Combined experimental and theoretical studies on metal-CeO$_2$ for NH$_3$-SCR of NO
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Abstract: Herein, we demonstrate that the degrees of catalytic performance of M-CeO$_2$-based catalysts (M= Mn, Cu, Ru or Zr) for NH$_3$ selective catalytic reduction (NH$_3$-SCR) of NO can be estimated using the three theoretical terms; (i) oxygen vacancy formation energy of catalyst, (ii) adsorption energy of NO and (iii) adsorption energy of NH$_3$. Those terms predict the trend of the catalytic performance in the following order; Mn-CeO$_2$ > Cu-CeO$_2$ > Ru-CeO$_2$ > Zr-CeO$_2$ > CeO$_2$. To verify the theoretical prediction, the catalyst synthesis and catalytic test were performed. The normalized NO conversion rates (mol·s$^{-1}$·m$^{-2}$) were measured at low temperatures (100-200 ºC) 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, respectively. The concept of structure-activity relationship analysis (SAR) shows a strong correlation between theoretical and experimental studies. Application of theoretical calculations to predict the catalytic performance of catalysts prior the catalyst synthesis is useful in catalyst design and screening by reductions of time and cost.

Keywords: De-NO$_x$; Density functional theory; Cerium Oxide; Nitrogen Oxide