Computational design of new materials for water electrolyzers

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Most of the energy consumed by human societies currently comes from fossil fuels such as coal, petroleum, and natural gas. When burned, these fuels generate CO_2 and CO, the atmospheric accumulation of which has led to a substantial and harmful imbalance in the carbon cycle.[1] This calls for the use of alternative fuels, such as hydrogen.

However, hydrogen is conventionally produced by steam reforming. As this energy-intensive process uses natural gas and its byproduct is carbon monoxide, it is not carbon neutral. A more convenient alternative is electrochemical water splitting, in which water molecules are catalytically transformed into hydrogen and oxygen using electricity.

Nevertheless, the low efficiency of this electrocatalytic process currently prevents the massive use of water electrolyzers. Therefore, active and stable catalysts for water splitting are required.

In this talk, I will present a computational strategy for the design of water splitting catalysts.[2] Interestingly, the methodology is based on simple and intuitive chemical concepts.[3] I will briefly discuss its advantages and limitations and show successful examples of its use.[4] Finally, I will talk about the future challenges in computational materials design for electrocatalysis.[5]

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