Small Cluster Catalysts for the electrochemical NH_3 Production: A DFT Study

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In this presentaion, for the NH_3 proudction, we examined the electrochemical nitrogen reduction reaction (N_2RR) on the small cluster metal catalysts embedded in support by using DFT calculation. We chose the single, double and triple atoms for the size of small clusters and also investigated the electrochemical N2RR catalysis for small multimetallic clusters through ligand engineering. For the support of small metal cluster catalysts, two dimensional materials such defective graphene and mexene are considered. In addition, the electronic structure was analyzed for the clear understanding of activity of small clusters toward ammonia production via electrochemical N_2 reduction. Our theoretical study provides the fundamental mechanism of NH_3 production catalysis on small clusters and gives the physical and chemical intuition for the next generation bimetallic small cluster catalysts for hydrogen storage applications.