



**Chemistry and Molecular
Sciences and Technologies
(CMST)**

Participating countries

A, BE, CY, CH, CZ, DE, DK, ES, FI,
FR, GR, IL, IRL, IT, NL, PL, PT, RO,
SE, TR, UK

Contact details

Chair of the Action

Benjamin Dietzek,
Professor,
Institute of Photonic Technology,
Germany
Benjamin.dietzek@ipht-jena.de

Science Officer

Dr Lucia Forzi
Science Officer Chemistry and
Molecular Sciences and Technology
COST Office
lucia.forzi@cost.eu

Website

www.perspect-h2o.eu

COST Action CM1202

PERSPECT-H2O

Supramolecular photocatalytic water splitting

2012 | 2016

Objectives

- Develop a fundamental understanding of the function determining light-induced elementary reactions in supramolecular photocatalytic water-splitting and develop novel spectroscopy- and theory-guided water-splitting supramolecular photocatalysts through understanding the underlying molecular interactions and energy decay mechanisms.
- Develop innovative functional systems operating in solutions, membranes or at surfaces, as well as in formulation of general design principles.

Main Achievements

- Successful scientific kick-off meeting (February 2013, Prague).
- First two STSMs have been granted.
- First joint papers have been published.
- Registration for WG1 and WG2 meeting (October 2013, Grenoble) has been opened.
- Website has been launched.
- CM1202 welcomed four new member states since kick-off meeting.
- *European Symposium on Current Challenges in Supramolecular Artificial Photosynthesis* is currently under preparation (March 2014, Jena).



Kick-Off meeting of CM1202, 22nd
November 2012, Brussels



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Working Group activities

Working Group 1

- Synthesis and characterization of lead structures of SPCs for water oxidation (based on Co, Ru, Ir units) and reduction (based on Pt, Pd and Rh polypyridine units), incorporation of earth abundant metals, e.g., Mn, Fe, Co, Ni and organic dyes
- Design of intramolecular electron relays and testing the catalytic activity of the integrated SPCs
- Synthesis of SPCs optimized for spectrally broad absorption, efficient energy and electron transfer, self-healing capacity and long-term stability.

Working Group 2

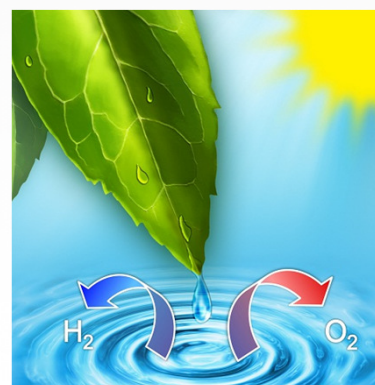
- Interfacing of hydrogen- (oxygen-) evolving SPCs with conductive oxides and other p- or n-semiconductors, and their photocatalytic characterization
- Photophysical studies of interfacial and intramolecular electron-transfer processes within the photoactive electrodes
- Development of theoretical tools to describe electronic states induced upon binding and their correlation with photoinduced electron transfer and catalytic properties
- Assembly of proof-of-concept functional photocatalytic cells

Working Group 3

- Joint experimental/theoretical investigations of ultrafast electronic and structural changes of SPCs and their photoactive building blocks upon photoexcitation, development of realistic computational tools, including solvation and supramolecular interactions

Working Group 4

- Spectroelectrochemical identification of intermediates and catalytically active species, spectroscopic characterization of long-lived intermediates (μs to min) within the catalytic cycle of SPCs
- Application of ab initio and TD-DFT methods to describe long-lived intermediates and supramolecular systems



Courtesy of E.S. Andreiadis/CEA:



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