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## Effects of Brønsted acid on the Selective Catalytic Reduction of NO with NH<sub>3</sub> on Ru-doped Ceria Catalyst

Reaction mechanism of selective catalytic reduction (SCR) of NO by NH<sub>3</sub> on the clean and Brønsted acid surfaces of Ru-doped CeO<sub>2</sub>(111) were investigated using density functional theory calculation corrected by on-site Coulomb interactions (DFT+U). The calculations were performed by Vienna Ab initio Program Package (VASP). The proposed reaction mechanism on the clean surface consists of two competitive catalytic pathways (ABCD and AED pathways), while that on the Brønsted acid surface follows FC pathway. The activation energy barriers of all elementary steps as well as the corresponding relative energies of all intermediates, reactants, and products were calculated. On the clean surface, an NH<sub>3</sub> molecule is preferentially adsorbed on the Lewis acid Ru-dopant site. The dissociation of the first N-H bond is broken spontaneously after the NH<sub>3</sub> adsorption and forms the NH<sub>2</sub> species. Then this NH<sub>2</sub> species readily interacts with a NO gas and converts to the NONH intermediate (IM:4). Note that IM:4 could be decomposed to H<sub>2</sub>O and N<sub>2</sub>O via step B or decomposed to N<sub>2</sub> and H<sub>2</sub>O via step E. The calculation results reveal that step B is more feasible in terms of lower activation energy barrier; 34 kJ/mol for the former and 129 kJ/mol for the latter. Therefore, the reaction on the clean surface is suggested to follow ABCD pathway. In addition, the NH<sub>3</sub>-SCR of NO over Brønsted acid surface of Ru-doped CeO<sub>2</sub>(111) were considered to study the effect of the presence of Brønsted proton on the catalyst surface. The reaction follows FC pathway, which occurs easily because of the substantial small activation barriers. The calculations reveal that the presence of Brønsted acid on the surface catalyst accelerates the decomposition of NO by NH<sub>3</sub> over Ru-doped CeO<sub>2</sub>(111) catalyst.

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