



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

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Publishable Summary Periodic Report 2

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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 30 months, we have divided our work in five scientific work packages (WP), to understand and identify the basic requirements, optimization strategies, and preferred assembly architecture for our A-LEAF prototype.

WP1 investigated into the surface states of electrocatalysts and their supports via the study of model systems with atomic resolution. The function, stability and doping effects on these materials were determined in situ after electrocatalytic CO₂ reduction or water oxidation.

WP2 optimized the electrocatalysts, electrode supports and working conditions to drive the two chemical reactions, water oxidation and CO₂ reduction. Faradaic efficiency, minimum overpotential and appropriate current densities matching the photovoltaic parts were common parameters for both reactions. On CO₂ reduction, parameters effecting the selectivity towards the different products were also identified.

WP3 gave computational support to define the key parameters limiting charge transfer, electrochemical activity and conversion rates on model and real electrocatalysts. This knowledge

allowed improving performance based on basic

WP4 investigated the development of multijunction Si light absorbers to match the working requirements from the electrochemical parts, and the optimum interface to minimize energy losses between light absorption and electrochemical performance in our A-LEAF integrated system.

WP5 was in charge of prototype design. A model electrochemical-only prototype was built to test the electrochemical parts developed through WP1-3 in flow/working conditions, as a platform to understand and optimize their performance. This prototype also allowed to investigate the influence of CO₂-gas feed to the selectivity and efficiency of the electroreduction.

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 geometrical currents achieved in Fe-decorated Ni foam electrodes, reaching $> 1 \text{ A/cm}^2$ in liquid electrolyte at overpotentials below 350 mV.
- We have developed a novel understanding tool allowing optimization of multicomponent catalysts by applying microfabrication, i.e., the set of techniques used in the fabrication of microchips.
- We have developed electrocatalysts reaching $> 75 \%$ selectivity for CO₂ to CO electroreduction, with low cell voltage in the range of 5-20 mA/cm² current densities, and excellent stability.
- We have produced all target catalysts in a practical form and prepared technical electrodes suitable for an electrolyzer configuration.
- We have confirmed the benefit of CO₂ gas feed for the selectivity and efficiency of the carbon reduction reaction in the electrolyzer configuration.

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: thermal treatment at low pressure, adsorption processes, water-based washing and filtering, and non-toxic solvents. 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



FUELS &
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