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Co-Catalyst-Free Photocatalytic Hydrogen Evolution on TiO₂: Synthesis of Optimized Photocatalyst through Statistical Material Science

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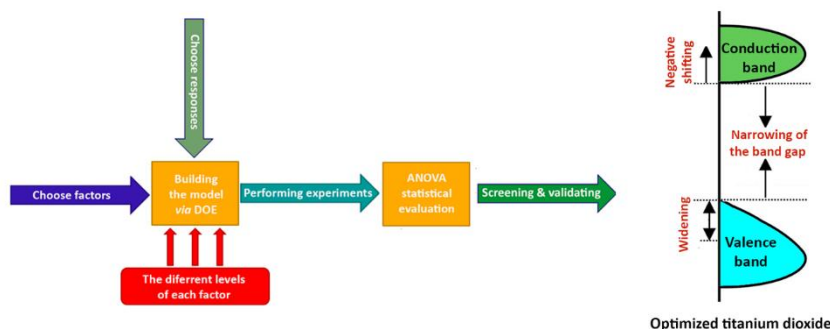
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Graphical abstract



Highlights

- A successful combination between statistical and material sciences was achieved.
- DOE offers a systematic statistical approach to synthesize TiO₂ via EISA method.
- A Photocatalytic hydrogen evolution on a co-catalyst-free TiO₂ was recorded.
- The anatase TiO₂ has a narrower band gap with a more negative potential of its E_{fb}.
- The optimized TiO₂ has high density of charge carriers exhibiting longer lifetime.

Abstract

An active TiO₂ for co-catalyst-free photocatalytic hydrogen evolution was successfully synthesized employing a simple Evaporation-Induced Self-Assembly (EISA) method that was developed and optimized with the help of Design of Experiment (DoE) coupled with Full Factorial Design (FFD) methodology. Coupling DoE with FFD provides a statistical tool for optimizing the synthesis process while carrying out the smallest number of experiments. This tool builds a statistical framework to determine the significance of the studied factors, i.e., titanium-precursor type, surfactant type and surfactant quantity, along with their potential interactions, as well as with their optimum levels. The choice of the titanium-precursor type is found to be the predominant factor affecting the efficiency of TiO₂ for hydrogen gas evolution. The interaction between precursor type and surfactant type is also statistically significant. The statistically optimized study identifies that combining F-108 amphiphilic block copolymers with titanium(III) chloride solution leads to TiO₂ exhibiting the highest photocatalytic efficiency for the generation of molecular hydrogen. The thus prepared TiO₂ shows relatively high photocatalytic hydrogen evolution rates (1.22 mmol.h⁻¹.g⁻¹) compared to the commercially available TiO₂ photocatalysts which are not active for hydrogen generation in the absence of a co-catalyst. Significant photocatalytic reforming of ethanol is achieved over the synthesized bare TiO₂ with the formation of acetaldehyde as the main by-product in the gas phase. This unexpected photocatalytic performance is mainly attributed to the shift of flat band potential towards more negative potentials as revealed from the characterization results in addition to the high density of charge carriers exhibiting longer lifetime shown by laser transient reflectance measurements. The latter showed the presence of a high number of trapped states, which are beneficial for the photocatalytic properties.

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