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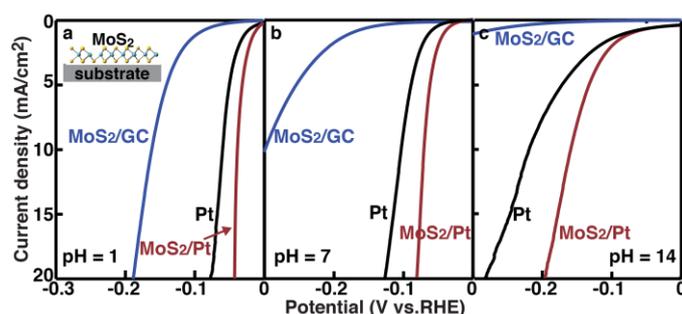
## Engineering MoS<sub>2</sub> for High-Performance Electrocatalytic Hydrogen Evolution

Developing catalysts better than Pt for the hydrogen evolution reaction (HER) consists of one holy grail in the field of clean energy. We demonstrate that monolayer MoS<sub>2</sub> films may be engineered to show better HER catalysis than Pt. This is realized by optimizing the density of sulfur vacancies in the film and leveraging proper interactions of the film with substrates. Pt substrate is used as an example to provide the proper interaction. The substrate does not participate the catalytic reaction, but may boost the activity of the film by forming a lower interface tunneling barrier and affecting the electronic structure of the film, such as through charge transfer. A minimal amount of Pt like 1 nm thick is enough to enable the superior performance at the film, and the performance of the film is very stable with no degradation for more than two months. This result indicates that MoS<sub>2</sub> may be engineered to be better than Pt in HER catalysis, although more studies would be necessary to find out non-noble materials as the proper substrate.

### References

- [1] All the catalytic active sites of MoS<sub>2</sub> for hydrogen evolution, Guoqing Li, Du Zhang, Qiao Qiao, Yifei Yu, David Peterson, Abdullah Zafar, Raj Kumar, Stefano Curtarolo, Frank Hunte, Steve Shannon, Yimei Zhu, Weitao Yang, Linyou Cao; *Journal of the American Chemical Society*; 2016, 138(51), pp 16632-16638;
- [2] Activating MoS<sub>2</sub> for pH-Universal Hydrogen Evolution Catalysis; Guoqing Li, Du Zhang, Yifei Yu, Shengyang Huang, Weitao Yang, Linyou Cao; *Journal of the American Chemical Society*; 2017, 139 (45), pp 16194-16200;

### Figures



**Figure 1. Better-than-Pt HER catalysis of monolayer MoS<sub>2</sub> films over a broad range of pH values.** (a) Polarization curves collected from a monolayer MoS<sub>2</sub> film on glassy carbon (GC) substrates (blue curve), a monolayer MoS<sub>2</sub> film on a Pt substrate (red curve), and the bare Pt substrate with no MoS<sub>2</sub> film (black curve) in 0.5 M H<sub>2</sub>SO<sub>4</sub>. Also given are the polarization curves collected from the monolayer MoS<sub>2</sub> film on Pt substrates (red curve) and the bare Pt substrate (black curve) in (b) neutral media (pH = 7) and (c) alkaline electrolyte (pH = 14). Inset in (a) shows a schematic illustration for the film on substrates.