Screening of Metal Halide for Selective CO Adsorption

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Refinery of various byproduct gases from many industries is essential to reduce greenhouse gas and wasted energy source. Particularly, environmentally hazardous carbon monoxide should be separated from byproduct gases, not only for eco-friendly environment but also for manufacturing value-added materials. In this study, for high adsorption performance of carbon monoxide, a porous adsorbent material impregnating metal halide, which consisted of highly electronegative metal cations (i.e., Fe, Co, Ni, Cu, Ru, Rh, Pd, Ag, and Au), was investigated. Through density functional theory (DFT) calculation, a variety of metal halides was screened to find the best performance of CO-selective adsorption. First, a systematic modeling of surface structures was conducted, and second, CO adsorption energies were calculated. The results showed that CO adsorption preference was not accurately predicted solely by electronic properties of bulk structures, and thus the adsorption structures of the surface should be simultaneously examined since the surface of metal halides containing many coordinatively unsaturated metal sites exhibited the higher preference on CO adsorption.