Department of Materials Science and Engineering Seminar Series 2025

Electronic States Engineering in Cobalt Oxyhydroxide for Efficient Water Oxidation

Zhang Xin

Date and time: 9 April 2026 (Thursday) 2 pm–4 pm

Venue: EA-02-15

Abstract

Electrochemical water splitting is a crucial technology for renewable energy conversion and storage, but its efficiency is limited by the sluggish kinetics of oxygen evolution reaction (OER). As such, it is essential to explore high-performance and low-cost catalysts to improve OER kinetics. Among various candidates, cobalt oxyhydroxide (CoOOH) has attracted considerable attention owing to its high activity, good durability, and versatile synthesis routes. Importantly, its catalytic performance is fundamentally governed by the electronic states near the Fermi level, the precise modulation of which remains insufficiently understood, thereby hindering the development of cobalt-based electrocatalysts. This thesis aims to enhance OER activity through electronic states engineering, by tuning the electronic states near the Fermi level from Co 3*d* t_{2g}^* to e_g^* in the first two studies, and shifting them from Co 3*d* to O 2*p* in the final work.

First, the electronic states near the Fermi level are tuned from t_{2g}^* to e_g^* orbitals, by introducing high-spin Co^{3+} in CoOOH, which enhances electron transfer ability from catalyst to external circuit. This spin transition is achieved by constructing coordinatively unsaturated Co sites at the edge of CoOOH, leading to significantly improved OER activity compared to

low-spin CoOOH. Then, the proportion of high-spin Co^{3+} is further increased by regulating the tetrahedral-to-octahedral Co ratio in precursors, thereby improving electron transfer ability. Despite these improvements, OER in these systems still follows a metal-centered redox pathway, limited by the scaling relationship between *OOH and *OH. In the final work, the electronic states near the Fermi level are shifted from Co 3*d* to non-bonding O 2*p*, through light-triggered electron transfer from oxygen to cobalt, thereby bypassing this bottleneck and enhancing OER activity. Overall, this thesis highlights the importance of electronic states engineering in designing efficient electrocatalysts.

Biography

Zhang Xin received her bachelor's and master's degrees in the Department of Materials Science and Engineering from Donghua University. She is currently a Ph.D. candidate in the Department of Materials Science and Engineering at the National University of Singapore under the supervision of Prof. Xue Junmin. Her research focuses on designing high-performance and durable electrocatalysts for next-generation alkaline water electrolysis.

Please join us!

HOST: Asst Prof Jing Yan