A Machine Learning and DFT - based Design of Sub-nanometer Ruthenium Clusters for Electrochemical Nitrogen 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 large amount of fossil fuels and releases CO_2 as a byproduct. Hence, electrochemical NRR at ambient conditions are considered a major alternative to this process.

We studied electrochemical NRR on the sub-nano sized Ru clusters. In this report, the optimized structure of Ru_n (n = 1-6) clusters and the adsorption energy of NRR intermediates were investigated using density functional theory (DFT) computation. From this result, we determined the NRR descriptor, reaction mechanism and the potential limiting steps on each catalyst. Furthermore, a three-layer artificial neural network (ANN) with geometrical and topological features was set up to predict NRR activities of Ru catalyst structures. This theoretical technique will provide efficient and high-throughput screening of sub-nano-scale clusters.