Sustainable Electrochemical Hydrogen Production

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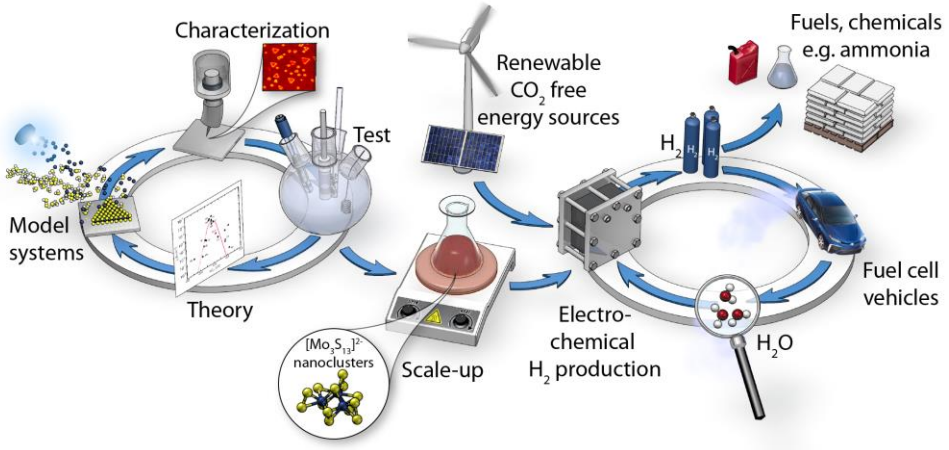
Molecular hydrogen (H_2) is one of the world's most important chemicals with a global production rate of approximately 50 billion kg per year. Today hydrogen is mainly used for petroleum refining and for synthesizing ammonia-based fertilizers but hydrogen also hold promise for the transportation sector using fuel cell vehicles. As hydrogen is mainly produced from fossil fuels, developing an alternative, renewable pathway to produce H_2 in a cost-competitive manner would have a significant impact in reducing fossil fuel consumption and CO_2 emissions. One attractive pathway for clean hydrogen production is through electrochemical processes coupled to renewable energy sources such as wind or solar.

The hydrogen evolution reaction (HER, $2H^+ + 2e^- \rightarrow H_2$) constitutes half of the water splitting reaction. To increase process efficiency, active catalysts for the HER are needed. Currently platinum is the best known HER catalyst as only small overpotentials are required to drive high reaction rates, but the scarcity and high cost of Pt may limit its widespread technological use. This has sparked a search for Earth-abundant catalysts that potentially could replace Pt - a search where the development of molybdenum sulfide (MoS_2)-based HER catalysts serves as an excellent example of theory-guided discovery and design of new electrocatalysts.

For decades, MoS_2 was believed to be inactive for the HER. However, inspired by hydrogen-producing enzymes such as hydrogenase and nitrogenase in nature, theoretical calculations predicted the edges of MoS_2 layers to be active. Guided by these calculations, several nanostructured MoS_2 catalysts have been synthesized to expose edge sites. In my talk, I will show this extraordinary development of non-precious metal HER catalysts and highlight a specific example of one such catalyst; $[Mo_3S_{13}]^{2-}$ nanoclusters.



Development of catalysts for electrochemical hydrogen production. *Left loop:* The interactive and interdisciplinary loop for discovering new catalysts in a rational manner. *Right loop:* Electrochemical conversion of water to hydrogen using energy from renewable sources.