Computational design of catalyst for nitrogen reduction reaction by controlling support effect

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Nitrogen Reduction Reaction (N_2RR) serves as both hydrogen supplier and carrier, and is expected to play an important role in decarbonization. However, conventional Haber-Bosch method required high operating condition and emitted CO_2 during operation. Here, Density Functional Theory (DFT) simulation is used to study electrochemical catalyst for N_2RR that exhibits high activity even in mild and carbon-free conditions. We first designed Ru-based small cluster catalyst, and defective graphene and MXene are selected as a support. Further, two different mechanisms are checked up and we acquired a descriptor in terms of the adsorption energy of $*NH_2$, which is used to measure the catalytic activity. To examine the catalytic activity, we controlled substituents, alloys, and size effects. We evaluated the catalytic performance by calculating N_2RR overpotential with the obtained free energy change in each reaction step. Hydrogen Evolution Reaction (HER) Onset potential was also considered in order to suppress competitive HER effectively. In addition, electronic structure and charge transfer were investigated to understand catalytic activity toward ammonia production.