MXene-based Catalysts for Electrochemical Nitrogen Reduction Reaction: a density functional theory (DFT) study

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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 MXene-based Ru single atom catalyst, and M_2CO_2 [M= Cr, Hf, Mo, Nb, Ta, Ti, V, W, Zr] is selected as a support. Further, two different mechanisms are checked up and we acquired a descriptor in terms of the adsorption energy of $*NH_2$ through the investigation of overpotential, which is used to measure the catalytic activity. In order to find a composition with more improved catalytic activity, screening was carried out by adjusting the type (Fe, Ru, Os) and size of atoms based on the descriptor. Hydrogen Evolution Reaction (HER) Onset potential was also considered in order to effectively suppress competitive HER. In addition, electronic structure and charge transfer were investigated to understand catalytic activity toward ammonia production.