Density Functional Theory Study on Catalytic Activation of Carbon Dioxide on Transition Metal Surfaces

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Since the Kyoto Protocol, CO_2 emission from fossil fuels has been one of the most important global issues. Therefore, CO_2 removal, capture, or conversion into useful chemicals became first priority for renewable energy research. Since CO_2 is thermodynamically stable, its activation on transition metal surfaces has been a main issue in this field. Although many researchers have studied the activation mechanism of CO_2 on transition metal surfaces, it is still controversial. Here, we carefully examined the CO_2 adsorption on a wide range of transition metal surfaces (Ni(111), Fe(110), Cu(111), Co (0001), Ir(111), Ru(0001), Pt(111), Pd(111), Rh(111), Au(111), Ag(111)) via density functional theory calculations with dispersion correction (DFT-D2). We first focused on the adsorption types (physisorption or chemisorption), and then analyzed what factors determine its adsorption behavior. Our results will provide a helpful insight to the catalytic activation of CO_2 in heterogeneous catalysis.