

# LIGHT-INDUCED HYDROGEN PRODUCTION FROM WATER USING NICKEL(II) CATALYSTS: THE ROLE OF THE NON-INNOCENT LIGANDS, THE REACTION MECHANISM, AND THE NUCLEARITY IN THE CATALYTIC EFFICIENCY

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Solar energy conversion to chemical energy through the process of light-induced water splitting to oxygen and hydrogen is a promising solution to meet the world's increasing energy demands. However, to make this transformation economically feasible, it is essential from one side to develop sustainable catalysts and on the other to influence the reaction mechanism, particularly in the case of molecular catalysts [1-3]. Biomimetic, non-innocent ligands can significantly enhance the reactivity and selectivity of the metal center, making them crucial components in the design of effective catalysts [4-5].

The focus of our study is to understand the relationship between non-innocent ligands and reaction mechanisms in the development of a high-performance molecular catalyst for hydrogen production. By combining experimental techniques such as spectroscopy and cyclic voltammetry with computational methods such as density functional theory calculations, we aim to investigate the role played by ligands and reaction mechanisms in light-driven water splitting. Our findings demonstrate that the presence of non-innocent ligands and the choice of reaction mechanism have a significant impact on the catalyst's efficacy. Additionally, we observed that the catalytic efficiency of the catalysts can be enhanced exponentially by increasing their nuclearity.

The insights gained from this study can be utilized in the development of more efficient and sustainable molecular catalysts for hydrogen production, ultimately contributing towards the development of clean energy sources.

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