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Effects of Brønsted acid on the Selective Catalytic Reduction of NO with NH3 on Ru-doped Ceria Catalyst

Reaction mechanism of selective catalytic reduction (SCR) of NO by NH3 on the clean and Brønsted acid surfaces of Ru-deoped CeO2(111) were investigated using density fuctionl theory calculation corrected by on-stie Coulomb interactions (DFT+U). The calculations were performed by Viena 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 corresponsing relative energies of all intermediates, reactants, and products were calculated. On the clean surface, an NH3 molecule is preferentially adsorbed on the Lewis acid Ru-dopant site. The dissociation of the first N-H bond is broken spontaneously after the NH3 adsorption and forms the NH2 species. Then this NH2 species readily interacts with a NO gas and converts to the NONH intermediate (IM:4). Note that IM:4 could be decomposed to H2O and N2O via step B or decomposed to N2 and H2O via step E. The calculation results reveal that step B is more feasible in term of lower activation energy barrier; 34 kJ/mol for the former and 129 kJ/mol for the later. Therefore, the reaction on the clean surface is suggested to follow ABCD pathway. In addition, the NH3-SCR of NO over Brønsted acid surface of Ru-deoped CeO2(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 substantail small activation barriers. The calculations reveal that the presence of Brønsted acid on the surface catalyst accerelates the decomposition of NO by NH3 over Ru-deoped CeO2(111) catalyst.

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