

Toward Precise Catalysis via Single-Atom Catalysts and Single-Cluster Catalysts

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Catalysis science is essential for chemical industries, pharmaceuticals, biological transformation, atmospheric processes, environment, energy, and human health, among others. The ultimate goal of catalysis science and technology is to achieve precise control of chemical transformation via green catalysts with high selectivity, stability, and activity for a target reaction. In recent years, with the rapid progress of research on single-atom catalysts (SACs) [1-4] and single-cluster catalysts (SCCs) [5-7], the dream of achieving precise catalysis via well-defined SAC and SCC active sites does not seem to be unrealistic. In this talk, we will present our recent theoretical and computational studies on SACs and SCCs in the field of heterogeneous catalysis and provide an overview and perspectives for the future development of precise catalysis via stable, well-defined, specific active sites.