



An Artificial Leaf: a photo-electro-catalytic cell from earth-abundant materials for sustainable solar production of CO₂-based chemicals and fuels

Deliverable D6.3

Publishable Summary Periodic Report 1

Lead Beneficiary	ICIQ
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1. PUBLISHABLE SUMMARY

Summary of the context and overall objectives of the project (For the final period, include the conclusions of the action)

Mimicking the photosynthetic function of green plants and algae is one of the major technological challenges scientists around the world are facing nowadays. Natural photosynthesis transforms water (H₂O) and carbon dioxide (CO₂) into oxygen and carbohydrates using exclusively the energy of the sun. An artificial photosynthesis scheme will work in an analogous way, absorbing sunlight to combine water and CO₂ into oxygen and chemicals, including fuels.

Fuels and fine chemicals are essentially produced from fossil reservoirs, whose retrieval and use have a deleterious impact on the environment. The combustion of fossil fuels (coal, oil and gas) is causing emissions of large amounts of “greenhouse gases” (GHGs) to the atmosphere, provoking global warming and affecting climate change.

A-LEAF European consortium seeks the realization of an artificial photosynthesis platform: for the capture and transformation of solar energy into chemical energy, as sustainable substitute for fossil resources.

Our multidisciplinary effort starts from atomic-scale studies to determine experimentally and theoretically the main parameters for optimization of the chemical transformations at surfaces to combine water and CO₂ into oxygen and energy-rich chemicals. This knowledge will be transferred and up-scaled into (photo)electrochemical set-ups to maximize performance. The champion components will be combined into a single photoelectrocatalytic(PEC) device: an artificial leaf. Our final aim is to validate our strategy and approach with respect to technological and industrial parameters, to assess the comparative advantages and disadvantages for the incorporation of A-LEAF into an economically viable, and environmentally sustainable energy cycle.

Work performed from the beginning of the project to the end of the period covered by the report and main results achieved so far (For the final period please include an overview of the results and their exploitation and dissemination)

During the first year, we have divided our work in four different work packages (WP), to tackle the basic requirements, understanding and optimization strategies for the future parts of our A-LEAF prototype.

WP1 investigated into the surface states of materials, including function and stability, via the study of model systems for the electrocatalytic production of oxygen from water, and fuels from CO₂ reduction.

WP2 optimized the electrocatalytic materials, electrodes and working conditions, to maximize performance.

WP3 gave computational support to identify the key parameters limiting charge transfer, electrochemical activity and conversion rates, to enhance prototype specifications.

WP4 dealt with the development of multijunction Si light absorbers, to match the working requirements from the electrochemical parts, to be combined into our A-LEAF integrated system.

Progress beyond the state of the art, expected results until the end of the project and potential impacts (including the socio-economic impact and the wider societal implications of the project so far)

Most of our technical results are still confidential, and subject to our assessment of their proper intellectual property position. At this time, we can publicly highlight the following achievements:

- We have confirmed the excellent surface stability of iron oxide surfaces under water and water oxidation conditions with spatially resolved microscopy and complementary techniques.
- We have identified the beneficial incorporation of Zn into water oxidation Fe-based oxides, by reducing overpotentials and increasing the density of active sites. This has been backed up by computational models, which have been able to identify the effect of these dopings.
- We have discovered the S-doping of Cu-based surfaces for the selective reduction of carbon dioxide to formic acid, identifying the optimum working conditions.
- We have developed new tools aiming to bridge surface science and electrocatalytic studies, which have already revealed the nature of the active phase in the highly efficient In-Cu catalyst for CO production.
- We have confirmed the need for a buffer layer between a light absorber multijunction and a catalyst to maximize charge extractions, and avoid energy losses.

In general, we have achieved all this progress exclusively studying abundant and non-critical materials: carbon, silicon, copper, iron, zinc or nickel. Also exclusively employing scalable and industrially-accepted processing methods. Our final objective is to validate our solar to fuels scheme as a viable and alternative energy vector, beyond the scientific and engineering challenge.

Address (URL) of the project's public website

<http://www.a-leaf.eu>

A-LEAF

