Department of Materials Science and Engineering Seminar Series 2025

COUPLED OXYGEN EVOLUTION MECHANISM AS A DUAL LIGHT-HARVESTING STRATEGY FOR PHOTOELECTROCHEMICAL WATER OXIDATION

An Hang

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Venue: EA-06-04

Abstract

Photoelectrochemical (PEC) water splitting is a promising technology for solar hydrogen production. The photocurrent of conventional semiconductor photoanodes is fundamentally limited by their optical absorption edge. Therefore, the development of strategies that can utilize a broader portion of the solar spectrum is critical for improving the efficiency of PEC water oxidation. However, conventional co-catalysts function primarily as kinetic promoters and do not contribute additional light harvesting.

In this thesis, the Coupled Oxygen Evolution Mechanism (COM) was established as a dual light-harvesting strategy for photoelectrochemical water oxidation. It was demonstrated that a light-responsive $Ni_{0.8}Fe_{0.2}OOH$ co-catalyst, when integrated with a $BiVO_4$ photoanode, absorbs long-wavelength photons that are transmitted by the semiconductor and thereby generates an additional oxidative equivalent under operating conditions. Systematic experiments, including directional illumination, TMA^+ inhibition, optical isolation, dual-light-source chronoamperometry, and operando ^{18}O differential electrochemical mass spectrometry, confirmed that the co-catalyst functions as an independent light-harvesting component. Based on this understanding, six Ni-based oxyhydroxides (M = Fe, Co, Cr, Cu, V, Mn) were systematically investigated to establish how the secondary metal modulates both intrinsic photon-utilization efficiency and interfacial electronic structure. Iron was identified as the optimal substituent. Further optimization of Fe content and photo-assisted

electrodeposition yielded a $BiVO_4$/ $Ni_{0.8}Fe_{0.2}OOH$ photoanode that delivers a photocurrent density of 8.25 mA cm^{-2} at 1.23 V versus RHE under simulated sunlight, exceeding the theoretical limit of pristine $BiVO_4$, with a projected levelized cost of hydrogen of 5.17 USD kg^{-1}. Finally, a hydrothermal reconstruction strategy was developed to convert Co-containing perovskites into chemically anchored photocatalyst–co-catalyst architectures, demonstrating a general route beyond the electrodeposited $BiVO_4$ system. The work redefines the role of the co-catalyst from a pure kinetic promoter to an active light-harvesting layer and provides design principles for higher-efficiency PEC systems.

Biography

An Hang received his bachelor's degree in Chemical Engineering from Fuzhou University and his Master's degree in Materials Science and Engineering from the National University of Singapore. He is currently a PhD candidate in the Department of Materials Science and Engineering at NUS under the supervision of Prof. Xue Junmin and Prof. Lu Li. His research focuses on photoelectrochemical water oxidation, and the design of dual light-harvesting photoanodes based on BiVO4 and Ni-based oxyhydroxides co-catalyst.

Please join us!

HOST: Asst Prof Jing Yan