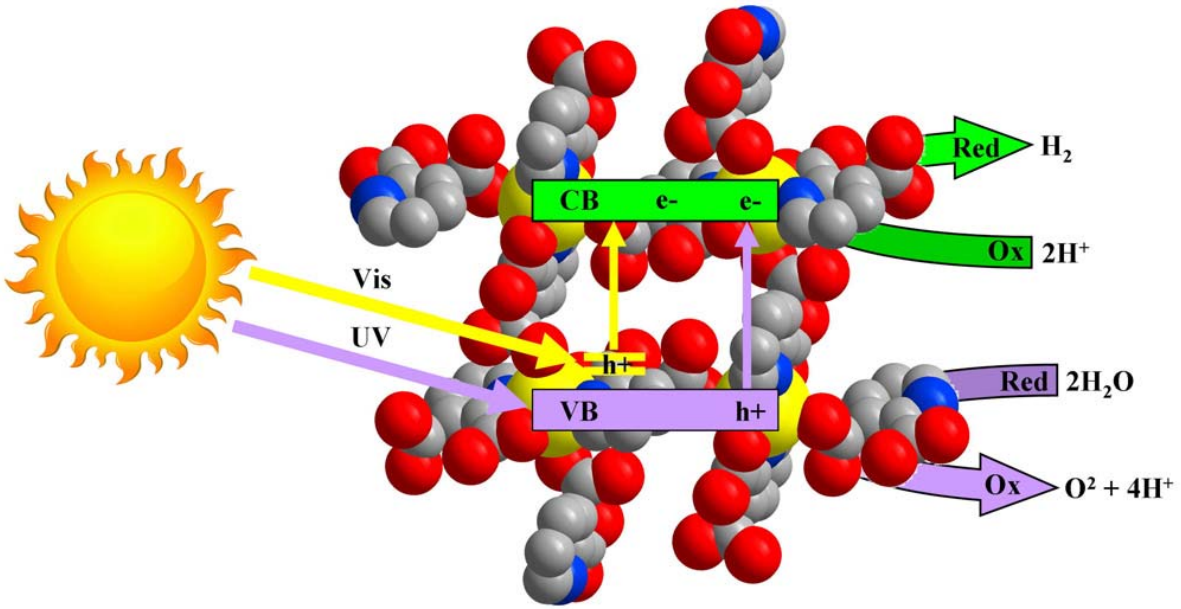
Project Details

Preliminary Registration Code	PD-2016-1708
Final Registration Code	PN-III-P1-1.1-PD-2016-1564
Project Title (Romanian)	Materiale fotocatalitice pentru scindarea apei: de la design la obținerea de hidrogen utilizând lumina solară
Project Title (English)	Next Level Photocatalytic Materials for Water Splitting: From the Drawing Board to Hydrogen Generation Using Solar Light
Project Acronym	PhotoCatSplit
Contracting Authority	UEFISCDI
Project Host Institution	University of Bucharest
Project Duration / Run Period	24 Months / 10.10.2018 - 09.10.2020
Total Funding	250.000,00 lei

Project Summary

In a world with ever-increasing energy demands, low-cost and clean alternatives of producing fuels are imperiously required. The use of sunlight as a source of free and virtually inexhaustible energy and of water as abundant and attractive raw material indicate that photocatalytic systems sensitive to solar light are a good candidate for hydrogen generation through photocalytic water splitting. However, despite recent progress, transition metal complexes have not yet achieved efficient photocatalytic water splitting, as they rely on sacrificial chemical oxidants or a potential bias. Moreover, turnover numbers and frequencies are not large enough, overpotentials are high, and best catalysts known today do not use earth-abundant elements, but rely on noble metals, therefore being costly and not sustainable.

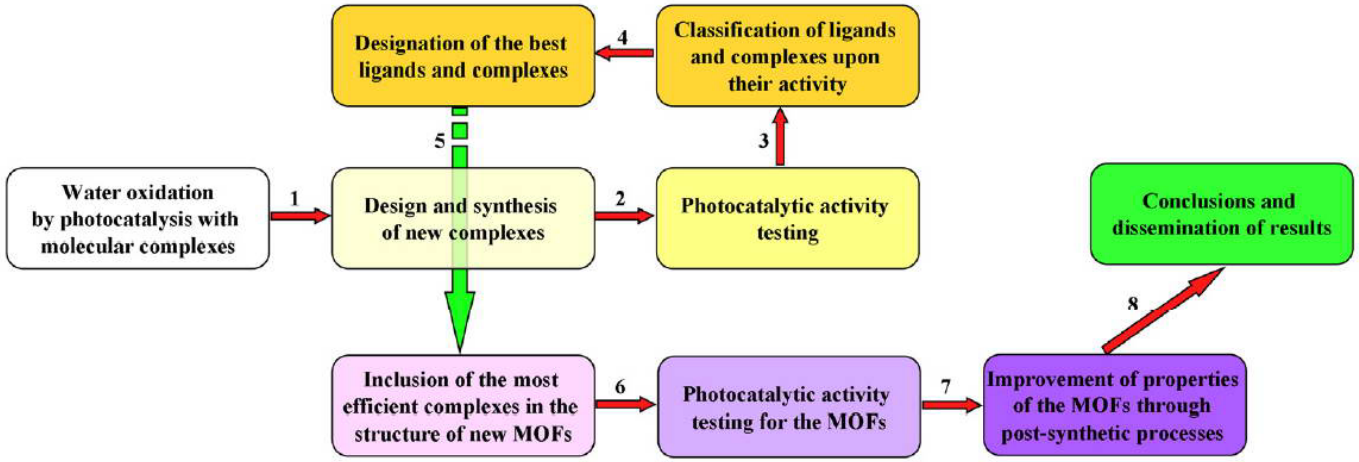


Scheme 1. The principle of action of a photocatalyst for water oxidation

Project Summary

The first part of the project focuses on the synthesis of new complexes containing 3d or 4d metal ions and Schiff-base, polypyridyl derivatives or diketones as ligands, followed by the study of their efficiency in photocatalytic water splitting. The comparison between complexes with $\{M_4O_4\}$ heterocubane core and the $\{Mn_4Ca\}$ oxygen-evolving complex from Photosystem II will help improving the design and photocalytic behaviour of the new materials. Following feed-back from photocatalytic activity testing, the most efficient complexes will be selected.

In the second part of the project, using the novel catalysts as nodes or spacers, new metal-organic frameworks (MOFs) will be obtained and their photocatalytic properties will be determined. MOFs will bring increased catalyst stability and recyclability and will allow a precise tuning of the excitation windows, thus making the new materials better candidates for flow production of hydrogen. The output of this project is represented by new efficient visible-light photocatalysts, which will be the subject of publications in the most relevant high impact factor journals.



Scheme 2. The flowchart of the project

The Implementation Degree of the Project

Phase I / 2018 (10.10.2018 - 31.12.2018): Synthesis of complexes to be used as starting materials

Activity 1.1. Synthesis and characterization of ligands and of complexes to be used as *building-blocks*

New complexes will be synthesized starting from metal ions of earth-abundant elements (Fe^{II}/Fe^{III}, Co^{II}/Co^{III}, Ni^{II}, Cu^{II}, Zn^{II}) or those of heavier elements shown to lead to highly active catalysts (Ru^{III}, various 3d-4f ion pairs). Polypyridyl ligands, macrocyclic ligands, and new Schiff-base ligands will be used in the process.

Deliverables

Phase report

The Implementation Degree of the Project

Phase II / 2019 (01.01.2019 - 31.12.2019): Synthesis of complexes to be used as starting materials, testing of their photocatalytical properties and their assembly into metal-organic frameworks

Activity 2.1. Synthesis and spectral characterization of the *building-blocks*
Activity 2.2. Structural characterization of the *building-blocks* and evaluation of their photocatalytical properties
Activity 2.3. Synthesis of metal-organic frameworks
Activity 2.4. Characterization of the synthesized metal-organic frameworks

Deliverables
Phase report
Scientific papers and communications

The Implementation Degree of the Project

Phase III / 2020 (01.01.2019 - 09.10.2020): Synthesis of complexes to be used as starting materials, testing of their photocatalytical properties and their assembly into metal-organic frameworks

Activity 3.1. Testing of photocatalytical properties (part two)
Activity 3.2. Synthesis and characterization of metal-organic frameworks (part two)
Activity 3.3. Testing of the photocatalytical properties and optimization of the properties

Deliverables
Phase report
Scientific papers and communications