Electronic Supplementary Material (ESI) for RSC Advances.

Selective catalytic reduction of NO over W-Zr-Ox/TiO2: Performance study of hierarchical pore structure

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Characterization

X-ray diffraction (XRD) patterns were obtained from an X-ray diffractometer (Smartlab TM 3 kW, Rigaku, Japan). The scan speed was 10 °·min^{-1} and the 2θ scans covered 10~85 °. The microstructural natures and element mapping of the catalysts have been investigated using a field emission scanning electron microscope (Carl Zeiss, Ultra 55) and transmission electron microscopy (JEOL, JEM-2010UHR). X-ray photoelectron spectroscopy (XPS) patterns were acquired by an AXIS ULTRA DLD instrument (Al-Kα radiation, 1486.6 eV), and the vacuum degree was maintained at 10^{-7} Pa. The samples were dried at 100 °C for 24 h to remove moisture and then were tested without surface treatment. The curve fitting was performed by using XPSPEAK 4.1 with a Shirley-type background.

The temperature programmed desorption of ammonia (NH_3-TPD) was conducted on the CHEMBET-3000 (Quantachrome) to obtain the surface acid properties. All the catalysts were preheated at 400 °C under a helium stream for 1 h, and then cooled to 50 °C for the ammonia adsorption. Afterwards, ammonia was desorbed from 50 °C to 550 °C at a heating rate of 10 °C·min^{-1}. The Semiautomatic Micromeritics TPD/TPR 2900 instrument was used for the temperature programmed reduction of hydrogen (H_2-TPR). All the catalyst carriers were preheated to 400 °C under an argon stream for 1 h, and cooled to 50 °C. Then 5% H_2/Ar flow was switched, and the temperature increased from 50 °C to 700 °C at a 10 °C·min^{-1} heating rate. The data were collected throughout the whole temperature range. The specific surface area and average pore diameter (BET method) of the samples were measured by N_2 adsorption/desorption isotherms at -196 °C using a surface-area analyzer (Micromeritics, 2020M V3.00H). All of the samples were degassed at 350 °C under vacuum for 3 h prior to the adsorption experiments.

In situ Diffuse Reflectance Infrared Fourier Transform Spectra (*in situ* DRIFTS) were also collected by a Nicolet IS50 spectrometer. For NH_3-SCR: 500 ppm NH_3 was pumped into the system for 10 min when the temperature was 300 °C. Then the flow of NH_3 was stopped and 500 ppm NO + 10% O_2 was pumped into the system for 10

min. After that, 500 ppm NH_3 + 500 ppm NO + 10% O_2 was pumped into the system for 10 min. At last, the temperature increased to 450 °C and 600 °C at the mixed flow of NH_3, NO and O_2, and stayed at each temperature point for 10 min.

Figure S1

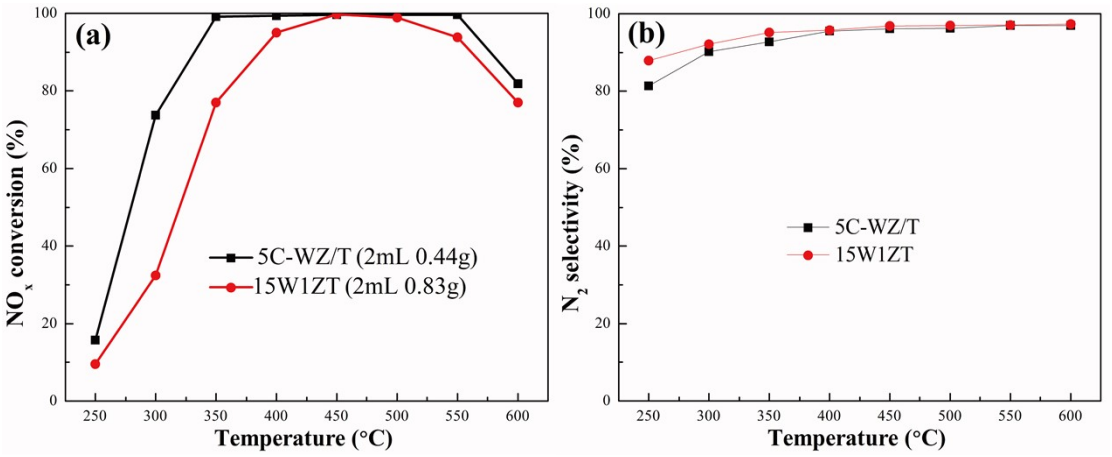

Fig.S1 (a) NO conversion and (b) N_2 selectivity of 5C-WZ/T and 15W1ZT catalysts. Reaction condition: 500 ppm NO, 500 ppm NH_3, 10% O_2, GSHV of 15000 h^{-1} and N_2 balance gas.

Figure S2

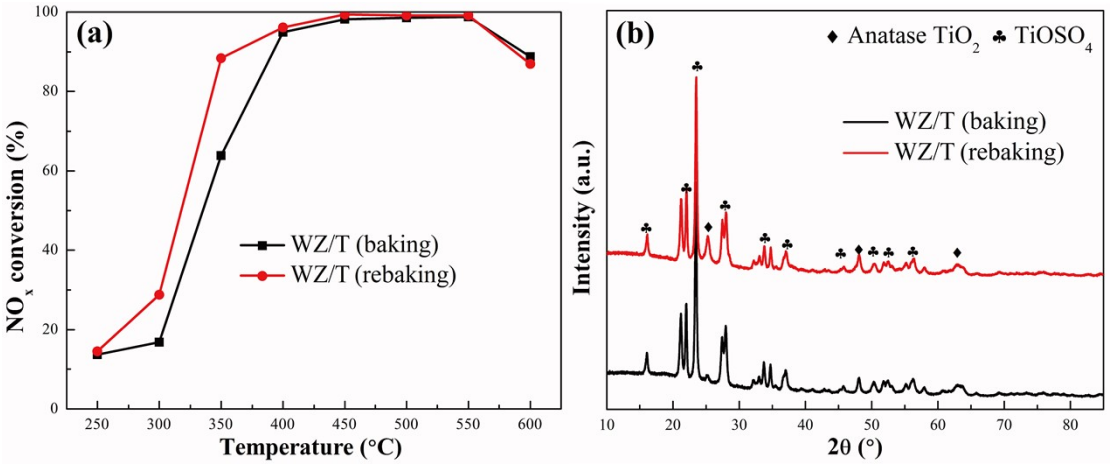

Fig.S2 (a) NO conversion and (b) XRD patterns of different catalysts.

Figure S3

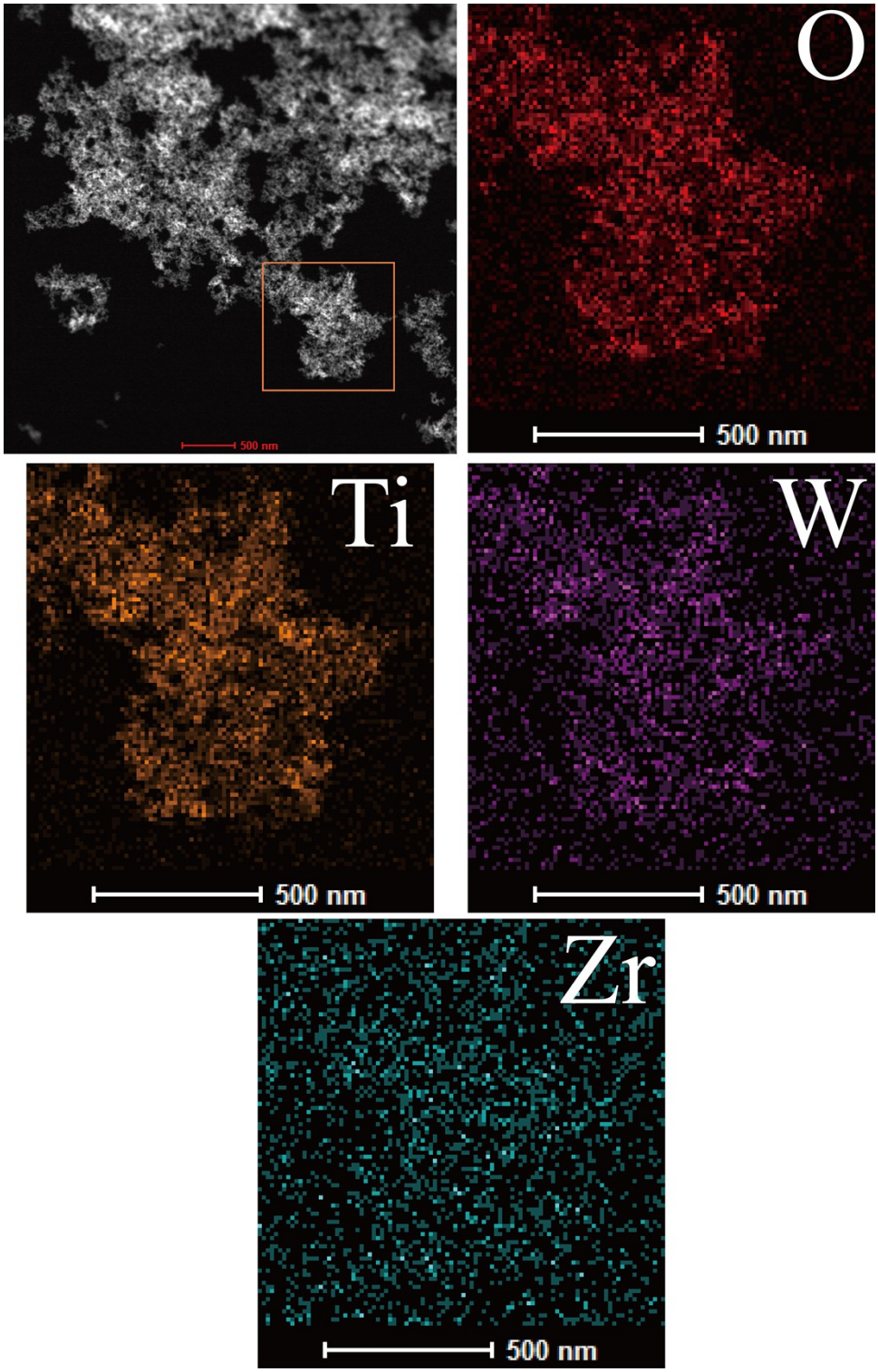

Fig.S3 Element mapping of 5C-WZ/T catalyst.

Figure S4

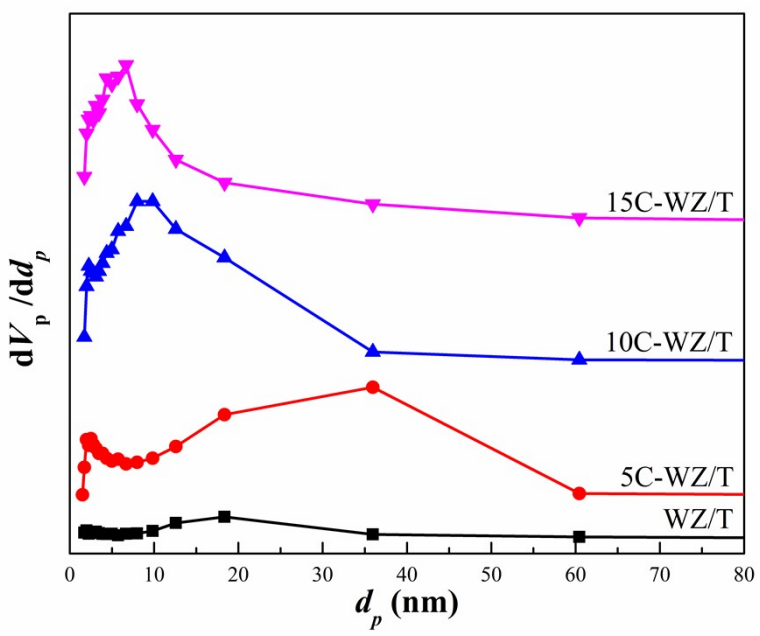

Fig.S4 Pore size distribution of different catalysts.

Figure S5

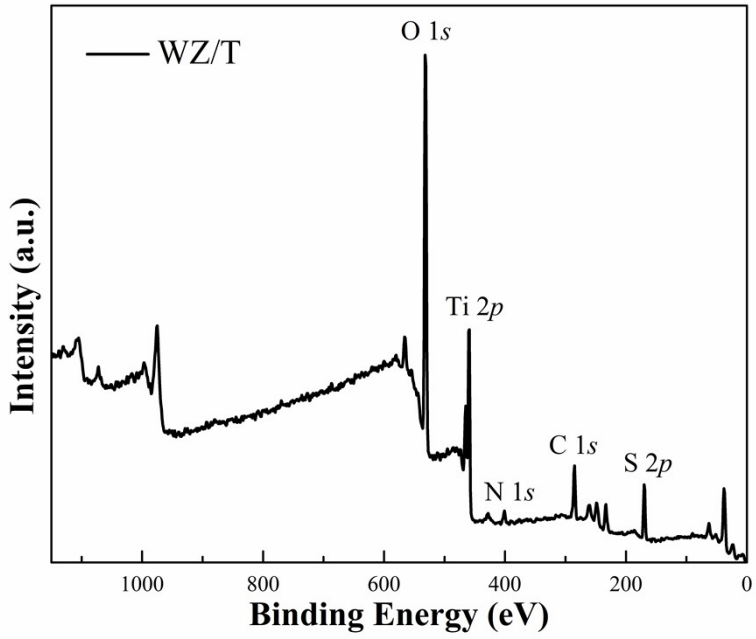

Fig.S5 SurveyXPS high-resolution scans spectra of WZ/T catalyst.

Figure S6

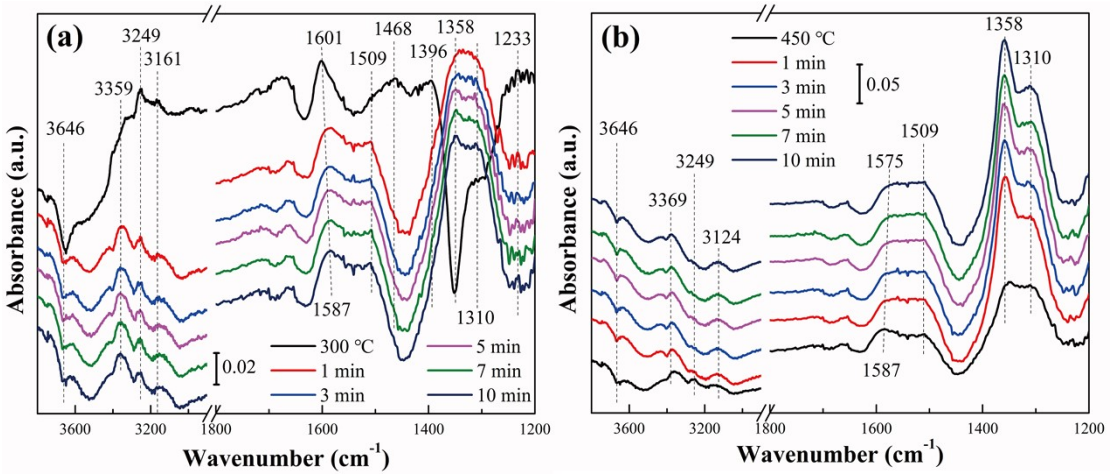

Fig.S6 *In-situ* diffuse reflection infrared spectrum of 5C-WZ/T catalyst: (a) NO+O_2 reacted with NH_3 at 450 °C, (d) NO+O_2 reacted with NH_3 at 600 °C.