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Electrocatalytic Enhancement Mechanism of Dual-Atom and Single-Atom MXenes-Based Catalyst in Oxygen and Hydrogen Evolution Reactions

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Abstract : Using single metal atoms has been considered an efficient way to develop new HER and OER catalysts. MXenes, a class of two-dimensional materials, have attracted tremendous interest as promising substrates for single-atom metal catalysts. However, there is still a lack of systematic investigations on the interaction mechanisms between various MXenes substrates and single atoms. Besides, due to the poor interaction between metal atoms and substrates resulting in low loading and stability, dual-atom MXenes-based catalysts have not been successfully synthesized. We summarized the electrocatalytic enhancement mechanism of three MXenes-based single-atom catalysts through experimental and theoretical results demonstrating the stronger hybridization between Co 3d and surface-terminated O 2p orbitals, optimizing the electronic structure of Co single atoms in the composite. This, in turn, lowers the OER and HER energy barriers and accelerates the catalytic kinetics in the case of the Co@V2CTx composite. The poor interaction between single atoms and substrates can be improved by a surface modification to synthesize dual-atom catalysts. The synergistic electronic structure enhances the stability and electrocatalytic activity of the catalyst. Our study provides guidelines for designing single-atom and dual-atom MXene-based electrocatalysts and sheds light on the origins of the catalytic activity of single-atoms on MXene substrates.

Keywords : dual-atom catalyst, single-atom catalyst, MXene substrates, water splitting
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