

Study on Preparation of Transition Metal Dichalcogenides by Low-temperature Plasma and Their Electrocatalytic Water Splitting Performance and Mechanisms

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Hydrogen production via electrocatalytic water splitting using renewable electricity is a promising route to clean energy utilisation and carbon-neutrality. The overall water splitting (OWS) consists of anodic oxygen evolution reaction (OER) and cathodic hydrogen evolution reaction (HER), and the lack of cost-effective and highly efficient catalysts greatly hampers the large-scale implementation of hydrogen energy. Transition metal dichalcogenides (TMDs) have emerged as viable candidates for replacement of platinum-group-metal-based catalysts. However, the electrocatalytic performance of TMDs, especially at high current densities, needs to be further improved for practical applications.

In this presentation, we report in situ plasma synthesis of nickel-iron layered double hydroxides/amorphous molybdenum tungsten sulphides (NiFe-LDHs/a-MoWS_x) as bifunctional catalysts toward OER and HER, with synergy between hydrogen spillover and vacancy engineering. NiFe-LDHs/a-MoWS_x possessed excellent electrocatalytic performance in alkaline electrolyte: for OER and HER, the overpotentials to reach a current density of 1000 mA cm⁻² were 300 mV and 545 mV, respectively. Assembled into a water electrolyser, the NiFe-LDHs/a-MoWS_x couple exhibited outstanding OWS performance: the cell voltage needed to deliver a current density of 1000 mA cm⁻² was 2.068 V, which was 12% smaller than that of the commercial Pt/C||RuO₂ couple. Density functional theory calculations demonstrated that hydrogen spillover from a-MoWS_x to NiFe-LDHs facilitated reaction kinetics and that iron vacancies generated during plasma synthesis lowered the energy barriers. This work paves the way towards batch fabrication of low-cost and efficient catalysts for industrial hydrogen production by water splitting.

References

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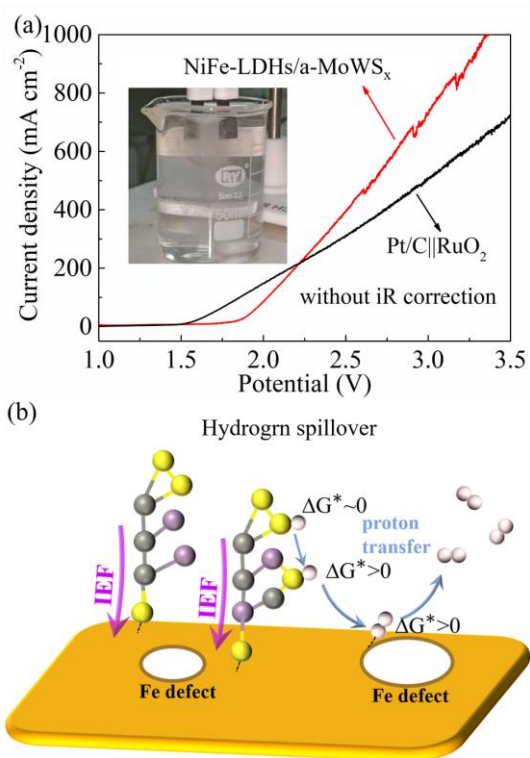


Figure 1. (a) OWS performance of NiFe-LDHs/a-MoWS_x. (b) Schematic of synergy between hydrogen spillover and vacancy engineering.