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Novel Strategies for Single-Atom Catalysts

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Heterogeneous metal catalysts play a vital role in industrial chemical synthesis, sustainable energy conversion devices and advanced biotechnologies. A key concept for catalyst design is the atomic dispersion of metals on solid supports, leading to so-called single-atom catalysts (SACs). Single-metal atoms hold promise for unique activity, selectivity, and atom utilization efficiency. The supports can also change the electronic structures of the single atoms. SACs can thus provide versatile pathways for efficient mass and charge transport, and bridge the gap between homogeneous and heterogeneous catalysis. However, fabricating SACs and maintaining the metal centers as atomically dispersed sites under synthesis and catalysis conditions are challenging. Moreover, most of the reported SACs have very low metal loading, so robust approaches for fabricating SACs with high metal loading (>2 wt%) have remained elusive. Here we introduce various concepts for synthesis of high-loading SACs including multilayer stabilization strategy, MOFs derives, and their applications in electro catalytic reactions such as oxygen reduction reaction, hydrogen evolution reaction and oxygen evolution reaction. The deciphered atomic structures of SACs were studied by advanced physical characterization such as aberration-corrected scanning transmission electron microscopy, synchrotron-based X-ray absorption spectroscopy. The struction-to-property correlation was established based on above advanced analysis in combination of calculation. Our work offers promising approaches toward high-performance carbon-based electro catalysts for energy conversion applications such as fuel cell, Zn-air battery and water splitting.