저온 일산화탄소 산화반응을 위한 금속산화물 촉매의 합리적 설계

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Ceria (CeO_2) is one of the most widely used materials as diverse oxidation catalysts due to its high oxygen storage capacity and high stability over a wide range of temperatures. In a field of automotive catalysis, enhancing or controlling of CO or hydrocarbon oxidation with reduction of NO_x has been main issues. One of the ways to enhance or control the catalytic activity of CO oxidation is doping of rare-earth metal or transition metal into the oxide catalysts. In this study, our combinatorial study of experiments and DFT shows the catalytic activities of CO oxidation on various rare-earth metals or transition metals. We found that the oxygen vacancy formation energy can be used as a simple descriptor to predict the whole reaction activity on both RE- or TM-doped CeO_2(111). In addition, we suggest a noble method of co-doping to overcome the limitation of single metal doped CeO_2. Our results will provide useful insight to enhance and predict the CO oxidation activity of ceria based catalysts.