

Density functional theory study of the competitive oxidation of CO and H₂ on CeO₂(111)

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Owing to the redox properties and stability, CeO₂ (ceria) has been spotlighted as a promising catalyst for automotive emission control and the reactions of a variety of fuel cells [1]. Our collaborators recently observed the preferential CO oxidation (CO-PrOx) reaction on CeO₂ surface under the mixed environment of H₂ and CO gas. Since the CO-PrOx reaction can be used to control the CO concentration in the mixed gas without the expense of H₂, it is essential for the enhancement of the performance of several kinds of fuel cells [2-3]. However, the mechanism behind the selective CO oxidation on CeO₂ has not been clearly revealed. We thus carried out density functional theory (DFT) calculations to examine the adsorption behaviors of CO and H₂ molecules on the CeO₂(111) surface, with which the mechanism of the CO-PrOx reaction is elucidated.

References

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