

Correlation between structural evolution of Ir Nanocrystals and Oxygen Evolution Reaction performance under Acidic media

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Ir and its oxide are the only available oxygen evolution reaction (OER) electrocatalysts with reasonably high activity and stability for commercial proton-exchange membrane electrolyzers. However, the structure-performance relationships for the design of better Ir-based electrocatalysts is hindered by their uncontrolled surface reconstruction during OER in acidic media. Herein, we monitor the structural evolution of two model Ir nanocrystals (one with a flat surface enclosed by (100) facets and the other with a concave surface containing numerous high-index planes). Operando X-ray absorption spectroscopy measurements reveal that the promotion of surface IrO_x formation during the OER by the concave Ir surface with high-index planes results in a gradual OER activity increase, while a decrease in activity and limited oxide formation are observed for the flat Ir surface. After the activation process, the Ir concave surface exhibits ~10 times higher activity than the flat surface. Density functional theory computations reveal that Ir high-index surfaces are thermodynamically preferred for the adsorption of oxygen atoms and the formation of surface oxides under OER conditions.