Electronic Supplementary Information (ESI)

Positive Effect of Ce Modification on Low-temperature NH_3-SCR Performance and Hydrothermal Stability over Cu-SSZ-16 Catalysts

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The Synthesis of the Catalysts

The organic structure directing agent (OSDA) used for the preparation of SSZ-16 is 1,4-diazabicyclo [2.2.2] octane-C4-diquat dibromide, which was synthesized from the reaction between 1,4-dibromobutane and 1,4-diazabicyclo [2.2.2] octane. Firstly, 12.8 g 1,4-dibromobutane was mixed with 6.6 g methanol (denoted as solution A). 20 g 1,4-diazabicyclo [2.2.2] octane was dissolved in 20 g methanol (denoted as solution B). After about 15 min, solution A was added dropwise to solution B in the ice bath under stirring condition and stirred for 1 h. The reaction solution was further mixed with 100 mL diethyl ether and continued to stir for 1 h, after that vacuum filtration and drying process were performed. When the above steps were completed, 1,4-diazabicyclo [2.2.2] octane-C4-diquat dibromide was obtained [1].

SSZ-16 was synthesized by using a reactant with the composition of SiO_2: 0.045 Al_2O_3: 0.11 OSDA: 0.8 NaOH: 20 H_2O at 150 °C for 9 days under rotation [1]. After that, white solid products were recovered, washed with deionized water and dried overnight at 100 °C. Subsequently, calcination in air at 290 °C for 2 h and then at 550 °C for 6 h was conducted to remove the OSDA.

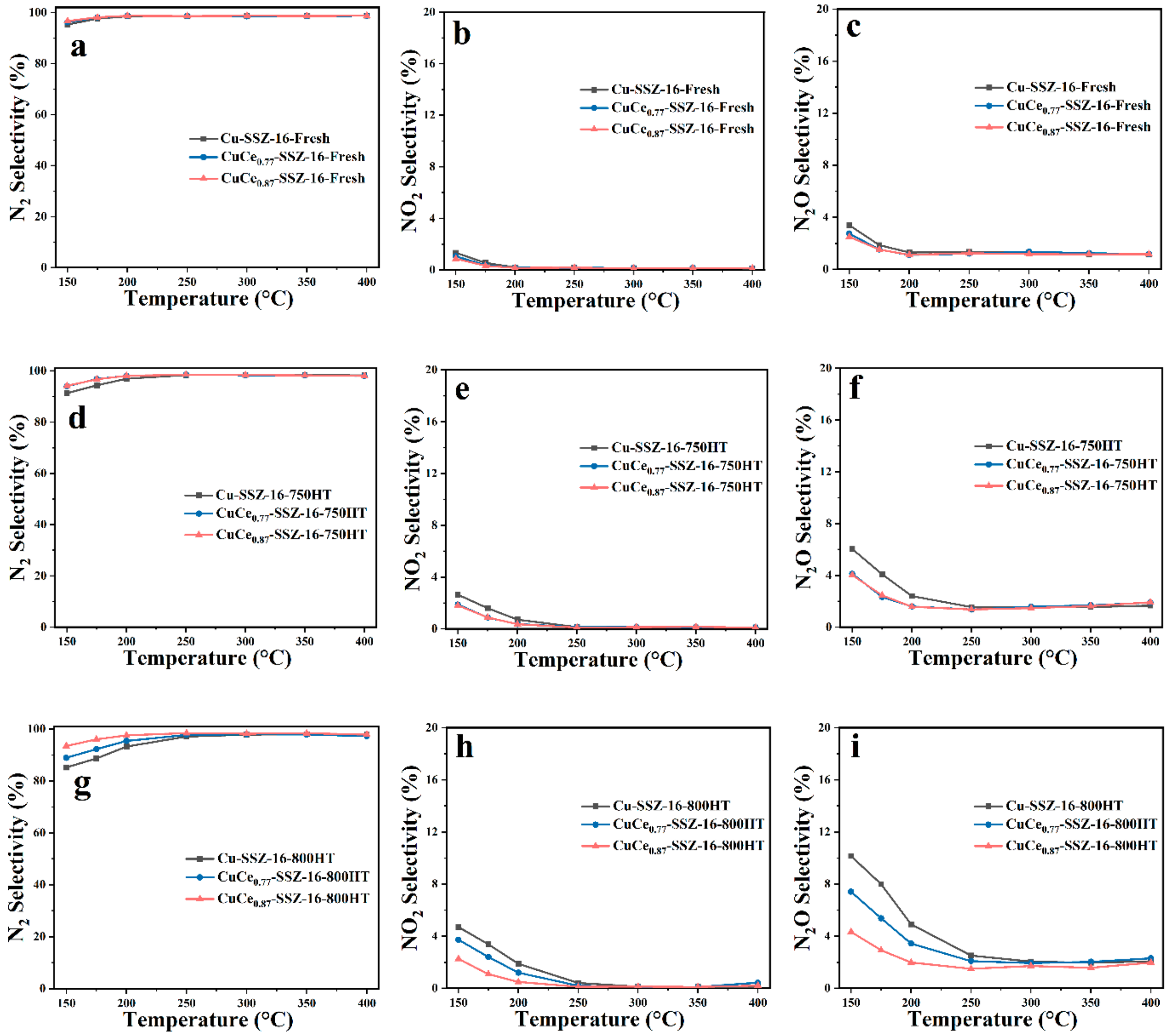

Figure S1. N_2, NO_2 and N_2O selectivity over Cu-SSZ-16, $CuCe_{0.77}$-SSZ-16, and $CuCe_{0.87}$-SSZ-16 before (a-c) and after hydrothermal treatment at 750 °C (d-f) and 800 °C (g-i).

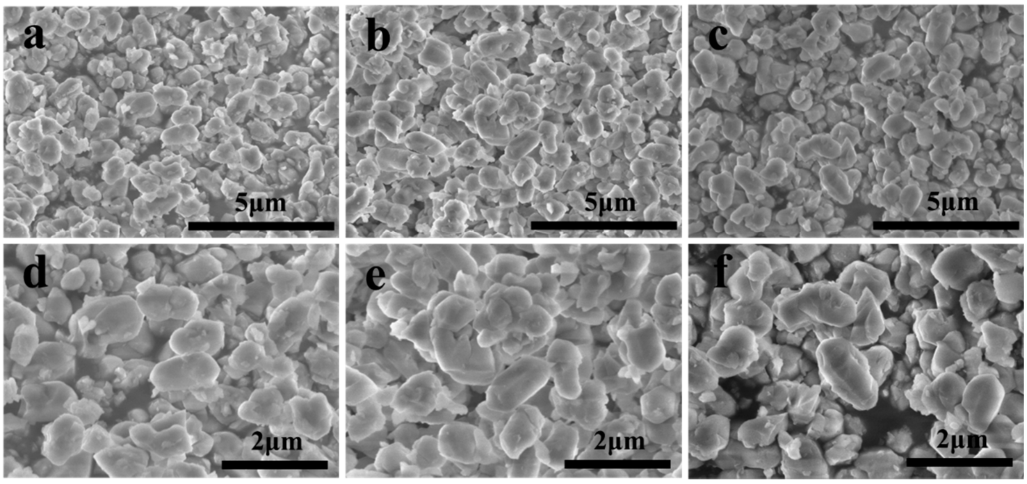

Figure S2. SEM images of Cu-SSZ-16-800HT (a, d), $CuCe_{0.77}$-SSZ-16-800HT (b, e), and $CuCe_{0.87}$-SSZ-16-800HT (c, f).

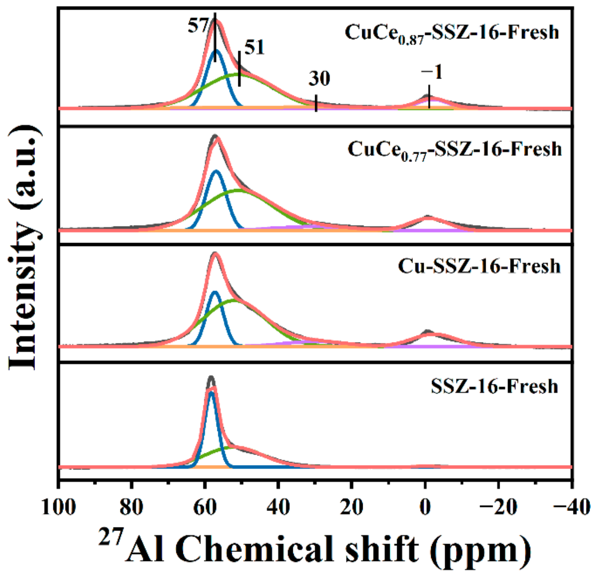

Figure S3. Deconvolution of ^{27}Al NMR spectra over SSZ-16-Fresh, Cu-SSZ-16-Fresh, $CuCe_{0.77}$-SSZ-16-Fresh, and $CuCe_{0.87}$-SSZ-16-Fresh.

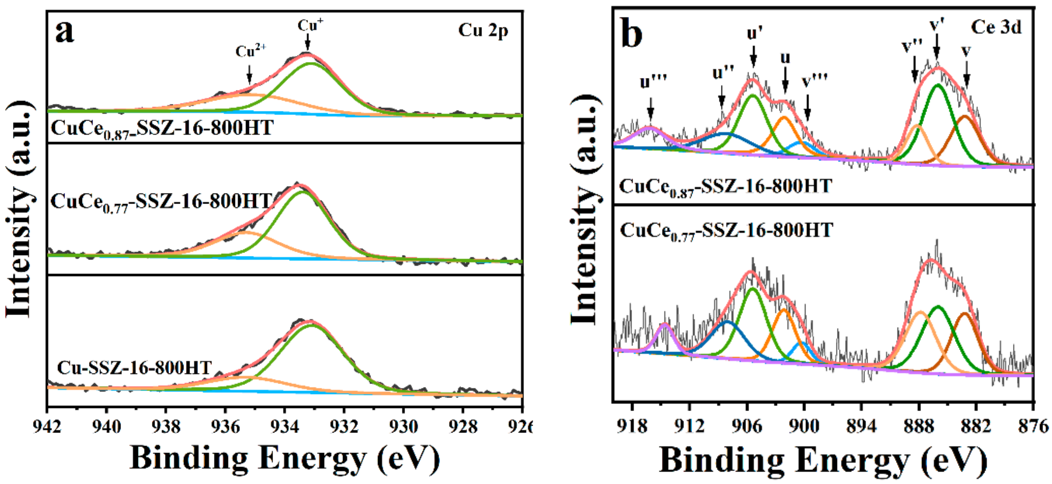

Figure S4. XPS spectra of Cu 2p (a) and Ce 3d (b) over Cu-SSZ-16-800HT, $CuCe_{0.77}$-SSZ-16-800HT, and $CuCe_{0.87}$-SSZ-16-800HT.

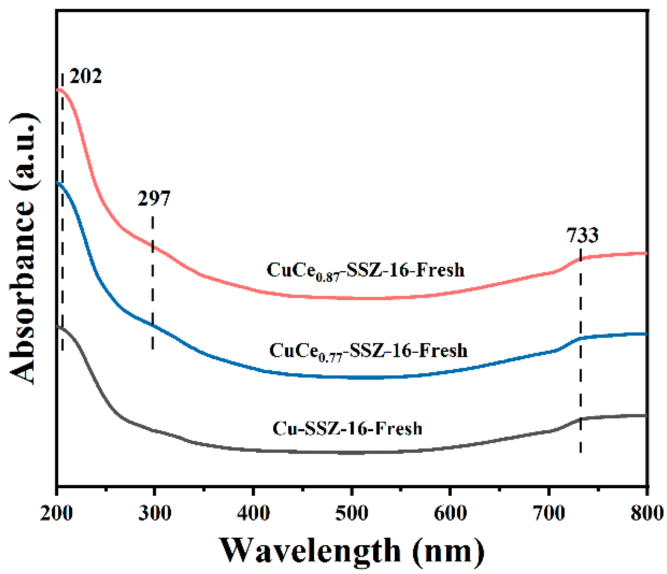

Figure S5. UV-vis spectra of Cu-SSZ-16-Fresh, $CuCe_{0.77}$-SSZ-16-Fresh, and $CuCe_{0.87}$-SSZ-16-Fresh.

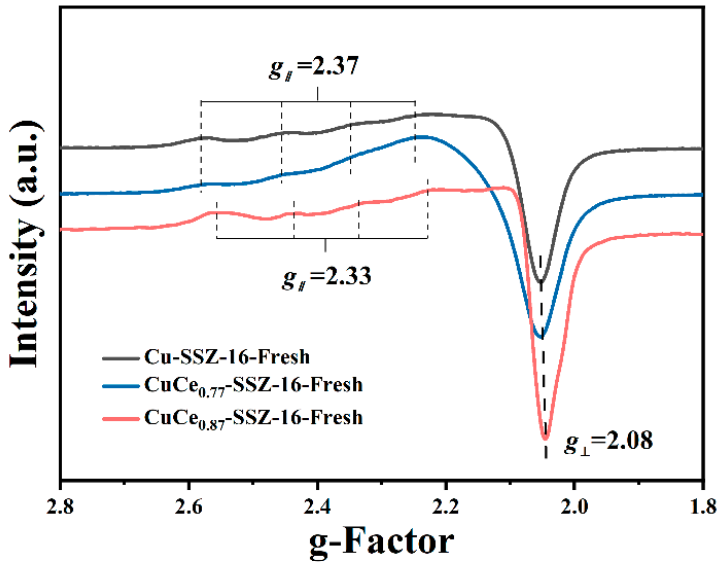

Figure S6. EPR spectra of Cu-SSZ-16-Fresh, $CuCe_{0.77}$-SSZ-16-Fresh, and $CuCe_{0.87}$-SSZ-16-Fresh.

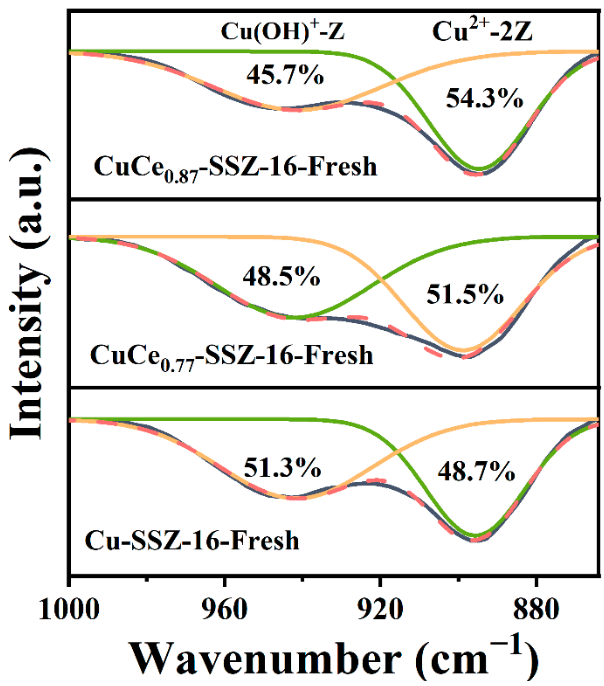

Figure S7. Deconvolution of in situ DRIFTS curves over Cu-SSZ-16-Fresh, $CuCe_{0.77}$-SSZ-16-Fresh, and $CuCe_{0.87}$-SSZ-16-Fresh.

Reference

1. Li, R.;Jiang, X.Q.;Lin, J.C.;Zhang, Z.P.;Huang, Q.T.;Fu, G.Y.;Zhu, Y.J.;Jiang, J.X. Understanding the influence of hydrothermal treatment on NH_3-SCR of NO_x activity over Cu_x-SSZ-16. *Chem. Eng. J.* **2022**,*441*,136021. https://doi.org/10.1016/j.cej.2022.136021