

# The Role of Thermodynamics in the Design of High-Efficiency Catalysts for Green Hydrogen Production

David Lewis\*

Department of Chemistry, University of Edinburgh, Edinburgh, Scotland

## DESCRIPTION

The pursuit of renewable and sustainable energy sources has increased its importance of hydrogen as a clean fuel that can be essential to the decarbonisation of the power, transportation, and industrial sectors. A possible route for "green" hydrogen among the several hydrogen generation techniques is water electrolysis, especially when employing renewable power. The creation of effective catalysts that can speed up the electrochemical processes that split water into hydrogen and oxygen is a main step in this process. In order to ensure that hydrogen generation is both economical and energy-efficient, thermodynamics the area of physics that studies the interactions between heat, work, and energy is essential to the design of these catalysts. Through two half-reactions, the Hydrogen Evolution Reaction (HER) and the Oxygen Evolution Reaction (OER), water electrolysis divides water molecules ( $\text{H}_2\text{O}$ ) into hydrogen gas ( $\text{H}_2$ ) and oxygen gas ( $\text{O}_2$ ) when an electric current is applied. Since both processes are endothermic by nature, energy must be added in order for them to proceed. However, a voltage across the electrolyser cell may be used to drive the whole process. The voltage needed to drive the reactions, which is established by thermodynamic parameters like the processes Gibbs free energy change ( $\Delta G$ ), determines how efficient this process is.

The over-potentials needed to get over the kinetic barriers connected to both HER and OER are directly related to the thermodynamic efficiency in the case of water electrolysis. The theoretical minimum voltage, which is around 1.23 V under normal circumstances, is not met by these. However, because of the inefficiency of the catalysts used in these processes, larger voltages are really required in practice. Catalysts are essential for lowering the energy barriers in electrochemical processes, which increases process efficiency. The design of catalysts for high-efficiency green hydrogen generation is influenced by both their intrinsic electrical and thermodynamic features. A catalyst has to have the ideal combination of characteristics to maximize the electrolysis processes' kinetic and thermodynamic aspects.

The most important steps that need to be completed correctly are the selection and optimization of the electro-catalyst. In order to enhance the synthesis of  $\text{H}_2$  from protons, HER requires a thermodynamic reduction in the hydrogen adsorption energy on the catalyst surface. Because of their ideal hydrogen binding energy, metals like platinum are very effective, but they are also costly and hard to find. Researchers are looking for substitute materials that have similar catalytic activity but are more readily available and reasonably priced, including metal alloys or transition metals. Effectively oxidizing water to oxygen is the thermodynamic difficulty for OER, and this is a more complicated process since it involves several electron exchanges. The production of high-energy intermediates, such hydroxyl and peroxide species, is especially detrimental to the OER. These catalysts, including ruthenium oxide and iridium, are uncommon and costly while having excellent thermodynamic efficiency.

The design of efficient catalysts is often based on the "Energy landscape" of an electrochemical reaction. A key thermodynamic concept is the reaction free energy, which determines the energy required for each step in the reaction mechanism. For both HER and OER, an ideal catalyst should provide favourable energy pathways that lower the activation energy and minimize over-potentials. This requires a careful balance between the adsorption energies of intermediates and the overall change in the Gibbs free energy of the reaction. Thermodynamic modeling and computational studies such as Density Functional Theory (DFT) have been invaluable tools in predicting and designing catalysts with optimal electronic structures that match the desired reaction energies. In addition to catalytic activity, thermodynamics also determine the stability and durability of a catalyst. Because electrolysis processes involve harsh conditions such as high voltages and acidic or basic environments, a highly efficient catalyst must be resistant to degradation over time. The thermodynamic stability of a catalytic material is important to ensure that it does not undergo phase changes, dissolution, or surface poisoning that would affect its performance and lifetime.

**Correspondence to:** David Lewis, Department of Chemistry, University of Edinburgh, Edinburgh, Scotland, E-mail: lewisDch@edin.ac.uk

**Received:** 21-Oct-2024, Manuscript No. JTC-24-35862; **Editor assigned:** 23-Oct-2024, PreQC No. JTC-24-35862 (PQ); **Reviewed:** 06-Nov-2024, QC No. JTC-24-35862; **Revised:** 13-Nov-2024, Manuscript No. JTC-24-35862 (R); **Published:** 20-Nov-2024, DOI: 10.35248/2157-7544.24.15.419

**Citation:** Lewis D (2024). The Role of Thermodynamics in the Design of High-Efficiency Catalysts for Green Hydrogen Production. J Thermodyn Catal. 15:419.

**Copyright:** © 2024 Lewis D. This is an open-access article distributed under the terms of the Creative Commons Attribution License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original author and source are credited.

Furthermore, creating catalysts that prevent undesirable side reactions requires an understanding of the thermodynamic stability of the reaction intermediates. To avoid the generation of hazardous species that might lower catalyst efficiency or induce deterioration, for example, the stability of oxygen intermediates during OER must be maximized. The design of high-efficiency catalysts for the creation of green hydrogen is

based on thermodynamics. Researchers may create catalysts that reduce energy barriers, improve reaction kinetics, and increase overall efficiency by comprehending the thermodynamic principles governing the electrochemical processes of water splitting. Finding a balance among material availability, cost-effectiveness and long-term stability, while optimizing catalytic activity thermodynamically is a persistent issue.