Theoretical Guidance and Experimental Confirmation on Catalytic Tendency of M-CeO_2 (M = Zr, Mn, Ru or Cu) for NH_3-SCR of NO

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Herein, we demonstrate that the degrees of catalytic performance of M-CeO_2-based catalysts (M=Mn, Cu, Ru or Zr) for an ammonia selective catalytic reduction (NH_3-SCR) of nitric-oxide (NO) can be estimated using three theoretical terms; (i) an oxygen vacancy formation energy of a catalyst, (ii) an adsorption energy of NO and (iii) an adsorption energy of NH_3. Those terms predict the trend of the catalytic performance as the order; Mn–CeO_2 > Cu–CeO_2 > Ru–CeO_2 > Zr–CeO_2 > CeO_2. To verify the theoretical prediction, the catalysts were synthesized and tested their performances on the NH_3-SCR of NO reaction. The normalized NO conversion rates at low temperatures (100–200 °C) were measured for Mn–CeO_2, Cu–CeO_2, Ru–CeO_2, Zr–CeO_2 and CeO_2 as 2.61–7.46, 1.30–6.82, 0.73–3.02, 0.81–3.31 and 1.55–2.33 mol s^{-1} m^{-2}, respectively. A concept of a structure-activity relationship analysis shows a strong relationship between theoretical terms predictions and experimental results at the lower tempertures (Figure 1).[1,2]

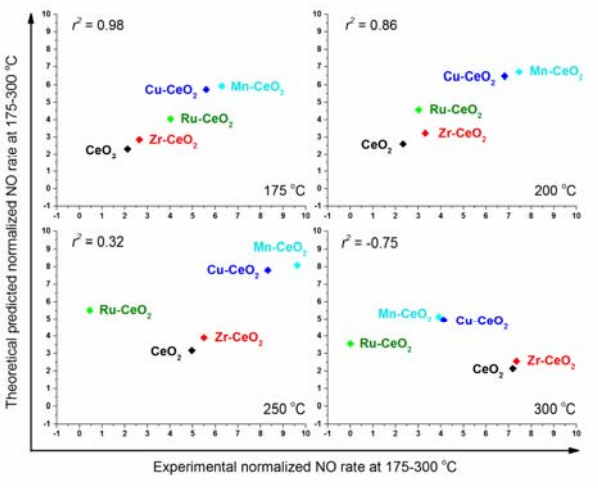

Figure 1. Experimental and predicted normalized NO conversion rate (*10^{-5} $mols^{-1}m^{-2}$) from 175 – 300 °C over the CeO_2, Zr-CeO_2, Ru-CeO_2, Cu-CeO_2 and Mn-CeO_2 catalysts.

References

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Acknowledgement

The authors acknowledge the support of the National Natural Science Foundation of China (21722704). All calculations were done at Nanoscale simulation laboratory, National Nanotechnology Center (NANOTEC), Thailand. P.M. would like to thank the Natural National Science Foundation of China (NSFC) Research Fund for International Young Scientists FY 2016 (21650110450).

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