Electrochemical reduction of nitrogen on 2-dimentional hetero-double atomic catalysts: a DFT study

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The electrochemical nitrogen reduction reaction (NRR) to ammonia is one of the most attractive and emerging chemical process in hydrogen storage and transportation. We studied NRR on 2-dimentional hetero-double atomic catalysts embedded in defective graphene (RuM/C) using density functional theory computation. First, we systematically investigated the energetically optimized geometries of RuM/C to elucidate the interaction between Ru, M and support C atoms. The Gibbs free energies of nitrogen dissociation were calculated to determine which mechanism to follow for NRR on RuM/C. In addition, we calculated the adsorption energy of possible reaction intermediates to identify the limiting potential for NRR on each catalyst. We found that RuM/C showed obviously enhanced activity for NRR compared to Ru single atomic and homo-double atomic catalyst due to the adequate adsorption energy of reaction intermediates caused by strain, ligand, and support effect. We also found that the most promising candidates, on the top of the volcano plots, are RuFe/C (−0.79 eV) and RuMn/C (−0.80 eV).