Hydrogen production using 2D MoS_2 electrocatalysts: The effect of applied potential and catalyst support

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One solution to reduce fossil fuel consumption over the next 50 years is a shift towards a hydrogen economy where H_2 is used to store, transport, and release energy. To realise this shift, H_2 must be able to be produced *via* electrocatalytic splitting of H_2O. One of the half-cell reactions in this process is the hydrogen evolution reaction (HER):

$$2H^+ + 2e^- \xrightarrow{\text{catalyst}} H_2$$

The most efficient catalyst for the HER is Pt, however it is scarce and therefore undesirably expensive for H_2 production on an industrial scale. As a result, there has been significant interest in designing alternative catalysts from abundant and inexpensive materials.[1] Nanoscale MoS_2 catalysts are one promising option, as they are cheaply synthesised and have shown encouraging catalytic activity towards H_2 evolution.[2] However, the mechanism for the HER on MoS_2 is not yet fully understood,[3] and the catalyst must be optimised to perform as well as Pt.[4]

This presentation will explore results from first-principals calculations examining the Tafel and Heyrovsky mechanisms of hydrogen evolution on MoS_2. Specifically, we focus on how these mechanisms, and thus the rate of hydrogen evolution, can be affected by different applied potentials and catalyst supports (e.g. gold and graphene). The results allow a more comprehensive understanding of the HER on MoS_2, and contribute to the optimisation of this key reaction for sustainable energy.

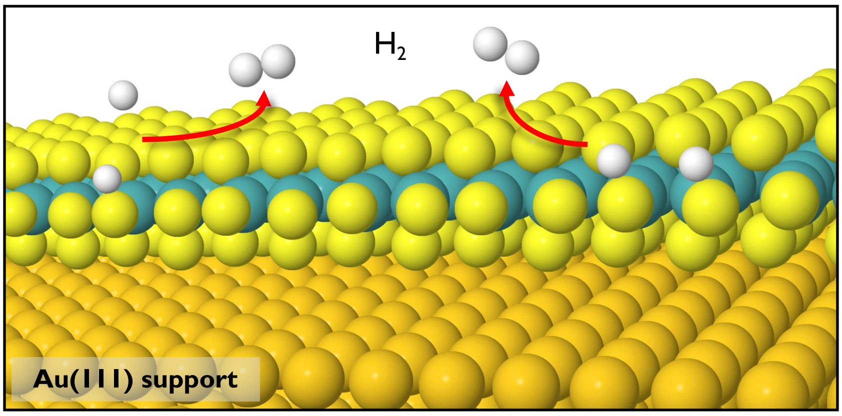

Figure
Two possible mechanisms for H_2 evolution on an MoS_2 edge. Key: Mo - green, S - yellow, H - white, Au - gold.

Left (Tafel): $H_{ads} + H^+ + e^- \rightarrow H_2$
Right (Heyrovsky): $2H_{ads} \rightarrow H_2$

References

[1] Greeley, J., Jaramillo,T., Bonde, J., *et al.*, *Nat. Mater.* **2006,** *5*, 909-913.
[2] Jaramillo, T., Jørgensen, K., Bonde, J., *et al.*, *Science* **2007,** *317*, 100-102.
[3] Huang, Y., Nielsen, R., Goddard, W., *et al.*, *J. Am. Chem. Soc.* **2015,** *137*, 6692-6698.
[4] Tsai, C., Abild-Pedersen, F., Nørskov, J. K., *Nano. Lett.* **2014**, 14, 1381-1387.