CO-assisted NOx reduction using IrRu bimetalic catalyst: Theoretical study

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Nitrogen oxides (NO_x) is one of the toxic gas exist in vehicle exhaust affecting environment and human health acutely. The NO_x emission can be catalytically reduced by CO, which is co-existing in the exhaust. In the present study, we prepared the IrRu bimetallic catalyst that selectively reduces NO into N_2 using CO as a reducing agent in the presence of excess O_2. A mechanistic insight using density functional theory calculation reveals that the IrRu alloy catalyst has moderate binding energies for all the adsorbates and intermediates, resulting in the acceleration of critical surface reactions, such as CO oxidation and N-NO disproportionation. In addition, a series of theoretical surface modelling also suggests that the selectivity promotion on the IrRu alloy surface originates from ensemble effect, while the ligand and strain effects are rather detrimental to the catalyst performance. This study will help to devise a design strategy of the bimetallic catalyst that can maximize the promotion effect and minimize the use of precious metals.