# A Review of the Current DFT Simulations and Experimental Work done on Solar Powered Water Splitting

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## Abstract

Over the last years, there has been a steadily increasing focus on clean, renewable energy sources as a way to hinder the irreversible climate change we are facing and to meet the continuously growing energy demand. The direct harvesting of solar light and its conversion into electrical energy in photovoltaic cells or into chemical energy by photoelectrochemical reactions are the most relevant technologies to address this challenge. Conventionally, both technologies rely on the collection of light in semiconductor materials with appropriate bandgaps, matching the solar spectrum and thus providing a high-energy conversion efficiency. In this presentation, we describe the most recent theoretical simulations and experimental work within this field, with the intention of providing a clear overview of the current state of solar driven hydrogen production and of the main issues to be addressed before the technology can become competitive. We will discuss various photocatalysts, including metal oxides, nitrides, sulphides, lanthanides, nanocomposites and doped materials, providing an evaluation of their strengths and shortcomings. The interesting case of $TiO_2$ is presented in a separate section, in which we address the well-known issues related to its too wide band gap, the quick electron-hole recombination time and the large overpotential for hydrogen evolution reaction. We propose a number of solutions, including a variety of dopants, surface modification, amorphization of the crystal structure, heterojunction catalysts and noble metal deposition. The tremendous increase of computational power over the last couple of decades, in combination with methodological improvements, has made it possible to guide the development of new materials using principles and calculations based on quantum mechanics. Model simulations can work as a great tool for screening a large database of materials, thus identifying new promising materials. Future work should focus on improving the current technology by enhancing visible light absorption, physical and chemical stability, lifetime as well as charge transfer.