Two-dimensional heterostructures toward high current density electrocatalysis

With the support by the National Natural Science Foundation of China, the research teams led by Profs. Liu BiLu (刘碧录) and Zou XiaoLong (邹小龙) at Tsinghua-Berkeley Shenzhen Institute (TBSI), Tsinghua University, addressed the challenge of developing non-expensive electrocatalysts that work well at high current densities, by exploring the roles of morphology and surface chemistry of two-dimensional material based electrocatalysts, which was published in *Nature Communications* (2019, 10: 269)

Hydrogen production by electrochemical water splitting, i. e., hydrogen evolution reaction (HER), is one of the most effective strategies toward renewable energy paths and to solve current energy crisis and environmental pollution. The biggest issue for large-scale implementation of this technique is high electricity consumption. Development of highly efficient electrocatalysts becomes the key issue for the water splitting technique in academia and industry. Platinum (Pt) has been recognized as one of the most efficient electrocatalysts for HER reaction. Unfortunately, limited reserves and high cost of Pt prevent its wide use. In recent years, much effort has been devoted to finding alternative electrocatalysts, the performance of which is still poorer than that of Pt-based catalysts. In addition, for the industrial use in practice, the performance of electrocatalysts at large current densities of 200—1 000 mA cm^{-2} is critical. However, it is still a grand challenge to design catalysts that can work well at large current densities and the underlying mechanism is not clear.

From the electrochemical basis, hydrogen evolution at large current densities differs from that at small current densities because of unavoidable effects of mass transfer on the catalytic performance. Liu's group explored the roles of surface chemistry and microscopic morphology of catalysts in the mass transfer of reactants and products at large current density HER using three model catalysts, i. e., flat Pt foil, two-dimensional MoS_2 microspheres, and MoS_2/Mo_2C heterostructures. Their intentionally-designed MoS_2/Mo_2C heterostructure catalyst shows much better activity for HER than Pt, with low overpotentials of 227 mV (in acidic media) and 220 mV (in alkaline media) at a large current density of 1000 mA cm^{-2}. They also found that the catalysts show good stability and durability at large current densities, and the catalytic performance is independent of pH, indicating a bright future for this catalyst for practical uses. Experimental and theoretical investigations have shown that Mo_2C modified by surface oxygen formed during the HER process not only promotes the interfacial mass transfer of reactants and hydrogen gas bubbles on MoS_2, but also speeds up water dissociation and hydrogen absorption kinetics, resulting in decent HER performance at high current densities. This work not only produces a highly efficient electrocatalyst, but also provides insightful understanding of the roles of nanostructuring and surface chemistry in HER kinetics. The results provide general rules to guide the design of high performance catalysts working in HER and in principle, many other electrochemical reactions and systems.

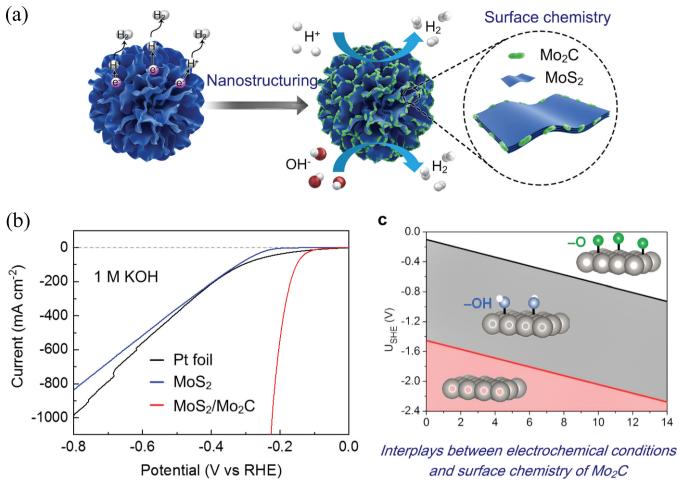

Figure (a) Design of efficient electrocatalysts for large current density HER based on combination of surface chemistry and morphology of catalysts. (b) Current-potential curves of the three electrocatalysts. (c) Interplays between electrochemical conditions and surface chemistry of Mo_2C, indicating modified active sites of Mo_2C during the HER process.