Design of Double Atom Catalysts for the Oxygen Evolution Reaction: A DFT Study

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In this work, our research group has investigated various double-atom catalysts(DACs) with 3d, 4d, and 5d metals on the basis of single cobalt atom catalyst supported on nitrogen doped graphene(Co@N_4/graphene), which has an overpotential of 0.40V for the oxygen evolution reaction(OER), through density functional theory(DFT) calculations. We looked closely into the Gibbs free energy changes at Co-Co double-atom catalysts(Co-Co@N_4/graphene), whose overpotential is 1.28V, during the reaction pathway and figured out potential limiting step implying the biggest endothermic reaction. Then, we built a descriptor and calculated its value representing catalytic activity to explore candidate materials that seem to have optimal descriptor value for improving the OER performance. We also carried out further DFT calculation to estimate the catalytic activity for candidate DACs and conducted additional analysis such as density of state and Bader charge to verify the enhancement of the catalytic activity. In conclusion, this research suggests another strategy of atomic catalysts design which could be outperforming single atom catalysts(SACs) in the future.