Theoretical Prediction of CO Selective Adsorption of the Activated Carbon (AC) - Supported Metal Halide Cluster

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Carbon monoxide (CO), which is one of byproduct gas exhausted from chemical plants and hazardous to environment, has potential application for producing value-added materials though adequate separation. In this study, activated carbon (AC) was impregnated with metal halide since this adsorbent was expected to have high porosity and high CO affinity for separating CO from carbon dioxide. To determine the best impregnated metal halide, we theoretically investigated CO adsorptivity of the atomically dispersed metal halide cluster, which was composed of 9 of highly electronegative metal cations. Using density functional theory calculation, optimal size and conformation of clusters were predicted to sort out effective candidates. Also, the effect of carbon support and moisture environment were investigated for screening high CO-selective adsorbent. We revealed that CO-selective adsorption to the cluster was induced by π back-bonding electron donation, which was confirmed by orbital distribution and density of states analyses. Through the structural and electronic properties of metal halides, we identified that the $RuCl_3$ is effective as a CO-selective adsorbent material.