Rational Design of Single-Atom Electrocatalysts for Hydrogen Evolution and Oxygen Reduction Reactions

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Single-atom catalysts (SACs) have aroused increasing interest for practical applications due to the low cost and the improvement of their intrinsic performance. In this talk, we use a combination of density functional theory (DFT) calculations and experimental approaches to explore the stability and electrocatalytic activity of a wide range of transition metal single atoms on the potential supports such as TiC or M-N-C. Specifically, we found a suitable reaction condition to stabilize SACs and explored the reaction mechanism on the SACs. The strategy developed in this study may have wide applications to various heterogeneous catalysis systems, including SACs for other applications.