Department of Materials Science and Engineering Seminar Series 2025

E_g^* BAND BROADENING IN NICKEL OXYHYDROXIDES FOR EFFICIENT WATER SPLITTING

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Date and time: 20 March 2025 (Thursday) 3:00PM - 5:00PM

Venue: EA-02-14

Abstract

Electrochemical water splitting to produce green hydrogen gas has emerged as a promising technology for addressing the intermittent availability of renewable energy sources such as solar, wind, and tidal energy. However, the industrial realization of the electrochemical water splitting has been significantly limited by its sluggish anodic reaction - oxygen evolution reaction (OER). As such, it is of great importance to explore highly efficient electrocatalysts to improve the OER kinetics. Among numerous electrocatalysts evaluated so far, Ni oxyhydroxide (NiOOH) based materials have been recognized as one of the best candidates due to their earth abundance, high activity and good durability. However, some fundamental issues i.e., the relations among the materials structure, kinetics of rate-determining step (RDS), and corresponding OER activity in NiOOH based materials remain ambiguous, which greatly hinders the further design of next-generation high-performing electrocatalysts.

In this thesis, we first investigate the structural origin of the OER activity in reconstruction derived X-NiOOH (X=NiS_2, $NiSe_2$, and Ni_5P_4). We find that a stronger strain leads to a greater extent of NiO_6 octahedron distortion in X-NiOOH, which results in a greater extent of e_g^* band (3d electron states with eg symmetry) broadening. The increase in e_g^* band broadening can facilitate the electron transfer by generating more electronic states around the Fermi level, which ultimately enhances the catalytic performance. Then, we propose a novel open circuit voltage combined pulse-voltammetry (OCV-PV) method to quantify the $^*OOH$ formation rate in NiOOH. The relationship between the materials structure, $^*OOH$ formation kinetics, and corresponding OER activity is further discussed by using $Ni_{1-x}Fe_xOOH$ ($x = 0, 0.05, 0.2$) as model samples. With the proposed OCV-PV method, it is found that a stronger e_g^* band broadening

could significantly accelerate the *OOH formation kinetics, hence resulting in a higher OER activity. Finally, the key role of e_g^* band broadening on the newly reported coupled oxygen evolution mechanism (COM) is studied. It is revealed that in low potential region, realizing stronger e_g^* band broadening could facilitate the *OH deprotonation. Meanwhile, in high potential region where the photon utilization is the rate-determining step (RDS), a stronger e_g^* band broadening would widen the non-overlapping region between d_{z^2} and a_{1g}^* orbitals, thereby enhancing photon utilization efficiency.

Biography

Zhong Haoyin received his bachelor's degree from Central South University in 2017 and master's degree from Shanghai Jiao Tong University in 2020. He is currently a Ph.D. candidate under the supervision of Assoc. Prof. Xue Jun Min and Adjunct Research Fellow Zhang Jun. His research focuses on electrocatalysts development for the electrochemical oxygen evolution reaction.

Please join us!

HOST: Prof Ding Jun