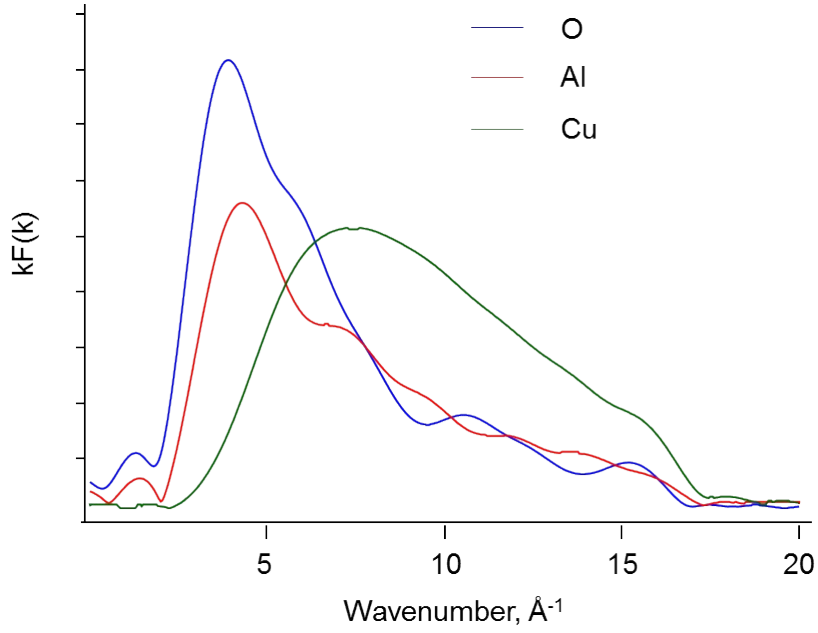

Fig. S6. Plot of the k-weighted backscattering amplitude factor calculated for single scattering paths with copper atom as absorber. For the calculations, dicopper mono-μ-oxo species located in an 8-membered ring of mordenite, optimized with density functional theory (DFT) was used.

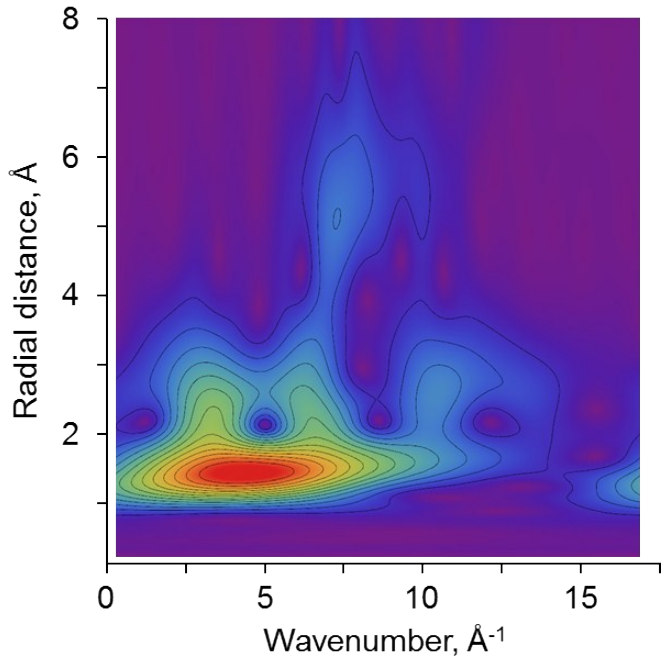

Fig. S7. 2D plots of WT EXAFS for k^2-weighted $\chi(k)$ data for CuO.

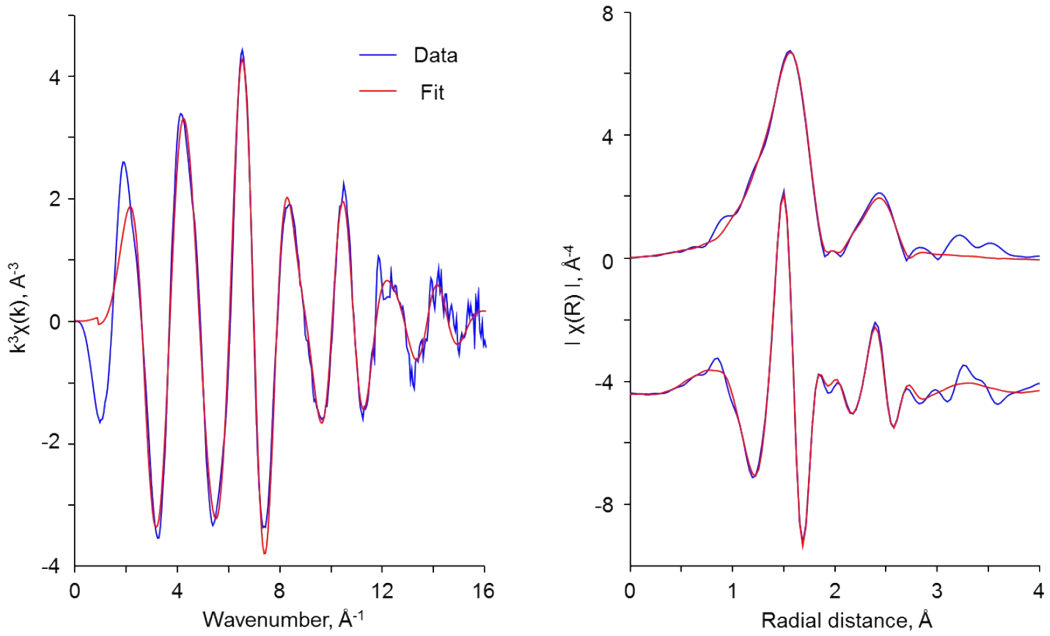

Fig. S8. Results of the fitting of k^3-weighted FT EXAFS spectrum of Cu(3.4)MOR(10). Left part corresponds to the fitted k-space and right part shows R-space magnitudes and real part of FT. The fit was performed in R-space, in the range of 1.0–3.0 Å, employing the k-range of 3.0–16.0 $Å^{-1}$ for the FT.

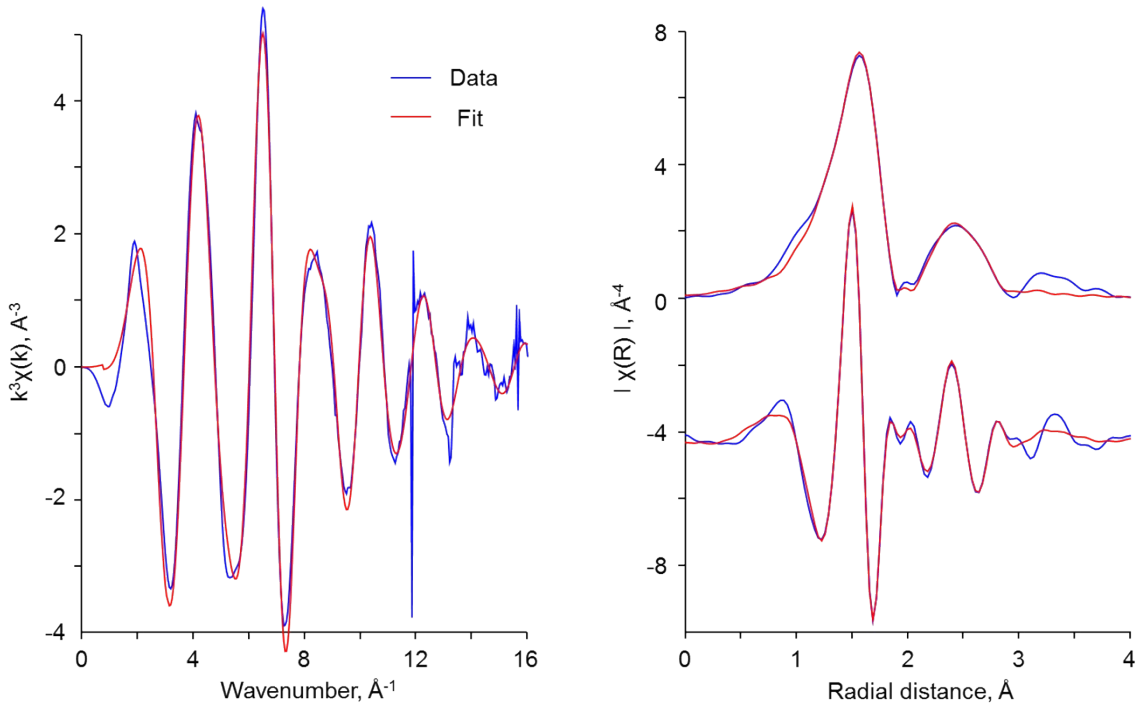

Fig. S9. Results of the fitting of k^3-weighted FT EXAFS spectrum of Cu(4.0)MFI(12). Left part corresponds to the fitted k-space and right part shows R-space magnitudes and real part of FT. The fit was performed in R-space, in the range of 1.0–3.0 Å, employing the k-range of 3.0–16.0 $Å^{-1}$ for the FT.

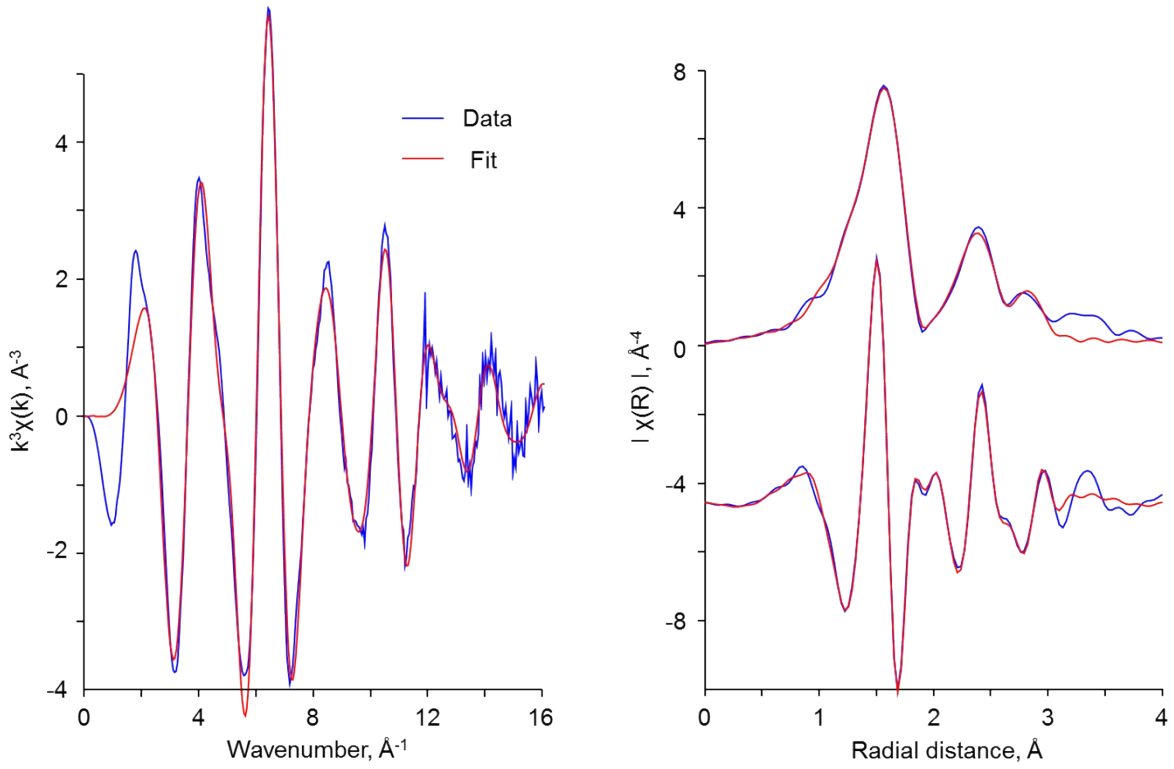

Fig. S10. Results of the fitting of k^3-weighted FT EXAFS spectrum of Cu(2.8)BEA(12). Left part corresponds to the fitted k-space and right part shows R-space magnitudes and real part of FT. The fit was performed in R-space, in the range of 1.0–3.2 Å, employing the k-range of 3.0–16.0 $Å^{-1}$ for the FT.

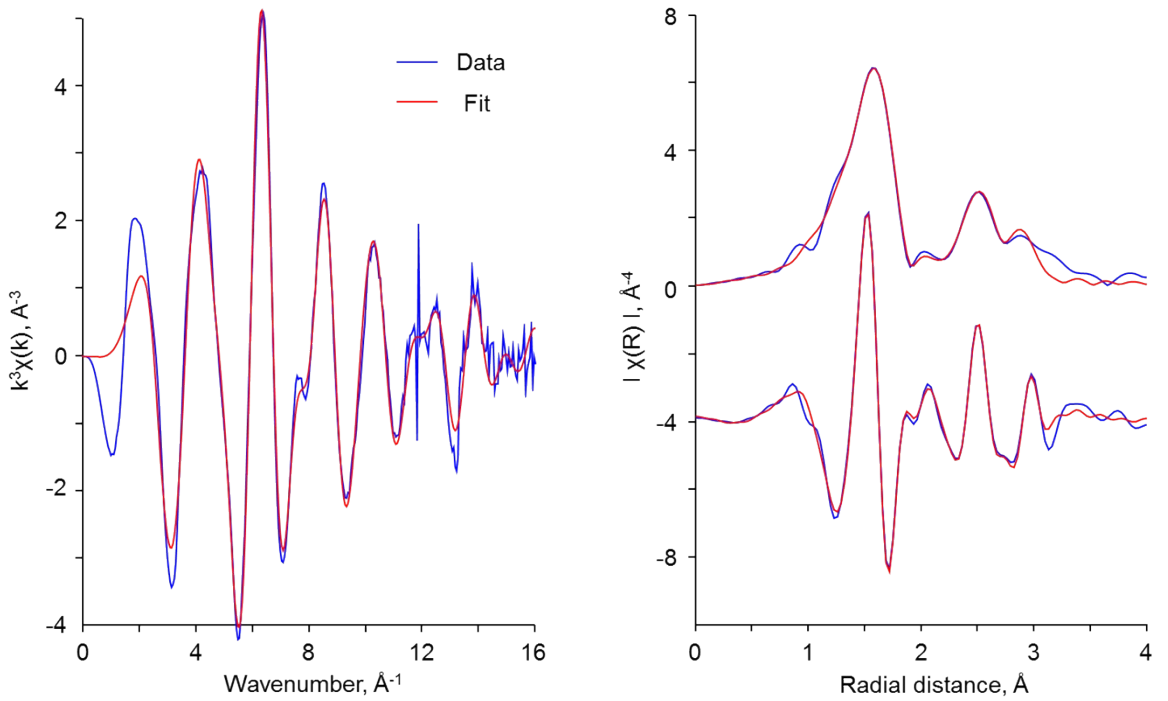

Fig. S11. Results of the fitting of k^3-weighted FT EXAFS spectrum of Cu(2.7)FAU(15). Left part corresponds to the fitted k-space and right part shows R-space magnitudes and real part of FT. The fit was performed in R-space, in the range of 1.0–3.2 Å, employing the k-range of 3.0–16.0 $Å^{-1}$ for the FT.

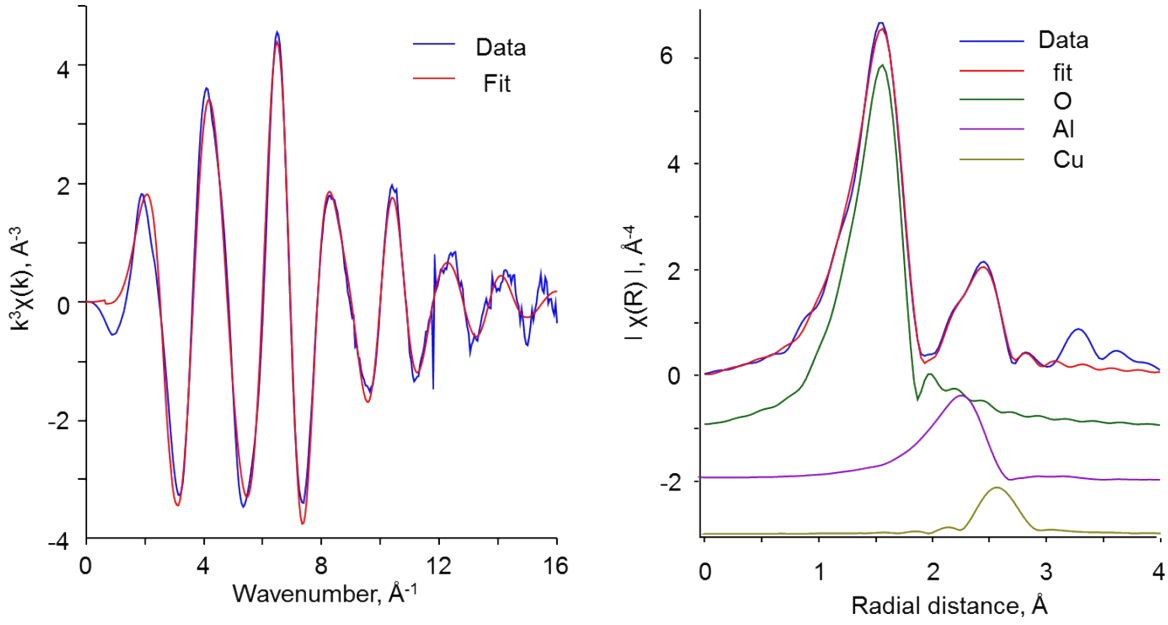

Fig. S12. Results of the fitting of k^3-weighted FT EXAFS spectrum of Cu(3.4)MOR(10) using both Al and Cu scatters contributing to the second coordination shell. Left part displays the k-space data and the resulting fit, while right part shows the magnitudes due to oxygen, aluminum and copper atoms, impacting to the resulting FT EXAFS.

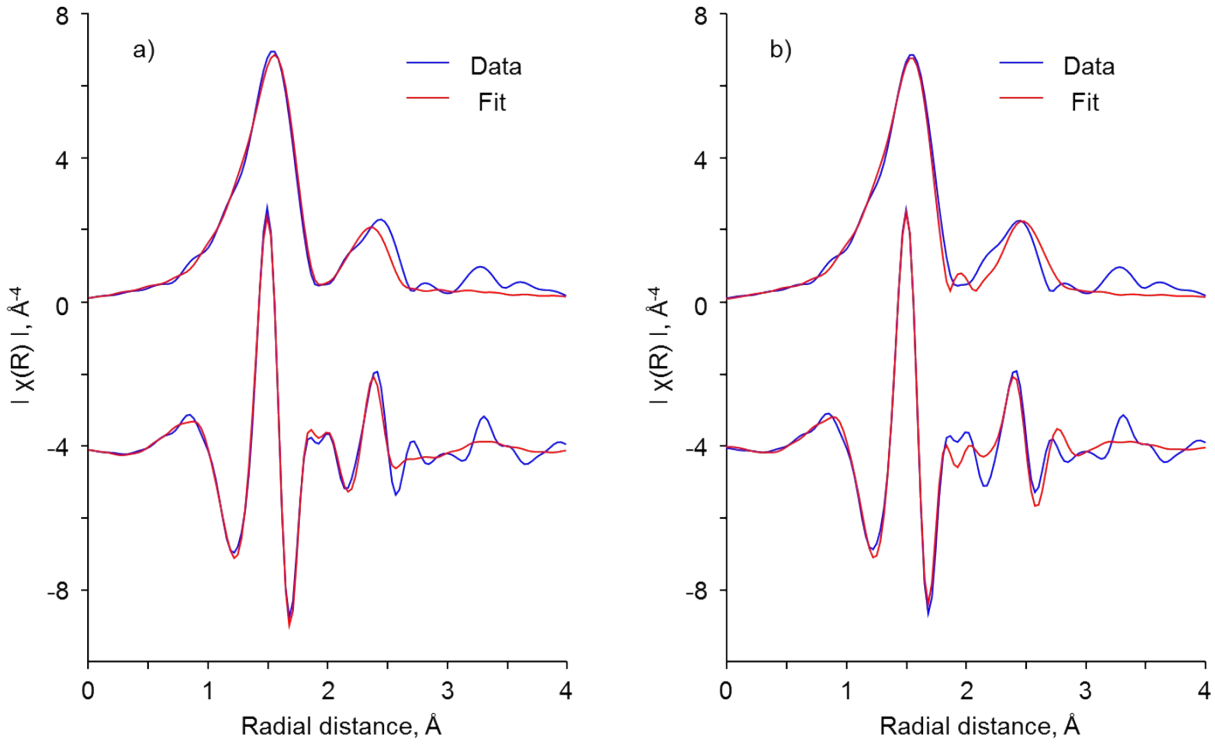

Fig. S13. Examples of k^3-weighted EXAFS fits of Cu(4.3)MOR(6) material: a) with exclusive contribution of Al in the second shell and b) with exclusive contribution of Cu. A clear misfits are visible, which can only be avoided by the fitting of the second shell with simultaneous contribution from both Al and Cu.

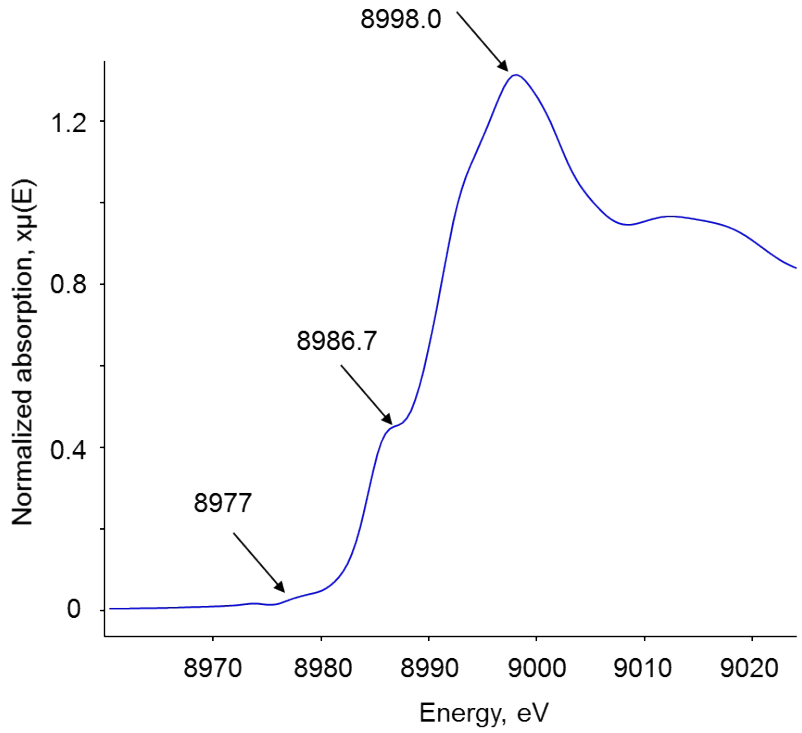

Fig. S14. Cu K-edge XANES spectrum of bulk CuO, measured at 298 K.

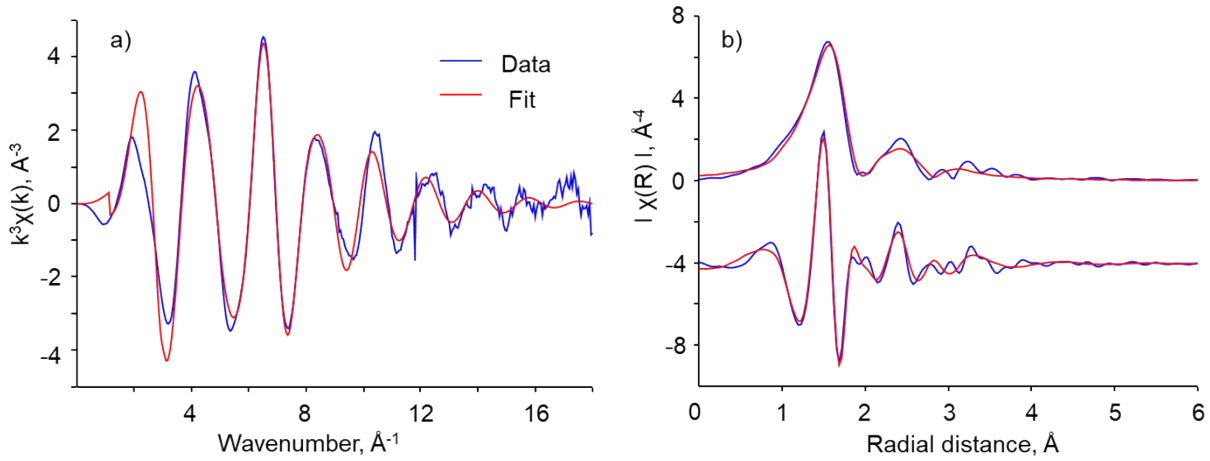

Fig. 15. Results of the fitting of k^3-weighted FT EXAFS spectrum of Cu(4.3)MOR(6) using the fit obtained for Cu(2.7)FAU(15) as the initial guess with fixed interatomic distances. Left part corresponds to the fitted k-space and right part shows R-space magnitudes and real part of FT.

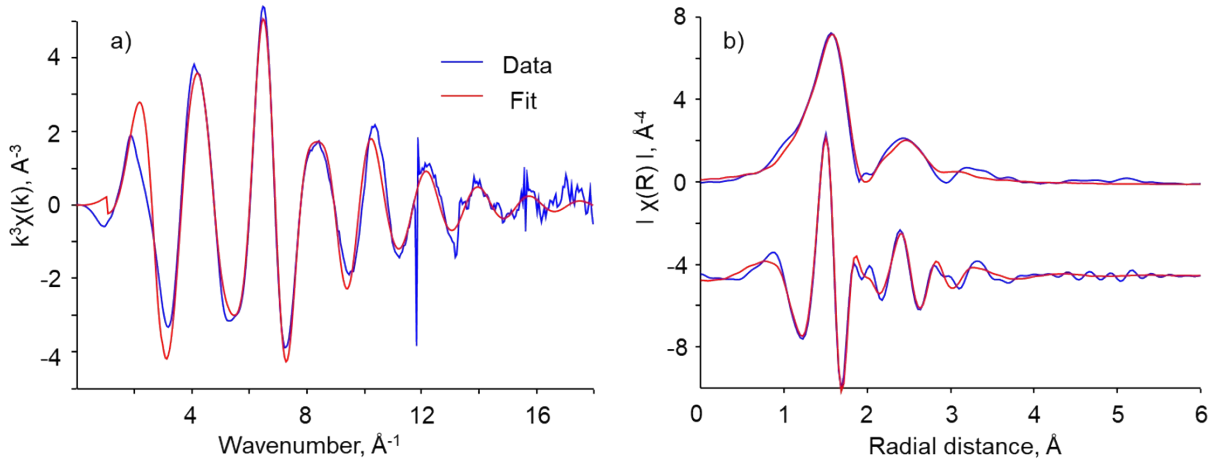

Fig. S16. Results of the fitting of k^3-weighted FT EXAFS spectrum of Cu(4.0)MFI(12) using the fit obtained for Cu(2.7)FAU(15) as the initial guess with fixed interatomic distances. Left part corresponds to the fitted k-space and right part shows R-space magnitudes and real part of FT.

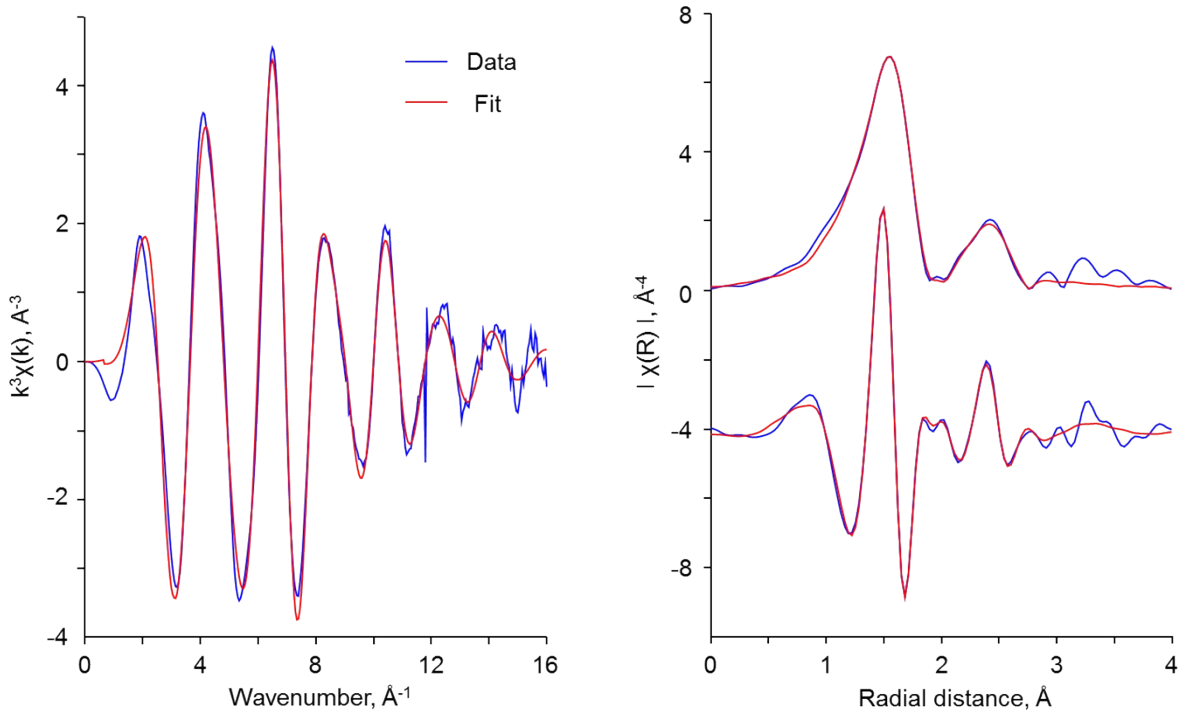

Fig. S17. Results of the fitting of k^3-weighted FT EXAFS spectrum of Cu(4.3)MOR(6). Left part corresponds to the fitted k-space and right part shows R-space magnitudes and real part of FT. The fit was performed in R-space, in the range of 1.0–3.0 Å, employing the k-range of 3.0–16.0 $Å^{-1}$ for the FT.

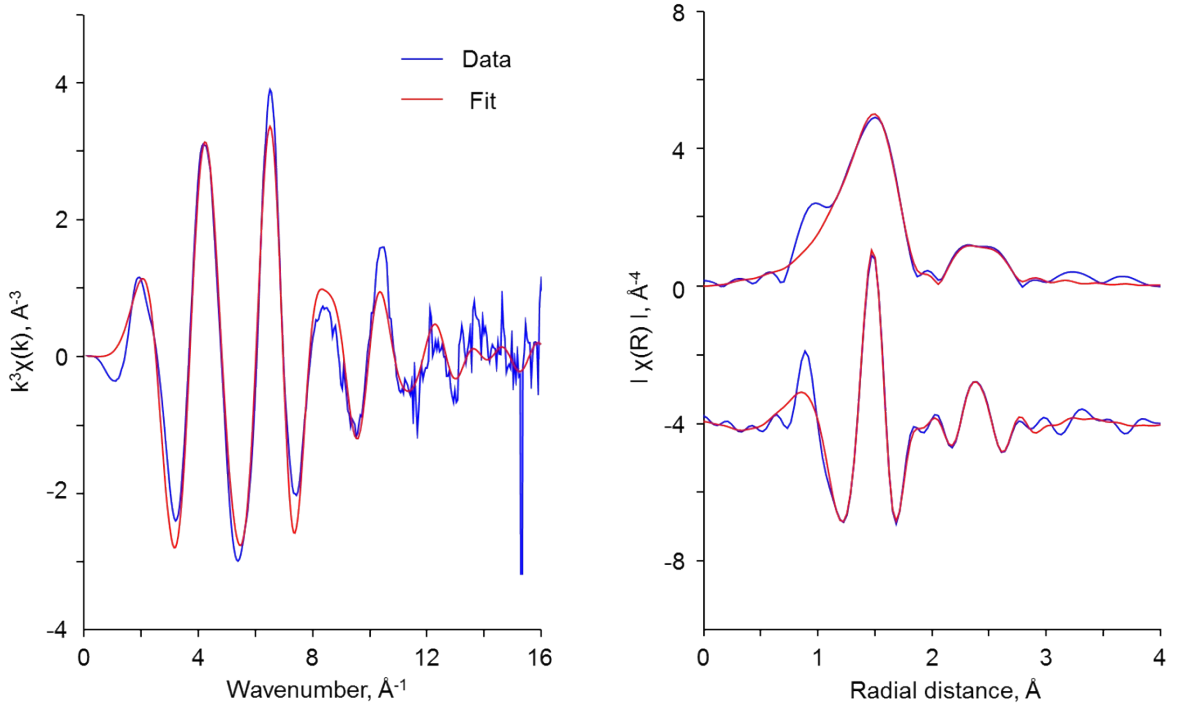

Fig. S18. Results of the fitting of k^3-weighted FT EXAFS spectrum of Cu(1.2)MOR(46). Left part corresponds to the fitted k-space and right part shows R-space magnitudes and real part of FT. The fit was performed in R-space, in the range of 1.0–3.0 Å, employing the k-range of 3.0–16.0 $Å^{-1}$ for the FT.

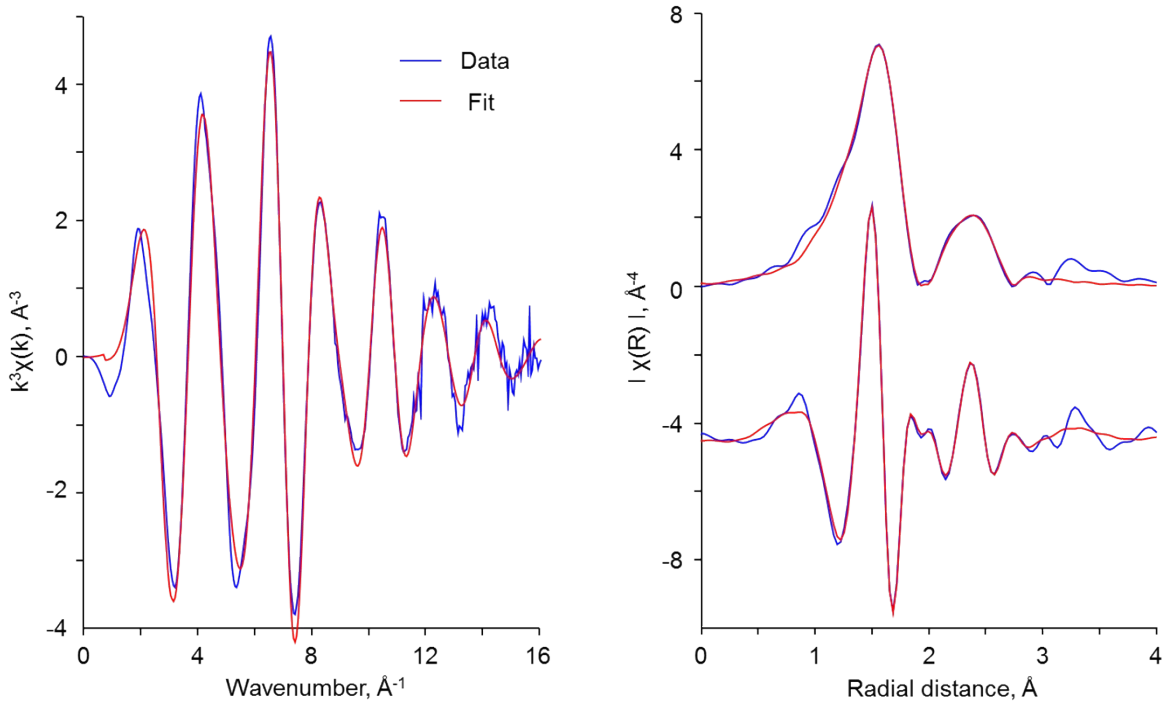

Fig. S19. Results of the fitting of k^3-weighted FT EXAFS spectrum of Cu(3.5)MOR(6). Left part corresponds to the fitted k-space and right part shows R-space magnitudes and real part of FT. The fit was performed in R-space, in the range of 1.0–3.0 Å, employing the k-range of 3.0–16.0 $Å^{-1}$ for the FT.

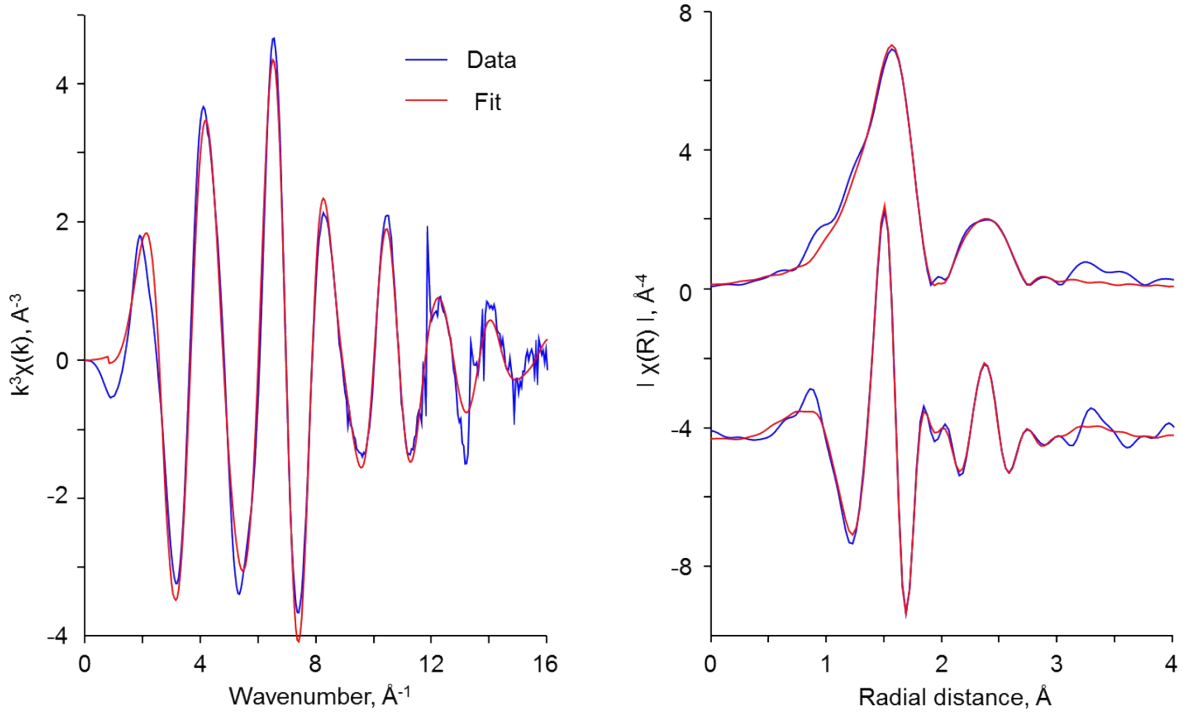

Fig. S20. Results of the fitting of k^3-weighted FT EXAFS spectrum of Cu(3.2)MOR(6). Left part corresponds to the fitted k-space and right part shows R-space magnitudes and real part of FT. The fit was performed in R-space, in the range of 1.0–3.0 Å, employing the k-range of 3.0–16.0 $Å^{-1}$ for the FT.

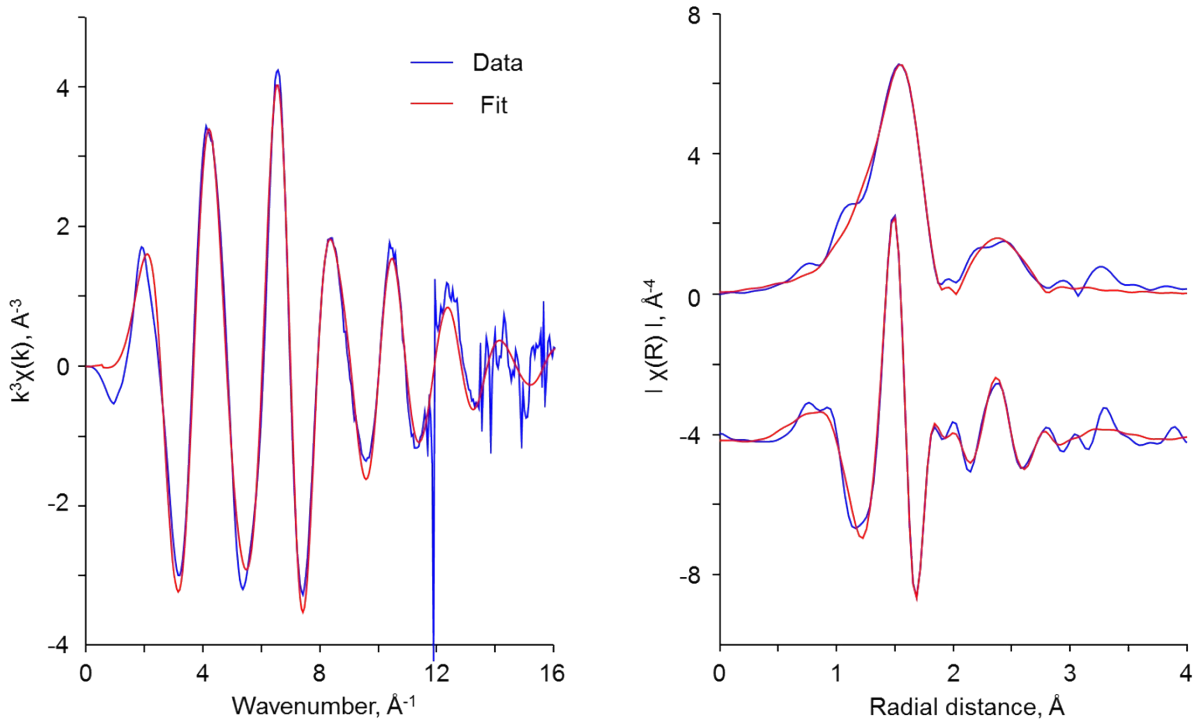

Fig. S21. Results of the fitting of k^3-weighted FT EXAFS spectrum of Cu(2.5)MOR(6). Left part corresponds to the fitted k-space and right part shows R-space magnitudes and real part of FT. The fit was performed in R-space, in the range of 1.0–3.0 Å, employing the k-range of 3.0–16.0 $Å^{-1}$ for the FT.

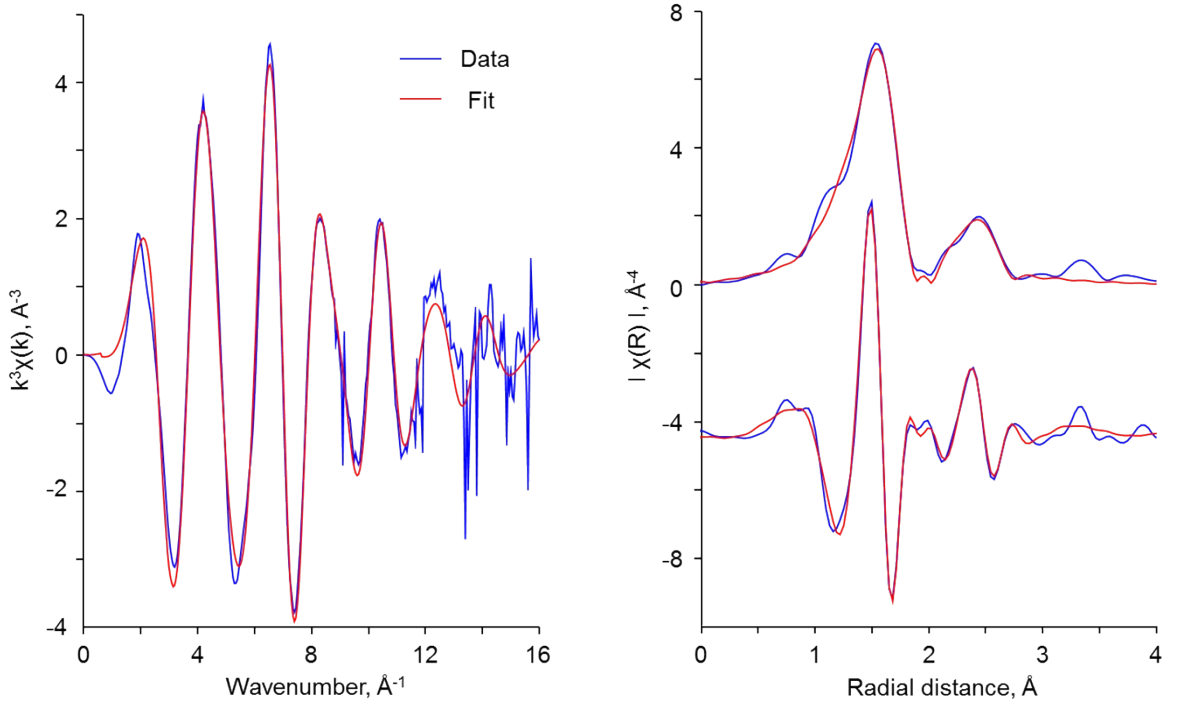

Fig. S22. Results of the fitting of k^3-weighted FT EXAFS spectrum of Cu(1.7)MOR(6). Left part corresponds to the fitted k-space and right part shows R-space magnitudes and real part of FT. The fit was performed in R-space, in the range of 1.0–3.0 Å, employing the k-range of 3.0–16.0 $Å^{-1}$ for the FT.

Table S1. Best-fit parameters optimized by EXAFS fits of the k^3-weighted spectrum of standard CuO. The tenorite crystallographic structure was used to generate scattering paths. Degeneracies were fixed according to the crystal structure. Other parameters, including Debye-Waller factors and effective radii were released. The fit was performed in R-space in the range of 1.0–3.3 Å, employing the k-range of 3.0–16.4 $Å^{-1}$ for the FT, resulting in a number of independent points $N_{ind} > 19$.

Parameter	Scatter	CuO
ΔE, eV		+0.1(9)
N_O		4
R(Cu-O_1), Å	O_1	1.953(5)
Debye-Waller factor, 10^{-3} $Å^2$		4(0)
N_{Al}		2
R(Cu-O_2), Å	O_2	2.74(6)
Debye-Waller factor, 10^{-3} $Å^2$		14(9)
N_{Cu}		4
R(Cu-Cu_1), Å	Cu_1	2.91(1)
Debye-Waller factor, 10^{-3} $Å^2$		8(1)
N_{Cu}		4
R(Cu-Cu_2), Å	Cu_2	3.06(5)
Debye-Waller factor, 10^{-3} $Å^2$		15(8)
N_{Cu}		2
R(Cu-Cu_2), Å	Cu_3	3.12(2)
Debye-Waller factor, 10^{-3} $Å^2$		6(2)
R-factor		0.012
χ^2-parameter		189

Table S2. Best-fit parameters optimized by EXAFS fits of the k^3-weighted spectrum of activated copper-exchanged MOR and MFI. The fit obtained for Cu(2.7)FAU(15) with fixed

atom coordinates was used as the starting guess. Other parameters, including Debye-Waller factors and amplitudes were released. The fit was performed in R-space in the range of 1.0–3.2 Å, employing the k-range of 3.0–16.0 $Å^{-1}$ for the FT, resulting in a number of independent points $N_{ind} > 16$.

Parameter	Scatter	Cu(4.3)MOR(6)	Cu(4.0)MFI(12)
ΔE, eV		+4.9(9)	+4.6(8)
N_O		4.2(5)	4.1(4)
R(Cu-O), Å	O	1.959(3)	1.959(4)
Debye-Waller factor, 10^{-3} $Å^2$		7.3(10)	6.5(1)
N_{Al}		12(7)	10(7)
R(Cu-Al, Si), Å	Al or Si	2.77	2.77
Debye-Waller factor, 10^{-3} $Å^2$		41(15)	40(16)
N_{Cu}		4.1(53)	4.3(26)
R(Cu-Cu_1), Å	Cu	2.93	2.93
Debye-Waller factor, 10^{-3} $Å^2$		28(14)	22(6)
N_{Cu}		-3.7(60)	-2.6(24)
R(Cu-Cu_2), Å	Cu	3.08	3.08
Debye-Waller factor, 10^{-3} $Å^2$		28(15)	22(6)
R-factor		0.025	0.0146
χ^2-parameter		1320	139

The obtained fits returned negative values for the second copper atom in the second coordination sphere, together with unrealistic coordination numbers for aluminum, indicating the absence of this scattering pathway in copper-exchanged MFI and MOR, hence confirming the different nature of copper-oxo species in zeolites of different structure.

Cartesian coordinates of the mono(μ-oxo)dicopper site in mordenite:

```
lattice_vector    18.25600000     0.00000000     0.00000000
lattice_vector     0.00000000    20.53400000     0.00000000
lattice_vector     0.00000000     0.00000000     7.54200000
atom       5.24642699    -0.10964989    -0.09536664 O
atom      13.95743362    10.39769246    -0.01163178 O
atom      12.96732457     0.18074116    -0.32314149 O
atom       4.18269061    10.43394489    -0.07714041 O
atom       4.95274291    -0.09710210     4.02627764 O
atom      14.53445099    10.65082711     3.89211269 O
atom      13.35787421     0.14517226     3.78595966 O
atom       3.88938607    10.09376579     3.52271479 O
atom       5.78268376     1.51043534     1.99546492 O
atom      15.54551403    11.81908162     1.66194991 O
atom      11.97503336     1.45019415     1.86468173 O
atom       3.19071922    12.08707331     1.84223244 O
atom       5.94224838    18.52355461     5.65607538 O
atom      15.04255323     8.71590677     5.67367657 O
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atom       2.80110678     8.94430633     5.73265246 O
atom       6.76156004     2.10495108     7.17330085 O
atom      15.86537859    11.96073413     6.55900319 O
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atom       2.65406467    12.62132954     6.87258865 O
atom       7.06269156    18.97920668     3.25248135 O
atom      16.24892350     8.62313814     3.31915091 O
atom      11.60623827    18.80579031     2.98617557 O
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atom       2.21074500     8.83494529     0.77271425 O
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atom       4.06402645     2.21943378     7.53319794 O
atom      13.67945385    13.06374351     7.75734893 O
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atom      13.57191315     8.21526949     3.45179172 O
atom      14.25279904    18.24489891     3.45437332 O
atom       4.22952603     7.51660640     3.91253904 O
atom      13.96719240    18.28462985     0.16888367 O
atom       4.55269274     7.78466567    -0.13296483 O
atom       4.23738297    18.02026881     0.13462424 O
atom      13.23322071     7.85241881    -0.08683814 O
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atom 4.80673581 12.53182791 3.96880927 O
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atom 6.03104204 6.62579108 2.16802657 O
atom 14.97926584 16.32506981 1.69718168 O
atom 12.22099125 6.22624364 1.81494721 O
atom 3.27943013 16.16675136 1.82597638 O
atom 6.27912977 14.01211017 5.58102930 O
atom 15.03722980 3.48666452 5.72818693 O
atom 12.46791821 13.82547479 5.47843536 O
atom 3.18422183 4.07511659 5.78472598 O
atom 4.57187837 4.81913593 0.41977863 O
atom 13.53856150 15.68716900 -0.47112359 O
atom 13.91120505 5.23448600 -0.05433667 O
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Cartesian coordinates of the copper oxide cluster site in faujasite:

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