Supporting Information

Reduction of NO with NH\textsubscript{3} over ferric oxide nanocrystals: The crystallographic facet-induced catalytic enhancement

Zhiwei Huang,* Yueyao Du, Jie Zhang, Xiaomin Wu, Huazhen Shen, Yuhao Qian and Guohua Jing*

\*Department of Environmental Science & Engineering, Huaqiao University, Xiamen 361021, P. R. China.

Corresponding Authors

zwhuang@hqu.edu.cn; zhoujing@hqu.edu.cn

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\textsubscript{2}⁻, are created during the activation process by the saturation of dangling bonds over the high energy facets with NH\textsubscript{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\textsubscript{x} over Fe\textsubscript{2}O\textsubscript{3}-hexagon, Fe\textsubscript{2}O\textsubscript{3}-diamond, and Fe\textsubscript{2}O\textsubscript{3}-rods.
Figure S2. $N_2$ selectivity, outlet $N_2O$, and $N_2O$ concentration as a function of temperature over Fe$_2$O$_3$-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$_2$O$_3$-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$_2$O$_3$-hexagon.