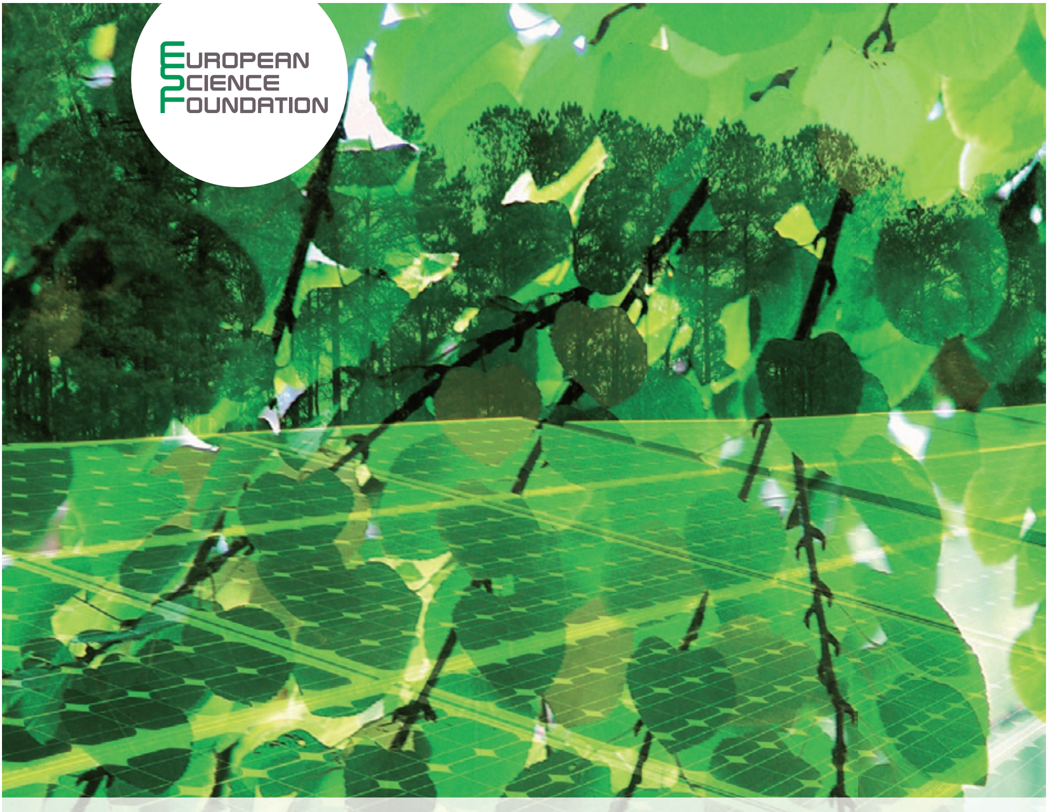
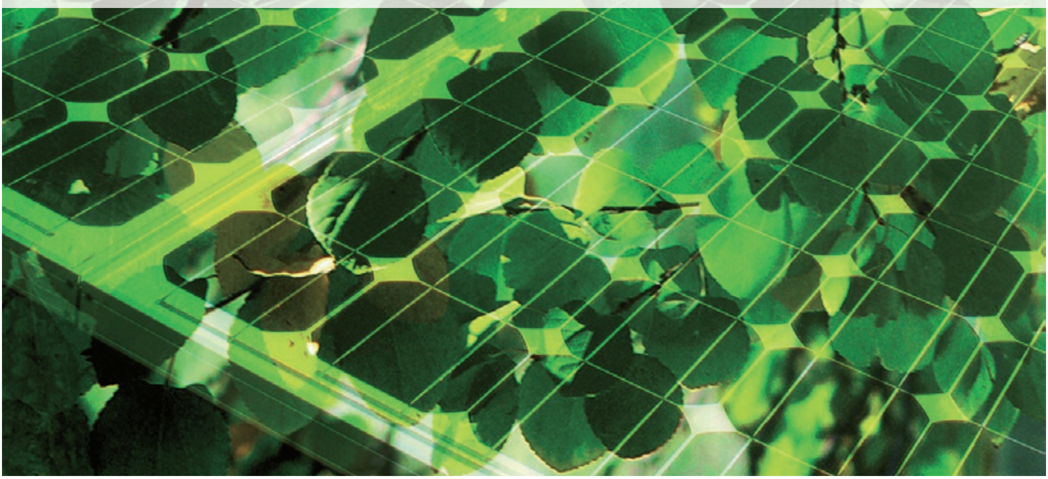


EUROPEAN SCIENCE FOUNDATION

EUROCORES Programme

EuroSolarFuels

Molecular Science for a Conceptual Transition from Fossil to Solar Fuels



Europe (and most of its individual countries) depends heavily on outside energy resources. These are dwindling and their supply can easily be jeopardised. Many dominating energy carriers are connected to environmental and social factors that clearly affect quality of life. In particular this concerns fossil fuels, with severe availability constraints, pollution problems and fast growing CO_2 emissions. Many citizens worry about large, future nuclear-power programmes. Therefore, a strong need is felt for substantial development of and investment in solar energy research. The term ‘solar fuels’ has become increasingly well established since the beginning of the new millennium. This introduction of the concept of solar fuels is spurred by worries about global warming and a decreased availability of oil and gas. The promising potential of solar fuels as important future energy carriers makes this a central theme that must quickly move up the global research agenda. The EuroSolarFuels programme intends to accelerate research on solar fuels on a pan-European scale.

The aim of EuroSolarFuels is to develop molecular science to produce a CO_2-lean solar fuel to meet the grand challenge of phasing out fossil fuels. A key concept in the research is solar energy conversion. All parts of the programme aim for direct conversion of solar energy to chemical energy in the form of a fuel. The solar fuel will be formed from water as electron source, using visible light in direct processes involving (i) photobiological solar fuel production in green algae and/or cyanobacteria that excrete the fuel; (ii) artificial photosynthesis in molecular systems and (iii) solar fuel production in nanostructured and semiconductor-based systems. To meet these goals, EuroSolarFuels has the ambition to develop solar fuels research into a powerful European field in a shorter time than would be possible with only individual or national initiatives. The programme is inclusive and brings together scientists active in relevant fields in Europe.

Collaborative Research Projects (CRPs)

Bio-inspired oxygen-evolving light-driven catalysts (BOLDCATS)

(BBSRC, MNiSW, NWO)

The major challenge in the area of renewable energy is to devise sustainable ways of making fuels, preferably dense portable fuels that can be used for applications such as aviation. There is one major biochemical/chemical process on Earth that can use solar energy to make fuels and this is photosynthesis. The problem, however, of using photosynthesis directly to make fuels (biofuels) is the rather low efficiency of conversion of solar energy into fuel. However, if it were possible to 'tap into' photosynthesis at the level of the primary reactions then, in principle, higher energy conversion efficiencies may be achievable. This is the idea behind the drive for artificial photosynthesis. Photosynthesis can be broken down into four partial reactions. Worldwide there has been a lot of work designed to understand the molecular details of these key four steps in photosynthesis. There has been excellent progress in understanding the science of photosynthesis; indeed there are now many artificial reaction centre and antenna mimics that function rather well. The major barriers to building systems capable of using solar energy to make fuels are our current inability to produce robust catalysts that can split water and use the reductant produced to synthesise a fuel. The main aims of this CRP are to work towards the production of novel devices that can overcome these barriers.

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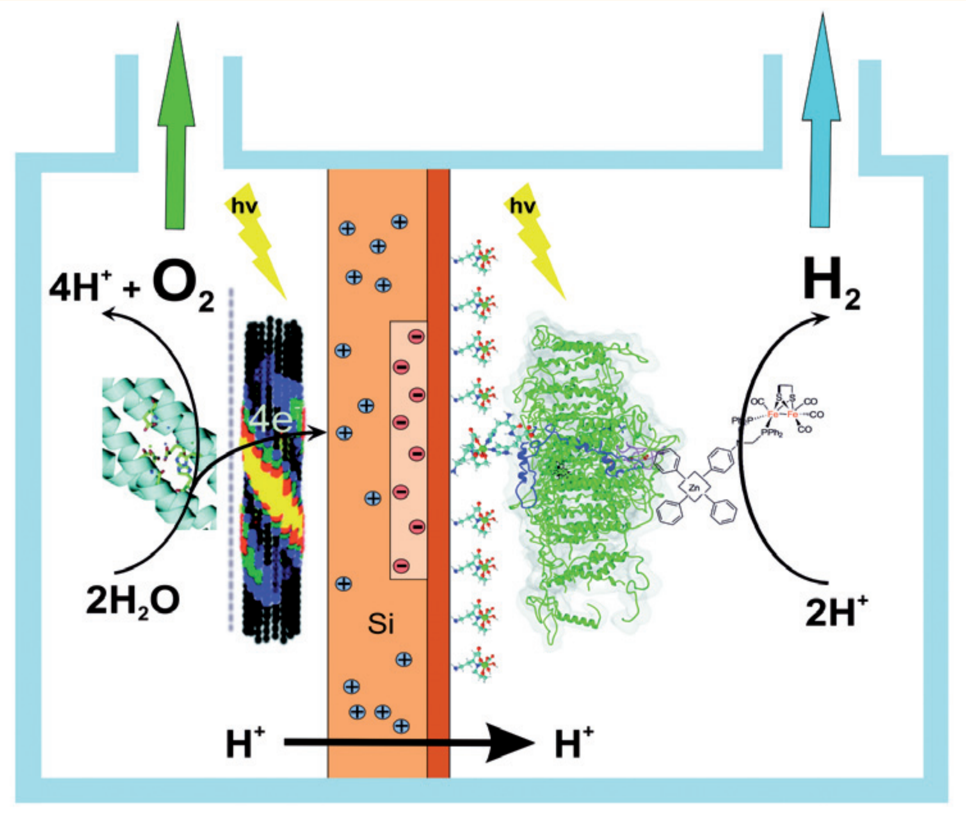
Modular design of a bio-inspired tandem cell for direct solar-to-fuel conversion (Solarfueltandem)

(BBSRC, CNR, MNiSW, MPI-Mülheim, NWO, TÜBITAK)

The principal objective of this CRP is the modular design of a bio-inspired nanostructured organic–inorganic heterojunction tandem cell for solar-to-fuel conversion. The vision is to work from a combination of natural and artificial modules for catalysis and charge separation and explore a range of different combinations for functional tandem device concepts. This allows us to work in parallel on modular systems integration and optimisation of components.
Self-assembled Zn chlorin nanocylinders forming excitations with internal charge transfer character will be aligned in an alumina solid membrane to form a supramolecular sensitiser for ultrafast charge separation and charge injection into a low-band-gap semiconductor. In this heterojunction system, two regions of the solar spectrum can be used in tandem to overcome the thermodynamic barrier for water oxidation and hydrogen production with visible light in a single device. Two complementary synthetic strategies will ensure access to a wide library of Zn chlorins.
Post-functionalisation of chlorophyll *a* and bacteriochlorophyll *c* will ensure rapid preparation of compounds for self-assembly and photophysical studies, including the use of ^{13}C labels. Total synthesis will give full control over the pattern of substituents for fine-tuning of all required physicochemical properties. We will use the most sturdy natural PS2 and Pt/



cobaloxime-modified PS1 complexes from *Cyanidioschyzon merolae* with a very high photosynthesis rate as working photocatalysts for optimisation of catalyst interfacing to semiconductors. In a parallel supramolecular approach, we will prepare homogenous Ru/Ir/Co water oxidation and Fe/Ni/Co hydrogen formation catalysts for immobilisation and interfacing to natural and artificial electron transfer units. Optical spectroscopy, NMR, EPR, electrochemistry, X-ray crystallography and modelling will be used to assess the kinetics of the multi-electron catalysis and dual band-gap electron transfer mechanisms to guide the design.
The final aim of the CPR is to give a proof of concept of a functional tandem device, as indicated schematically in the figure.

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  Netherlands Organisation for Scientific Research, The Netherlands
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  The Scientific and Technological Research Council of Turkey, Turkey
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