ELECTRONIC SUPPLEMENTARY INFORMATION

Insights into sulfur poisoning and regeneration of Cu-SSZ-13 catalysts: In situ Cu and S K-edge XAS studies

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Contents

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S1 S K-edge XAS of reference compounds

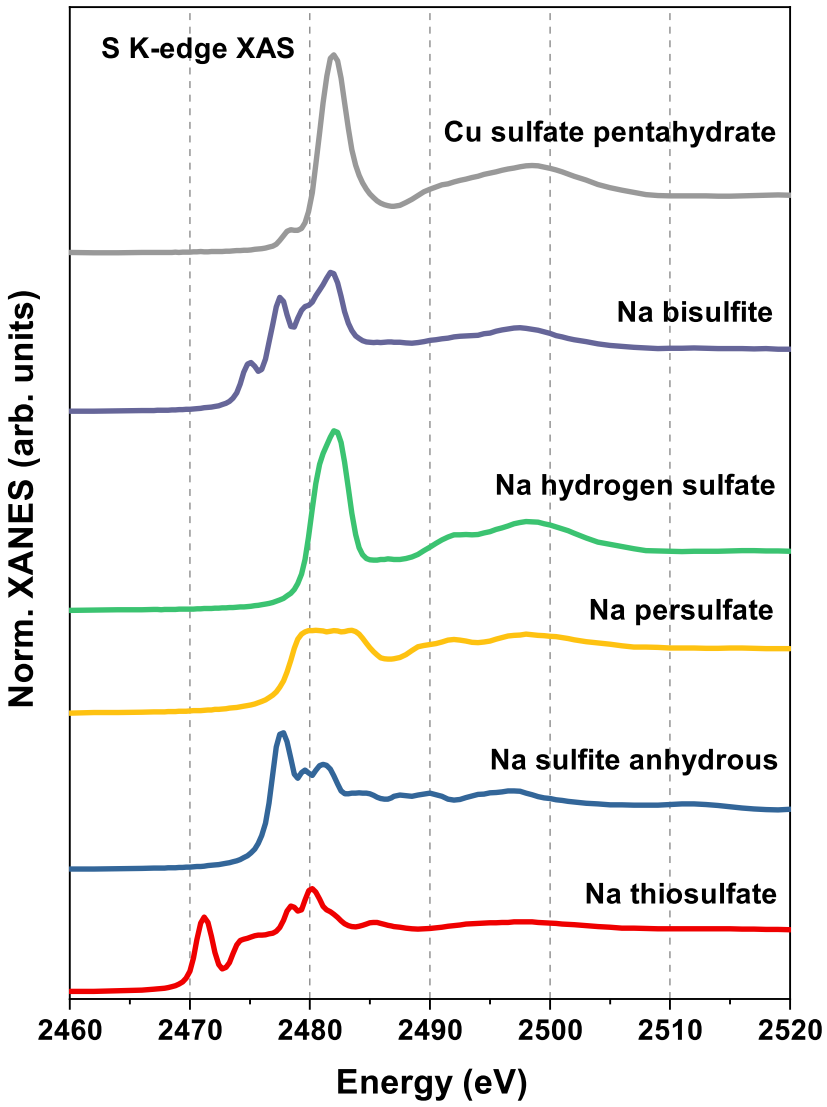

Fig. S1 Sulfur K-edge XANES spectra of reference compounds. Spectra were measured in fluorescence yield detection mode under vacuum at RT.

S2 3D plots of Cu K-edge XAS data

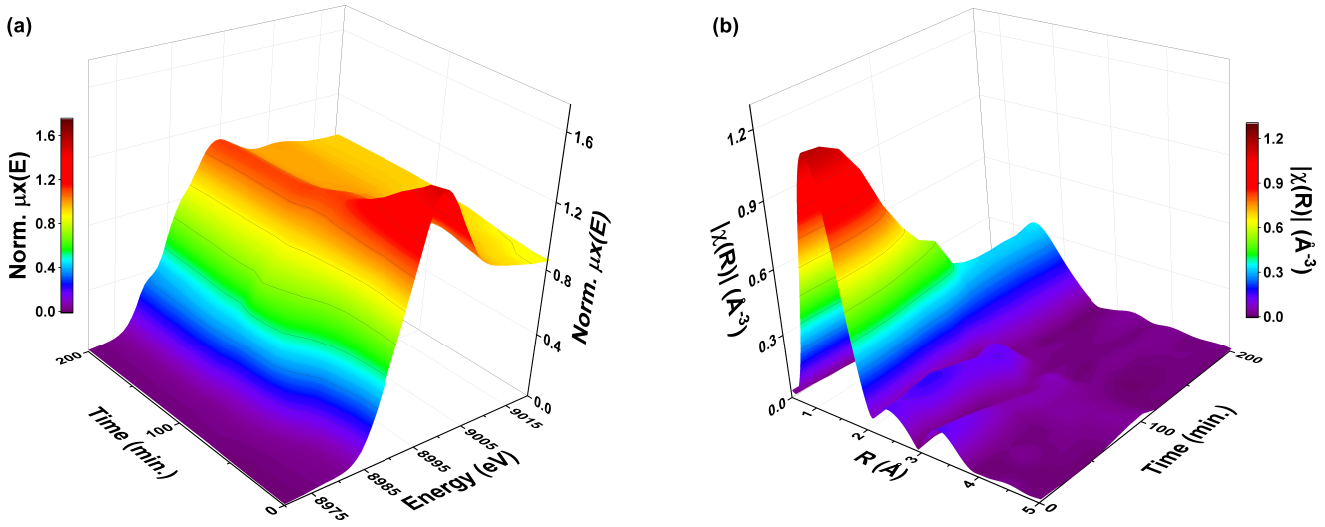

Fig. S2 3D plots of in situ Cu K-edge XAS data collected for the fresh Cu-SSZ-13 catalyst during heating in He and subsequent cooling in 5% CO/He. Parts (a) and (b) present the XANES and FT EXAFS, respectively.

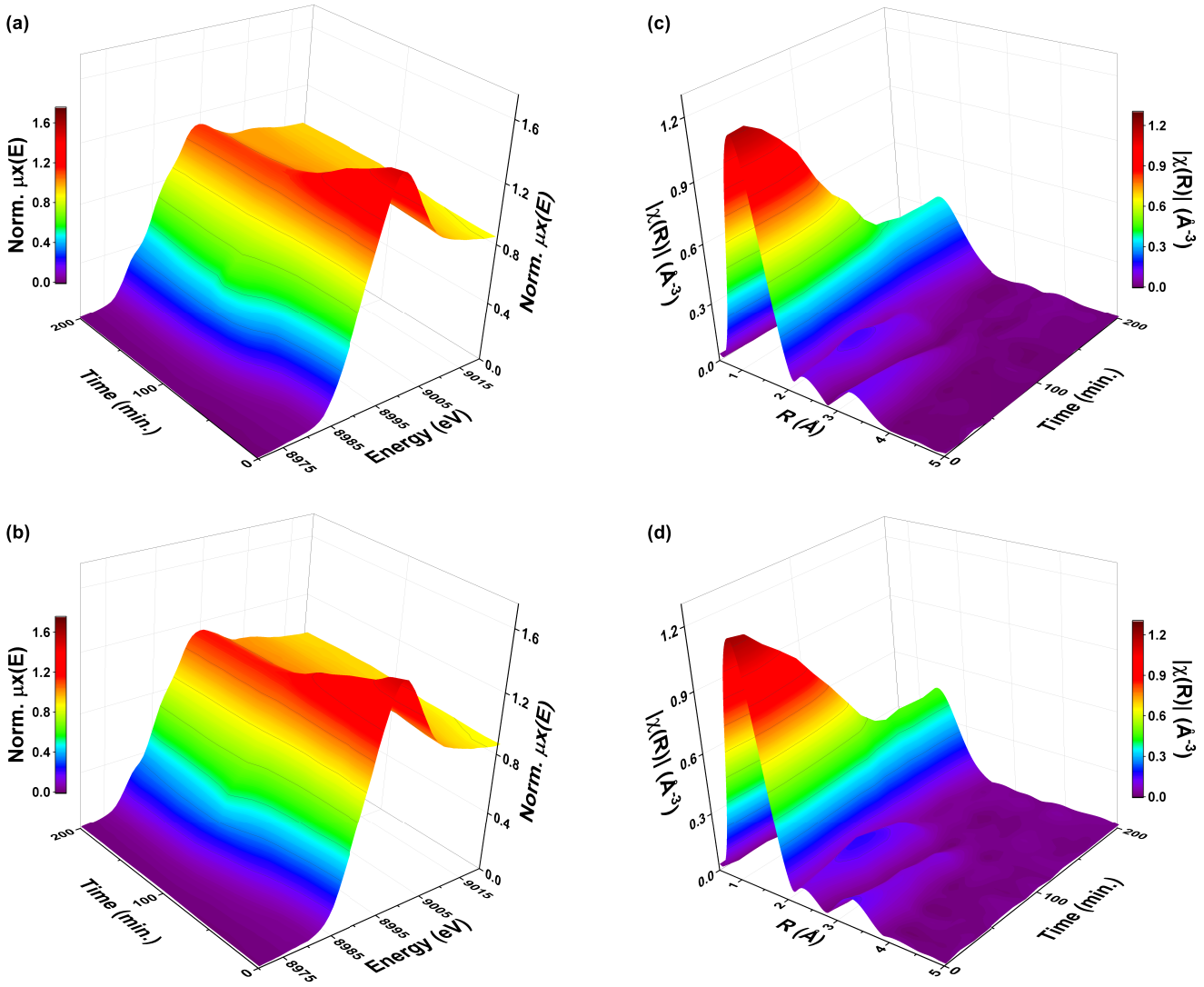

Fig. S3 3D plots of in situ Cu K-edge XAS data collected for sulfur-poisoned Cu-SSZ-13 catalysts during heating in He and subsequent cooling in 5% CO/He. The left part shows the XANES for (a) S-200 and (b) S-500. The right part shows the FT EXAFS for (c) S-200 and (d) S-500.

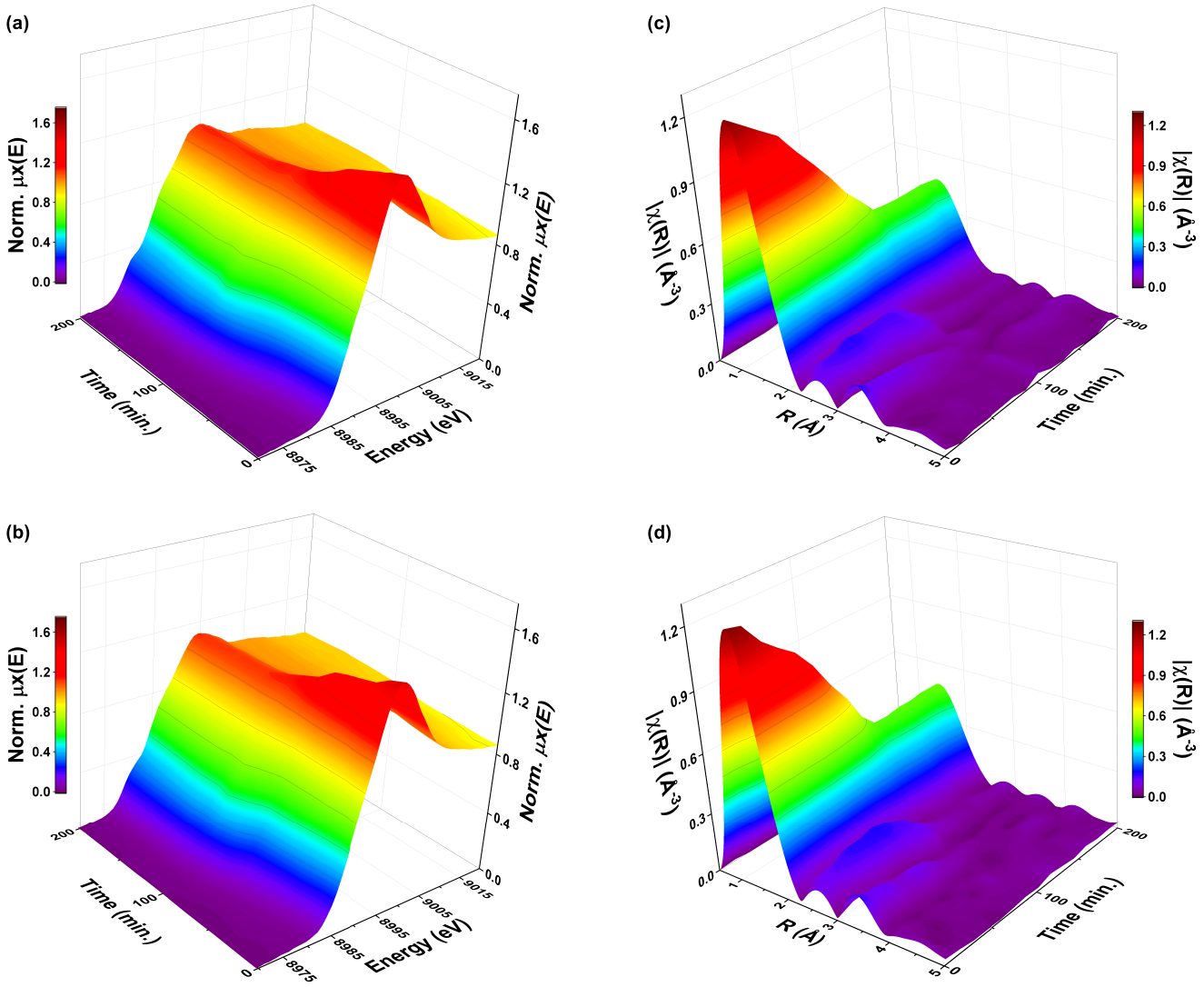

Fig. S4 3D plots of in situ Cu K-edge XAS data collected for regenerated Cu-SSZ-13 catalysts during heating in He and subsequent cooling in 5% CO/He. The left part shows the XANES for (a) R-200 and (b) R-500. The right part shows the FT EXAFS for (c) R-200 and (d) R-500.

S3 PCA of Cu K-edge XAS data

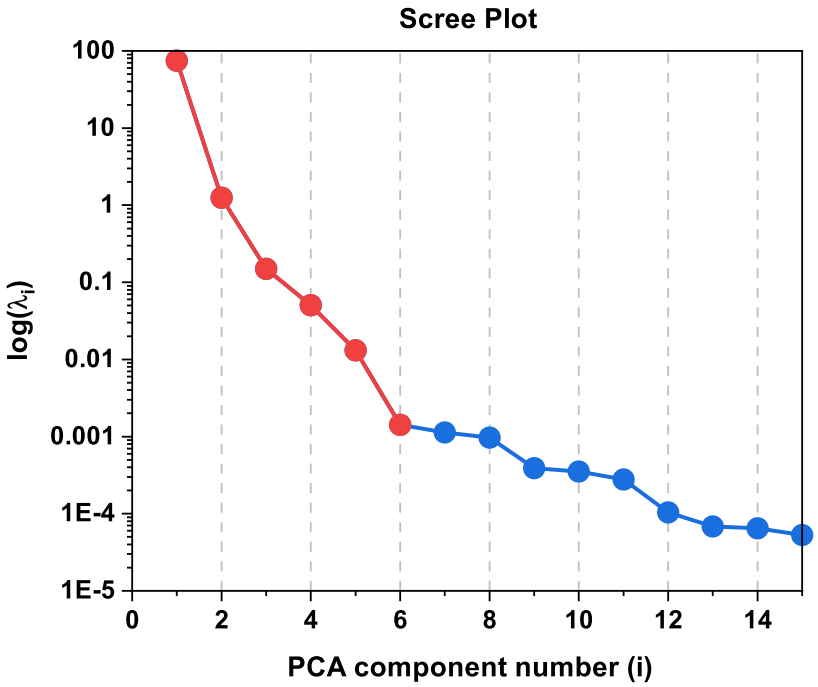

Fig. S5 Scree plot of the eigenvalues obtained from PCA of the combined XAS dataset containing the spectra of fresh, sulfur-poisoned, and regenerated Cu-SSZ-13 catalyst samples. The eigenvalues are presented on a log scale. Significant components are marked by red.

S4 FT EXAFS of pure components

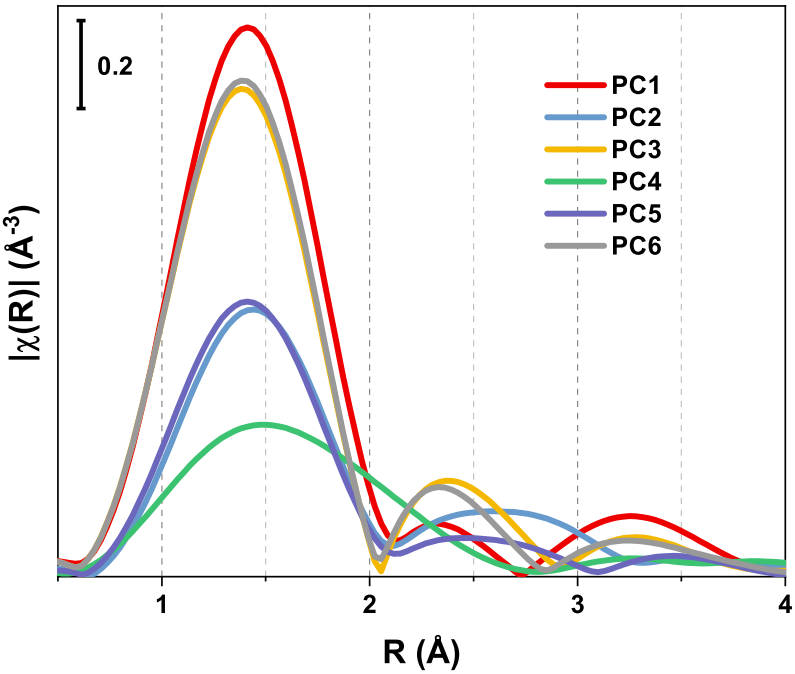

Fig. S6 FT EXAFS region of six pure components derived from the MCR-ALS analysis of the combined XAS dataset containing the spectra of fresh, sulfur-poisoned, and regenerated Cu-SSZ-13 catalyst samples.

S5 WT EXAFS of pure components

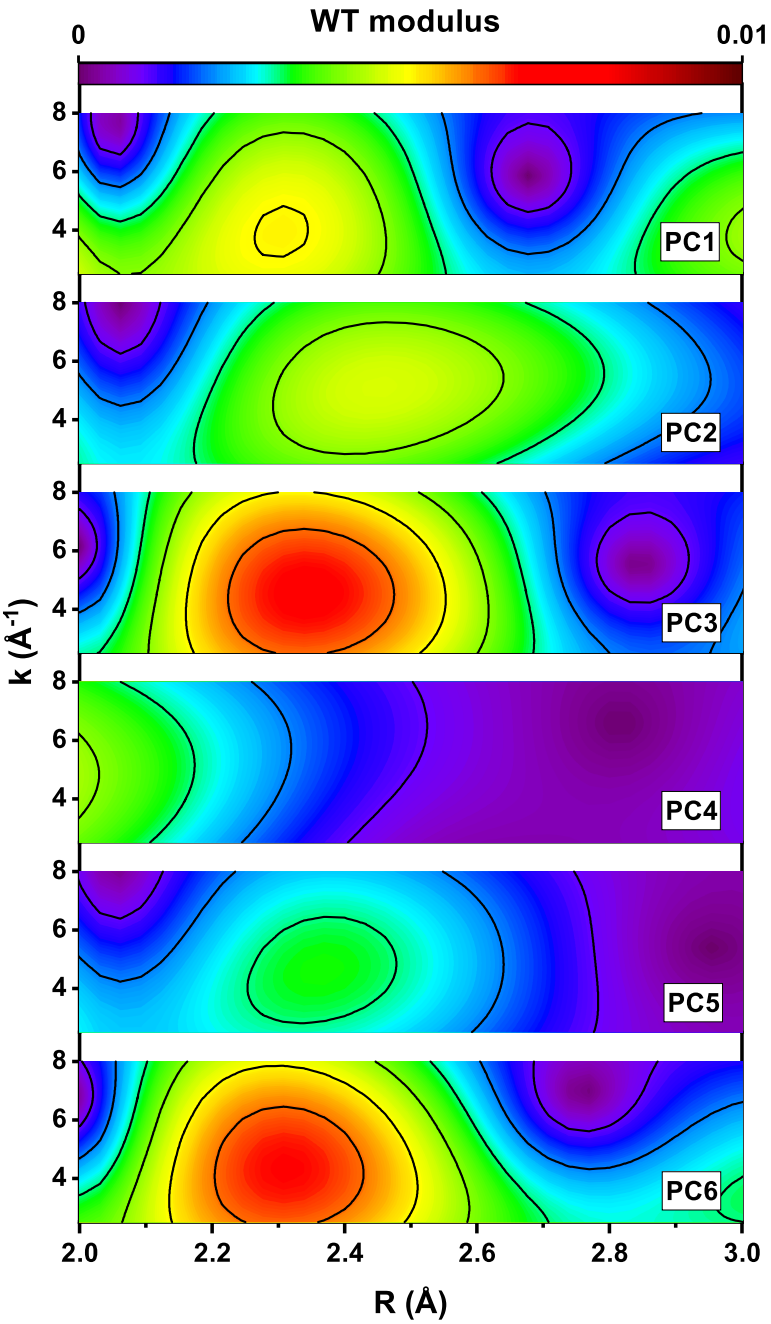

Fig. S7 WT EXAFS region of six pure components derived from the MCR-ALS analysis of the combined XAS dataset containing the spectra of fresh, sulfur-poisoned, and regenerated Cu-SSZ-13 catalyst samples. Only the region of the second lobes between radial distances from 2 to 3 Å is shown.

S6 Backscattering amplitude factors

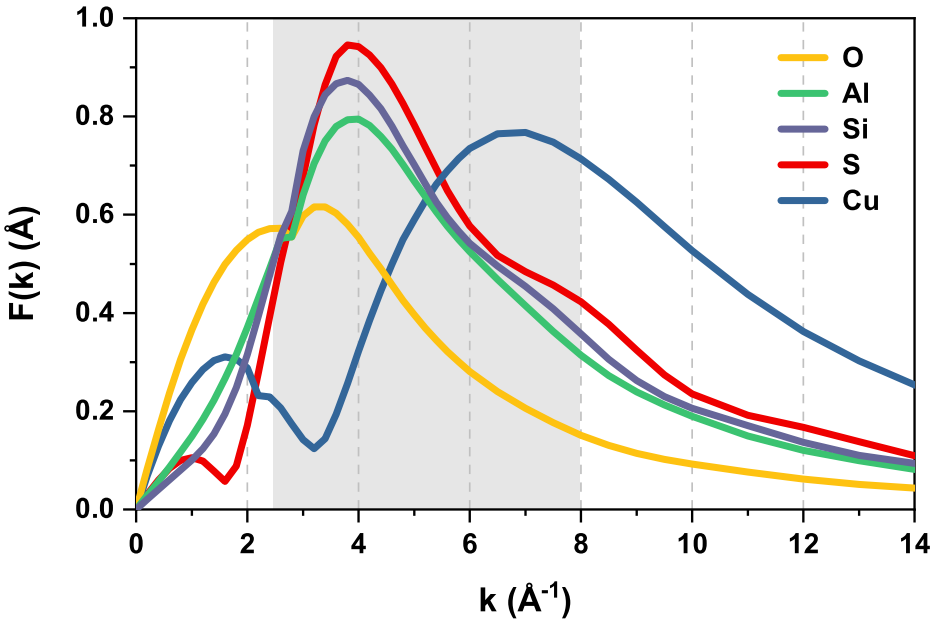

Fig. S8 Backscattering amplitude factors associated with chemical elements present in the studied catalyst samples. The light gray box shows the range of wavenumbers used for the comparison of pure components. The results were obtained in our previous study[1], using the FEFF code[2].

S7 MCR-ALS using five components

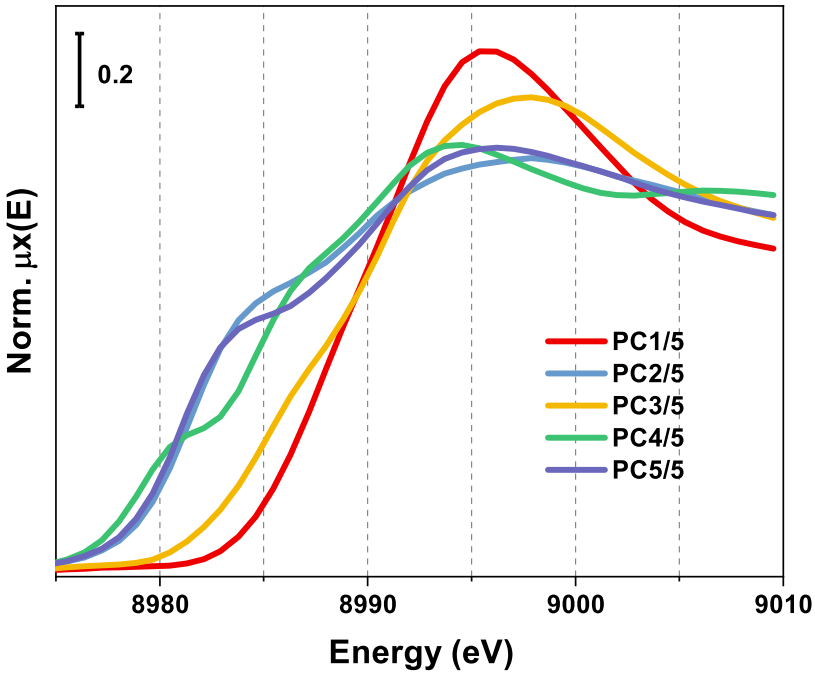

Fig. S9 Cu K-edge XANES region for the five components derived from the MCR-ALS analysis of the combined dataset containing the spectra of fresh, sulfur-poisoned, and regenerated Cu-SSZ-13 catalyst samples. A smaller number of components than identified by PCA was used.

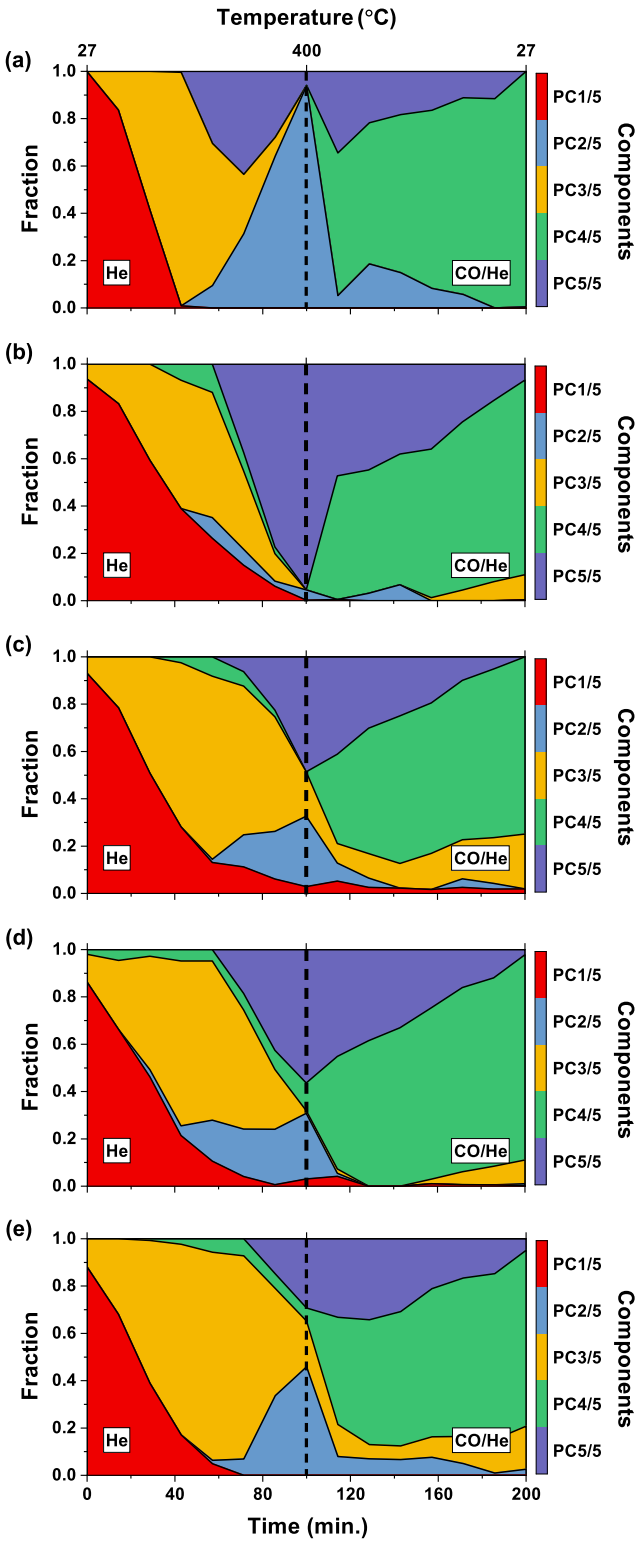

Fig. S10 MCR-ALS concentration profiles of the five components for (a) fresh catalyst, (b) S-200, (c) S-500, (d) R-200, and (e) R-500. Vertical dotted lines indicate the substitution of He with CO/He. The component numbers increase with a decrease of their eigenvalues. A smaller number of components than identified by PCA was used.

References

1 V. V. Mesilov, S. L. Bergman, S. Dahlin, Y. Xiao, S. Xi, M. Zhirui, L. Xu, W. Chen, L. J. Pettersson and S. L. Bernasek, *Appl. Catal., B*, 2021, **284**, 119756.

2 J. J. Rehr and R. C. Albers, *Rev. Mod. Phys.*, 2000, **72**, 621–654.