Supporting Information

Facet-activity Relationship of TiO_2 in Fe_2O_3/TiO_2 Nanocatalysts for Selective Catalytic Reduction of NO with NH_3: *In Situ* DRIFTs and DFT Studies

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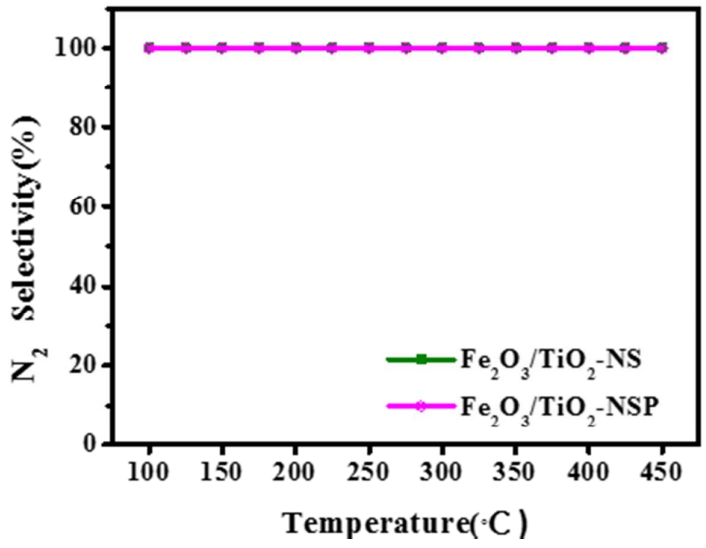

Figure S1. N_2 selectivity *versus* reaction temperature over the Fe_2O_3/TiO_2-NS and Fe_2O_3/TiO_2-NSP nanocatalysts. Reaction conditions: [NO] = [NH_3] = 500 ppm, [O_2] = 3 vol %, N_2 balance, and GHSV= 25 000 h^{-1}.

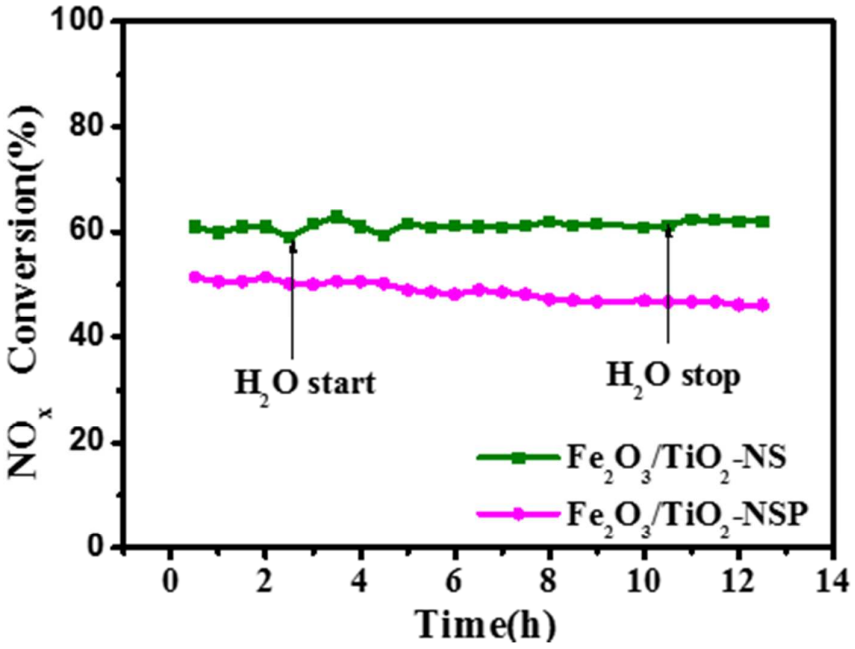

Figure S2. NO_x conversion versus reaction time on stream in the presence of 8 vol%H_2O, Reaction conditions: [NO] = [NH_3] = 500 ppm, [O_2] = 3 vol %, N_2 balance, and GHSV= 25 000 h^{-1}.

The N_2 selectivity of Fe_2O_3/TiO_2-NS and Fe_2O_3/TiO_2-NSP nanocatalysts during the NH_3-SCR reaction was shown in **Figure S1**. It can be found that both Fe_2O_3/TiO_2-NS and Fe_2O_3/TiO_2-NSP nanocatalysts exhibited remarkable performance in N_2 selectivity during the NH_3-SCR reaction. The H_2O resistance of Fe_2O_3/TiO_2-NS and Fe_2O_3/TiO_2-NSP under 250 ^oC was evsaluated in **Figure S2**. The values of NO_x conversion of the two catalysts remained unchanged in the presence of 8 vol. % H_2O, revealing that the catalytic performance of Fe_2O_3/TiO_2-NS and Fe_2O_3/TiO_2-NSP was slightly affected in the presence of H_2O.

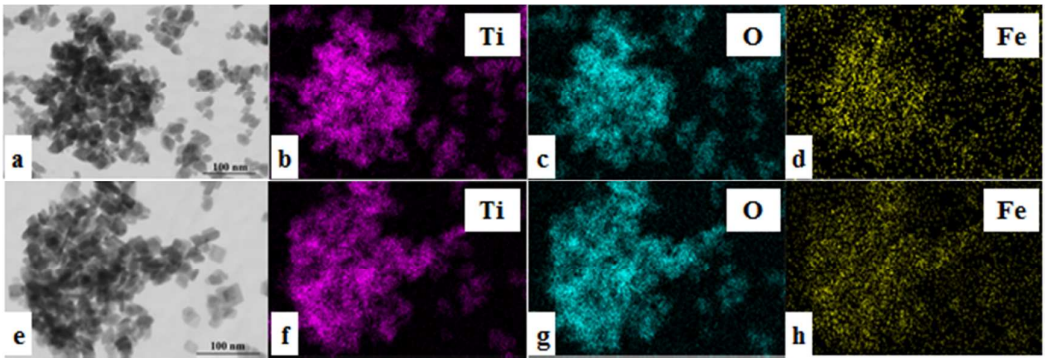

Figure S3. (**a, b, c, d**) STEM and EDS mapping images of Fe_2O_3/TiO_2-NSP nanocatalyst; (**e, f, g, h**) STEM and EDS mapping images of Fe_2O_3/TiO_2-NS nanocatalyst.

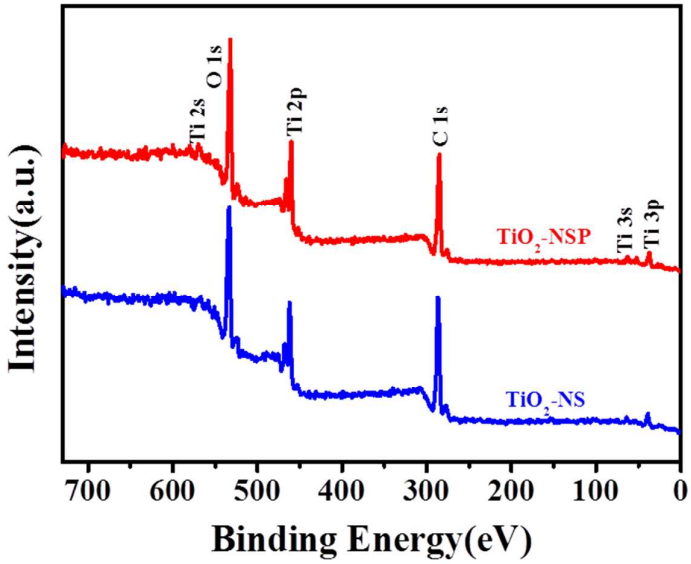

Figure S4. Full scan XPS spectra of TiO_2-NS and TiO_2-NSP.

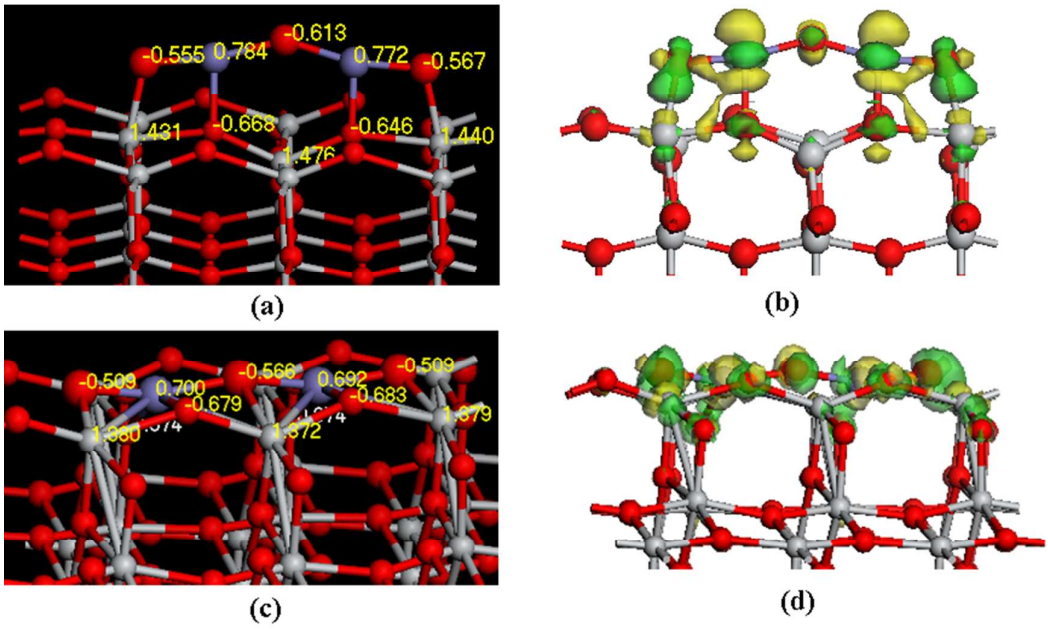

Figure S5. Charge on atoms (left) and electron density difference plot (right) of (**a**, **b**) $Fe_2O_3/TiO_2\{001\}$ and (**c**, **d**) $Fe_2O_3/TiO_2\{101\}$.