## Designing Nanostructures and Active Sites of 2D Materials for Enhanced Water Splitting Activity

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Sustainable and large-scale production of hydrogen from water using the efficient and cost-effective electrocatalytic/photocatalytic/photoelectrocatalytic water splitting devices, e.g., water-splitting electrolysers, is greatly promising for future hydrogen economy.<sup>[1]</sup> To this end, efficient, durable, and low-cost electrocatalysts are requisite for reducing the kinetic overpotentials of hydrogen evolution reaction (HER) and oxygen evolution reaction (OER). To date, precious metal platinum (Pt) and iridium (Ir)based catalysts remain as the most active and robust HER and OER electrocatalysts, respectively. Unfortunately, the large-scale applications of noble metal-based catalysts for hydrogen production is seriously hindered by its scarcity and high cost.

Recently, due to its high specific surface area and short charge transfer distance, 2D nanomaterials are emerging as a promising class of electrocatalysts for the HER and OER.<sup>[2]</sup> In order to achieve а hiah electrocatalytic water splitting performance, rationally designing nanostructures and electronic properties of 2D nanomaterials is essential for offering large surface area and optimal active sites. Herein, we will present our recent efforts on the design and synthesis of 2D nanomaterials as noble metal-free electrocatalysts for the HER and especially fabrication OER, of 2D hierarchical nanostructures,<sup>[3]</sup> interfacial engineering of 2D heterostructures<sup>[4]</sup> as well as tailoring water dissociation active sites.<sup>[5,6]</sup> We will highlight their great potentials for significantly enhancing the electrocatalytic

water splitting performance by designing rational nanostructures and electronic properties. Moreover, we also try to reveal the relationship among kinetic reaction steps, electronic properties of active sites and electrochemical water splitting performance.

## References

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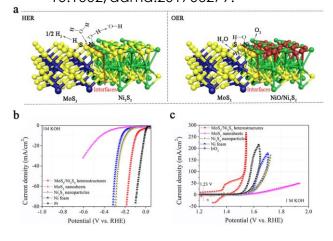


Figure 1: a) The proposed mechanisms of the dissociation of  $H_2O$ , OH, and OOH intermediates on the  $MoS_2/Ni_3S_2$  heterostructures; b) the HER and c) OER polarization curves of the electrocatalysts.