Correlating adsorption characteristic and catalytic activity of CeO_2-based catalyst in CO oxidation using DFT calculation

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Regulation on greenhouse gas emission are requiring the advanced combustion technics. However, it is difficult to meet both fuel efficiency and emission standards for such pollutants (CO, hydrocarbons, NOx and particulate matters) with commercial catalytic systems. Thus, such challenges to achieve total conversions of pollutants at low temperature (<150ºC) are ongoing.

CeO_2-based catalyst is widely known for its reducibility and oxygen adsorption on oxygen vacancy producing active oxygen species. Additionally, its promotional effect on metal dispersion enables to implement 'Single-Atom' catalysts which shows excellent activity at low temperature. Moreover, Lei Nie et. al reported that atomically dispersed Pt (Pt^{2+}) showed both high CO oxidation activity and thermal stability (750ºC). In this respect, CeO_2-based catalysts with atomic dispersion can be a promising catalyst to solve emission problem.

Since the characteristic of 'Single-Atom' catalyst is still undiscovered research area, we investigated CO and O_2 adsorption of metal-doped CeO_2 using DFT calculation. Then, activity test was performed to relate catalytic activity to DFT calculation results.