Electrocatalysis by Atomically Precise Metal Nanoclusters

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Metal nanoclusters containing a few to a few hundreds of metal atoms have received much attention as materials with many practical applications because of promises offered by their unique optical, electrochemical, and catalytic properties. These ligand-protected metal nanoclusters exhibit unique redox properties and size-dependent catalytic activities. While stable nanoclusters to date are rather limited to gold and silver systems, such as $\text{Au}_{25}(\text{SR})_{18}$, $\text{Au}_{38}(\text{SR})_{24}$, and $\text{Ag}_{25}(\text{SR})_{18}$, where SR is a thiolate ligand, bimetallic nanoclusters prepared by doping a foreign metal into the stable nanoclusters have opened a new avenue to the fine-tuning of the cluster properties. Recent progress in the computational design of solid catalysts has revealed the importance of engineering of the structure and adsorption energies for catalysis at surfaces. Studies of electrocatalysis by the bimetallic nanoclusters provide many important design principles for the development of electrocatalysts with tailored cluster structure and adsorption energy. These principles are illustrated with nanocluster-based electrocatalysts for water splitting and $\text{CO}_2$ conversion.

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