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Synthesis and characterization of Mo₂C-Cu composites as an electrocatalyst for the hydrogen evolution reaction

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Abstract:

The catalysts with metal particles as active sites play an important role for the understanding of hydrogen reaction mechanism for rational design of electrocatalysts. Recently, the application of metal organic frameworks (MOFs) in electrochemical hydrogen production has significantly increased. Here, a molybdenum-copper metal-organic framework (Mo-Cu MOF) was prepared by a simple wet chemical mixture as a precursor, followed by high-temperature carbonization. The molybdenum source was carbonized into molybdenum carbide nanocrystalline particles in the confined space of the Mo-Cu MOF, and the copper in the Mo-Cu MOF nodes for internal electron transfer to increase the efficiency of hydrogen production through electrocatalysis. X-ray diffraction analysis revealed the formation of η -MoC phase at a heat treatment temperature of 800°C. The MoC nanoparticles size increases from 3.8 nm to 23.73 nm with increase of synthesis temperature to 900°C due to change of original η -MoC phase into β -Mo₂C phase. The microstructure analysis by transmission electron microscopy revealed a gradual change of octahedral structure of Mo_xC-Cu with the increase of temperature. The structure of the MOF changed with the increase of temperature leading to a significant decrease in pore surface area and pore volume. The electrocatalytic hydrogen generation showed that the η -MoC-Cu material synthesized at 800°C exhibited an overpotential (η_{10}) of -233 mV and a Tafel slope of 73 mV/dec. This indicates the role of copper in facilitating electron transfer within the material. Details about hydrogen production and mechanism will be explained during presentation.

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