Department of Materials Science and Engineering Seminar Series 2025

DESIGN OF MOF-DERIVED CO-BASED NANOSTRUCTURES FOR ELECTROCATALYSIS

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Abstract

Water splitting technologies are limited by sluggish oxygen evolution reaction (OER), and many advanced electrocatalysts reconstruct under bias, obscuring designed structure–activity relations. Metal–organic frameworks (MOFs) offer well-defined architectures and compositional tunability, yet conventional MOF conversions typically destroy the original scaffold and yield poorly controlled active phases. In this thesis, a “capping-layer” strategy was developed that links synthesis, operando reconstruction, and performance in MOF-derived OER electrodes. Using Co-based MOF as a model, capping layers are pre-installed that provide robust OER-active sites, improve interfacial charge transport, and stabilize the MOF-derived framework, while steering the surface region to evolve into active species. Integrated structural/spectroscopic analysis and electrochemical testing, together with density functional theory, show that the capping layers host active Co sites and exhibit a narrowed electronic band gap. These features lower the potential-determining step and help explain the faster OER kinetics and improved durability relative to uncapped or converted controls. Overall, the work establishes surface capping as a practical design principle for architected MOF-derived OER electrodes and offers a framework to apply to more complex catalyst architectures.

Biography

Liu Weihao received his bachelor's degree in Materials Physics from Jilin University and his master's degree in Materials Science and Engineering from the National University of Singapore. He is currently a Ph.D. candidate in the Department of Materials Science and Engineering at NUS, under the supervision of Prof. John Wang. His research focuses on MOF-derived electrocatalysts for the oxygen evolution reaction (OER), with an interest in surface reconstruction. His work aims to develop stable, high-performance catalysts for next-generation electrochemical energy systems.

Please join us!

HOST: Asst Prof Jing Yan