Theory Guided Design of $MoO_3/NiMoO_4$ Heterostructures Hybridized Active Pt co-catalyst for Efficient Water Splitting

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Electrochemical water splitting is a promising, environment-friendly approach to produce hydrogen (H_2) fuel, as an energy storage medium for renewable energy systems. Water splitting requires a voltage higher than 1.23 V due to the sluggish kinetics of both hydrogen evolution reaction (HER) and oxygen evolution reaction (OER). While noble metals-based catalyst, such as Pt, RuO_2, and IrO_2, demonstrate excellent catalytic activity for enhancing the kinetics of water splitting. The challenge is that these noble metals are expensive and scarce, limiting their industrial applications. An ideal strategy to reduce the cost of catalyst production is the reduction of the overall noble metal content without compromising the entire catalytic activity.

In this study, an excellent bifunctional catalyst based on vertically aligned $MoO_3/NiMoO_4$ heterostructured nanorod arrays coupled with super-active Pt ultrafine nanoparticles for both HER and OER toward industrial-grade water splitting is developed using a combined computational and experimental approach. Through first-principles based density functional theory (DFT) calculations, we demonstrate the combination of MoO_3 and $NiMoO_4$ creates a metallic heterostructure with outstanding charge transfer ability. The DFT calculations have also revealed an excellent chemical coupling effect between the $MoO_3/NiMoO_4$ and Pt that synergistically optimizes the charge transfer capability and Gibbs free energies of intermediate species, leading to improved reaction kinetics for water electrolysis. The Pt-$MoO_3/NiMoO_4$ catalyst was synthesized and tested for electrochemical water-splitting performance. The Pt-$MoO_3/NiMoO_4$ electrocatalyst was found to perform better than noble-metals catalysts, such as Pt/C and RuO_2, at the industrial-grade current level ($\geq$1000 $mAcm^{-2}$). It shows extremely small overpotentials of 38.3 and 267.6 mV at 10 $mAcm^{-2}$ for the HER and OER, respectively. When used simultaneously as a cathode and anode, the proposed material yields 10 $mAcm^{-2}$ at a remarkably small cell voltage of 1.55 V and has shown extraordinary durability for over 50 h.