Supplementary Information

Design of Prussian blue analogues derives double-cone structure Ce-Fe catalysts and their enhanced performances for the selective catalytic reduction of NO_x with NH_3

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NH_3-SCR activity measurements

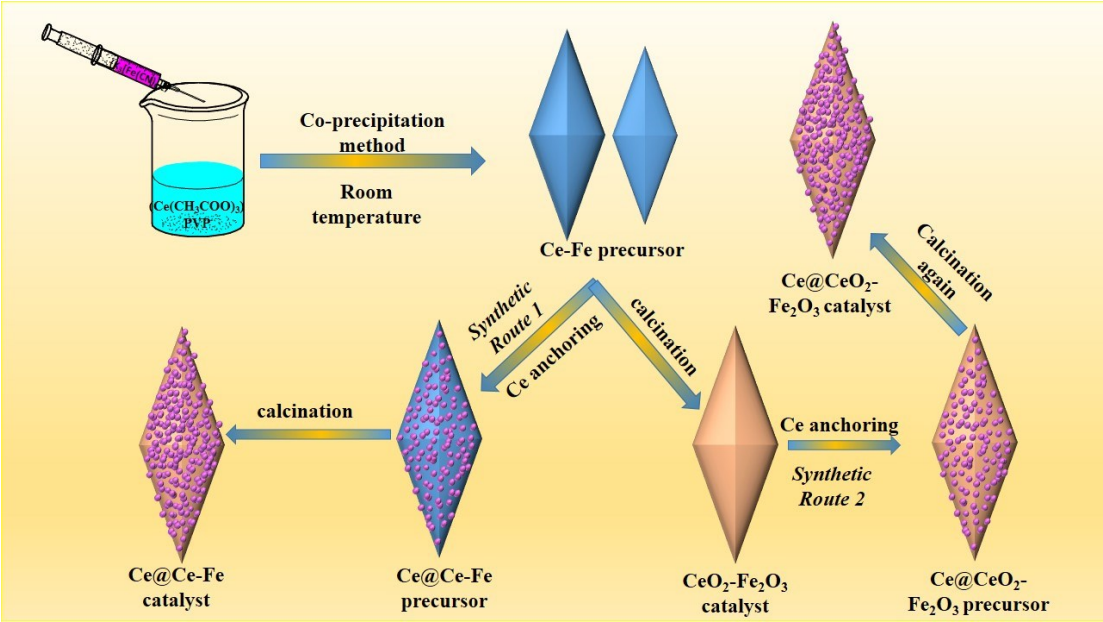
The NH_3-SCR activity measurement was performed in a fixed bed reactor with 0.40 g catalyst (40-60 mesh), which was carried out under a gas hourly space velocity (GHSV) of 30,000 h^{-1}. In addition, the reaction was following simulated gas: 500 ppm NH_3, 500 ppm NO, 100 ppm SO_2 (when used), 5 vol. % H_2O (when used), 5 vol. % O_2 and balance N_2. Meanwhile, the total flow rate was 200 mL min^{-1}. Finally, the product gas was analyzed using a flue gas analyzer (KM9106), a N_2O detector (G200) and an NH_3 detector (DR95C). For the concentration of the gases at steady state, the NOx and N_2 selectivity and NH_3 conversion were calculated as follows:

$$NO_x \text{ Conversion } (\%)=\frac{[NO_x]_{in}-[NO_x]_{out}}{[NO_x]_{in}}\times 100\% \quad (1\text{-}1)$$

$$N_2 \text{ Selectivity}(\%)=\left(1-\frac{2[N_2O]_{out}}{[NO_x]_{in}+[NH_3]_{in}-[NO_x]_{out}-[NH_3]_{out}}\right)\times 100\% \quad (1\text{-}2)$$

$$NH_3 \text{ Conversion}(\%)=\frac{[NH_3]_{in}-[NH_3]_{out}}{[NH_3]_{in}}\times 100\% \quad (1\text{-}3)$$

Where $[NO_x]_{in}$ and $[NH_3]_{in}$ are the initial concentrations of NO and NH_3, and $[NO_x]_{out}$, $[N_2O]_{out}$ and $[NH_3]_{out}$ are the concentrations after reaction at steady state.



Scheme S1 Schematic illustration of fabrication of catalysts.

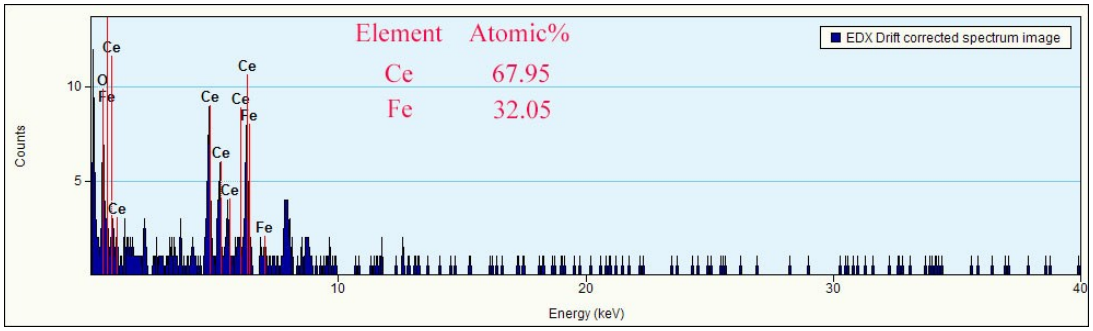


Figure S1 EDX spectrum of Ce@Ce-Fe catalyst.

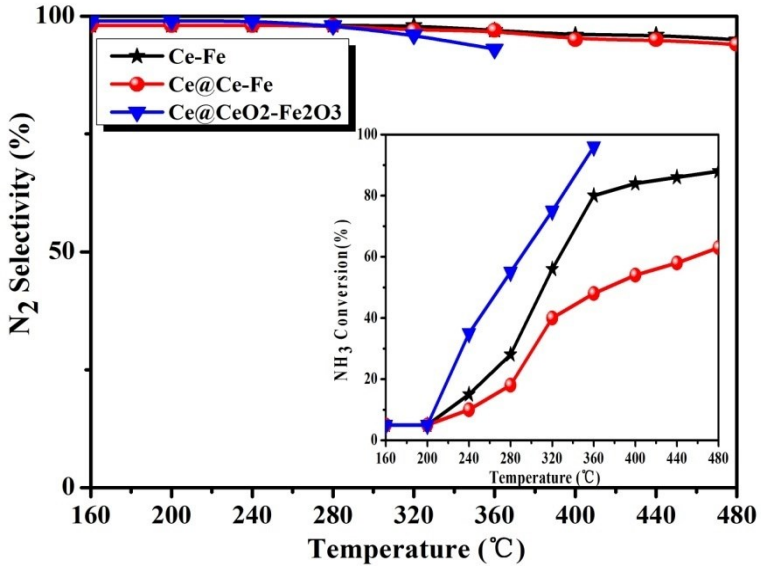


Figure S2 N_2 selectivity and NH_3 conversion (inner picture) of different catalysts.

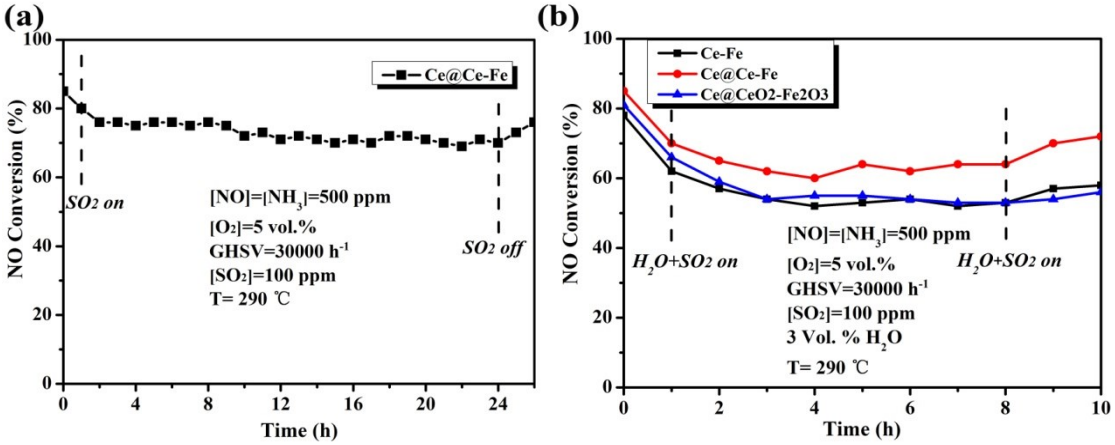


Figure S3 NO conversion of Ce@Ce-Fe under SO_2 conditions of 24 h (a) and NO conversion under H_2O and SO_2 conditions of different catalysts (b).

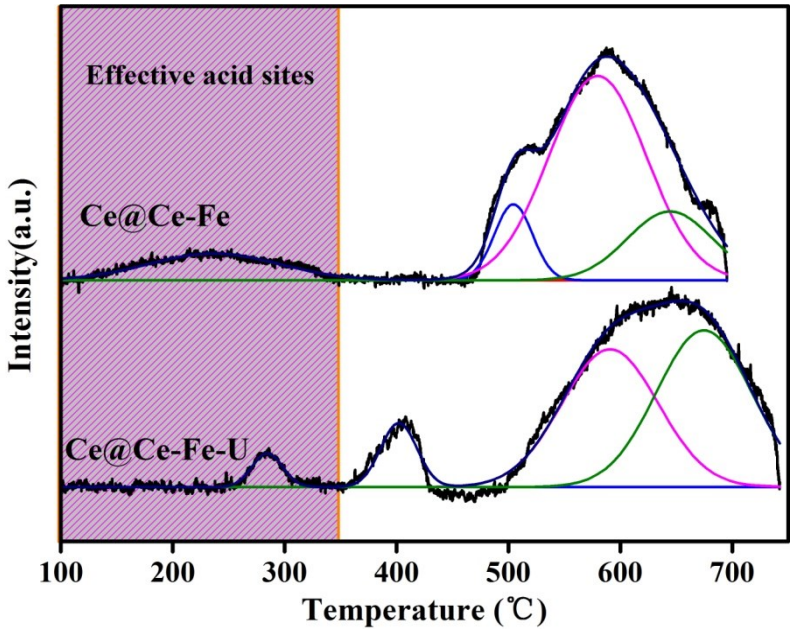


Figure S4 NH_3-TPD profiles of Ce@Ce-Fe and Ce@Ce-Fe-U (U represented the used catalyst) catalysts.