First-Principles Calculations for CO_2 Activation and Dissociation on Pure and Bimetallic Surfaces

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Recently, CO2 conversion into useful chemicals has been paid attention as a promising carbon resource. Due to its thermodynamic stability, one of the main issues in this filed is to activate the CO2 molecule on transition metal (TM) surfaces. However, the processes of CO2 activation and/or dissociation on the surfaces have been still under. Here, we performed DFT calculation to understand the CO2 activation process and suggest more reliable dissociation pathways on TM surfaces. Firstly, CO2 adsorptions on pure TM surfaces were investigated with the analyses of adsorption energetics and geometrics. Then, to identify the activated state of CO2, we analyzed vibrational frequencies, charge transfers and density of state on CO2 adsorption. In addition, we identified the Brønsted–Evans–Polanyi relations between reaction and activation energy and the scaling relations of adsorption strength for the reaction intermediates. Finally, the trends on CO2 dissociation on both bimetallic and pure metal surfaces were estimated by combining these relations and surface mixing rule which is a prediction method for the adsorption energies on bimetallic surfaces. Our results will contribute to designing TM catalysts for CO2 dissociation and CO2-related catalytic reactions.