Machine Learning and DFT Studies on the Ru-based Sub-nanometer Clusters for Electrochemical N_2 Reduction Reaction

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Ammonia synthesis via nitrogen reduction reaction (NRR) is one of the promising techniques to store and transport hydrogen. However, the Haber-Bosch process, the conventional approach for NH_3 production, is considered one of the main reasons for global warming because it consumes a large amount of fossil fuel and releases CO_2 as a byproduct. Therefore, electrochemical NRR at ambient conditions is considered a major alternative to this process.

We studied electrochemical NRR on the Ru-based sub-nano-sized alloy clusters. In this report, the adsorption energy of NRR intermediates was investigated, and the structures were optimized on the support or gas-phase, using density functional theory (DFT) computation. From this result, we determined the NH_2 adsorption energy as a descriptor of the catalytic reactivity and set up a dataset by extracting the features concluding the geometry, adsorption, and support information for machine learning. Hence, an artificial neural network (ANN) machine learning model composed of fully connected layers was constructed for NH_2 adsorption energy prediction of bimetallic small clusters with unknown composition.