Supporting Information

Reduction of NO with NH_3 over ferric oxide nanocrystals: The crystallographic facet-induced catalytic enhancement

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1. Correlation between the surface energy and the reaction rate

The surface atoms of a catalyst possess dangling bonds which cost energy. The existence of these dangling bonds is the leading cause of the surface energy. The high energy facets will have a larger fraction of low-coordinated surface atoms, and thus, their average binding energy per surface atom is higher. A large number of intermediates, such as NH_2^-, are created during the activation process by the saturation of dangling bonds over the high energy facets with NH_3. Given this relation, the surface energy analysis allows an evaluation of the probability that a given catalyst with high-energy surfaces may have a reaction rate higher than that of catalyst terminated with low-energy facets.

However, we should not expect a simple linear relation between the energy of the facet and the reaction rate. An obvious shortcoming of this simple approach is its neglect of all other possible source of parameters, such as the possible size effect, surface area, and reaction mechanism.

2. Supplementary figures

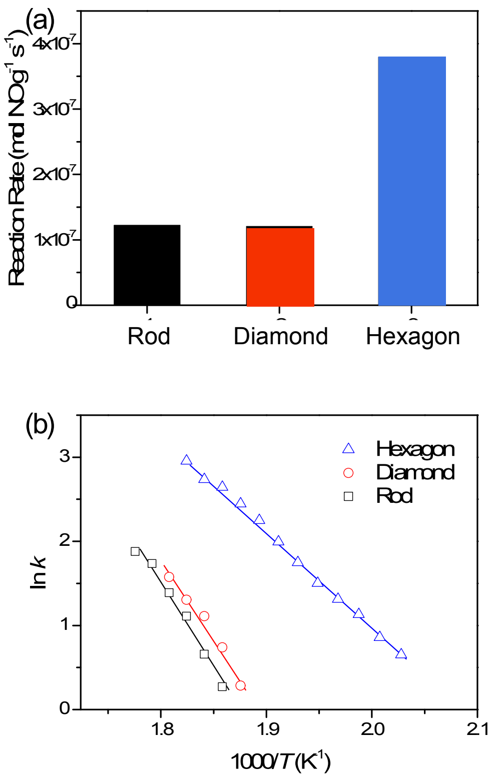

Figure S1. (a) Catalytic activities (at 300 °C) and (b) Arrhenius-type plots for selective catalytic reduction of NO_x over Fe_2O_3-hexagon, Fe_2O_3-diamond, and Fe_2O_3-rods.

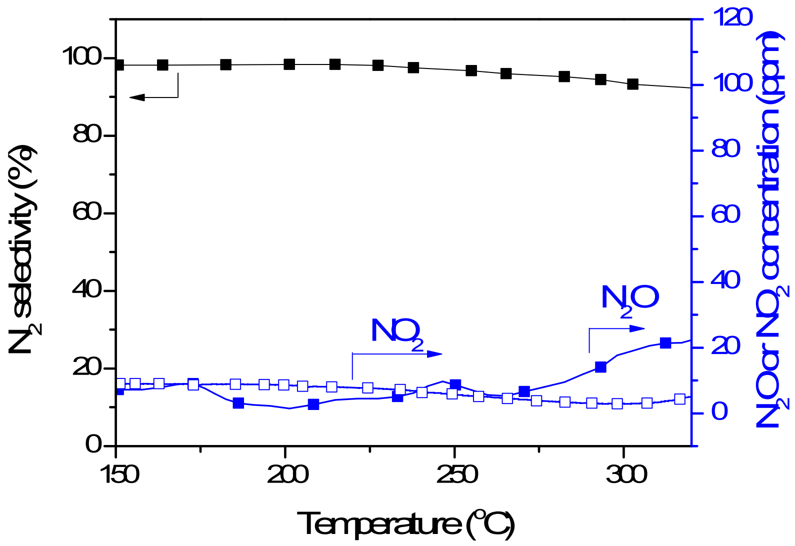

Figure S2. N_2 selectivity, outlet N_2O, and N_2O concentration as a function of temperature over Fe_2O_3-hexagon. Reactant feed contains 600 ppm of NO, 600 ppm of NH_3, 3 vol% O_2, balanced with N_2.

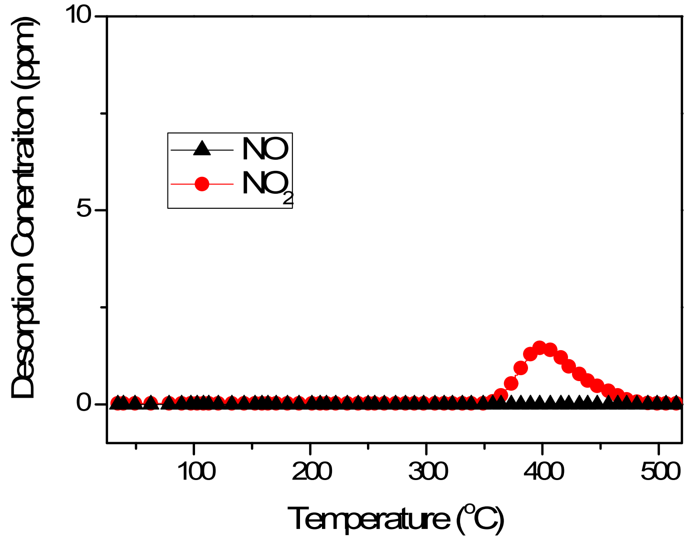

Figure S3. TPD spectra of NO and NO_2 taken after exposing the Fe_2O_3-hexagon sample to a saturation dose of $NO/3\%O_2/N_2$.

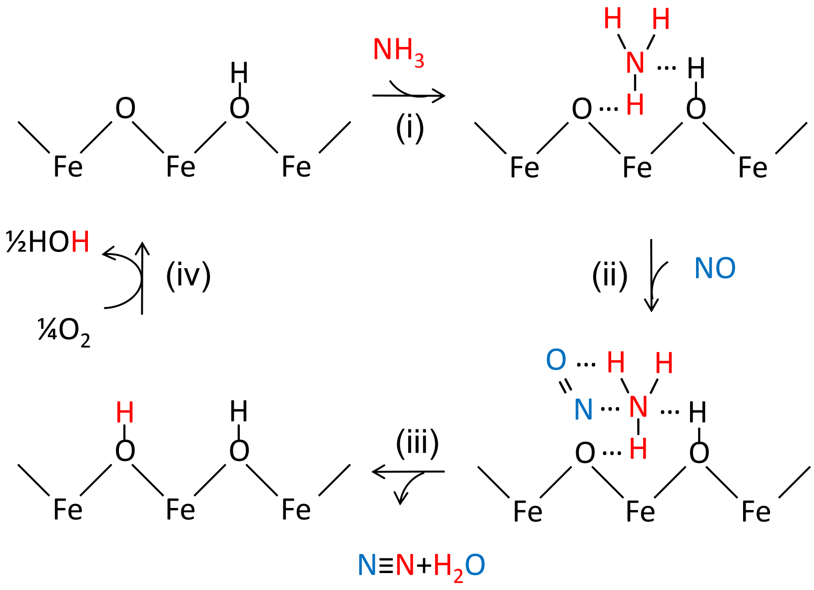

Figure S4. A plausible reaction mechanism of NH_3-SCR on Fe_2O_3-hexagon.