

Theoretical Study on the Electronic Properties of Metal Halide Cluster for CO Selective Adsorption

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Refinery of byproduct gases from industries is essential to reduce greenhouse gas and wasted energy source. Especially, carbon monoxide (CO) should be separated for manufacturing value-added materials such as acetic acid or methanol. In this study, CO adsorption capacity on the metal halide, which included metal cations (i.e., Fe, Co, Ni, Cu, Ru, Rh, Pd, Ag, and Au) with high electronegativity, was theoretically investigated. Additionally, in the impregnating process of metal halide into a porous-adsorbent material to enhance the CO adsorption, the metal halide turns to atomically dispersed clusters. Here, the size and structural stability of the metal halide clusters were screened through density functional theory calculation to sort out the effective CO adsorption candidates. We revealed that CO was adsorbed on the cluster by π back-bonding electron donation, which was confirmed by orbital distribution and density of states analysis. Also, the probability of CO adsorption was increased when the π back-bonding was strong. Particularly, we presented the descriptor for predicting the CO adsorption capacity from physical and electronic structure of metal halide from this study.