

M2/Engineering Internship: Detailed modelling of a hybrid PEC/PV system for the production of solar fuels

General information:

Location: PROMES-CNRS – 7 rue du Four Solaire, 66120 Font-Romeu-Odeillo-Via, France.

Supervision: Jean-François Cornet, Jérémie Dauchet, Thomas Vourc'h (Institut Pascal, Clermont-Ferrand), Alexis Vossier, Maxime Giteau (PROMES, Odeillo), Rodolphe Vaillon (LAAS, Toulouse)

Salary: ~€630/month.

Start date and duration: Flexible (between February/March and September 2026, up to 6 months).

Keywords: Solar fuels, photoelectrochemical systems, detailed balance calculations, theoretical limits

Scientific context:

The production of hydrogen and solar fuels by photoelectrochemical means (Photo-Electrochemical Cell, PEC) is one of the most promising approaches for storing solar energy in the form of clean, carbon-free chemical molecules[1].

These devices are based on photoelectrochemical cells capable, under solar illumination, of splitting water into hydrogen and oxygen through oxidation and reduction reactions occurring on a semiconductor photoanode and a metal cathode. This approach is known as "artificial photosynthesis". One of the major challenges of this technology is the high value of the redox potential difference for water dissociation (1.23 eV), which limits the choice of photoactive materials with a wide bandgap, which are often inefficient at absorbing the solar spectrum. To overcome this constraint, one strategy is to spectrally separate (on the same capture surface) the solar flux, with the UV-Visible portion feeding a PEC and the infrared portion feeding a photovoltaic (PV) cell, which provides the additional overvoltage required for photochemical reactions. However, this elegant solution first requires a detailed understanding of the physical phenomena at work in each of the subsystems (PEC and PV), and then in a hybrid system coupling the two. These phenomena are radiation transfer, the photogeneration of electron-hole pairs, their migration by drift-diffusion-reaction, their transfer to interfaces and, in the case of PEC, their participation in artificial photosynthesis reactions.

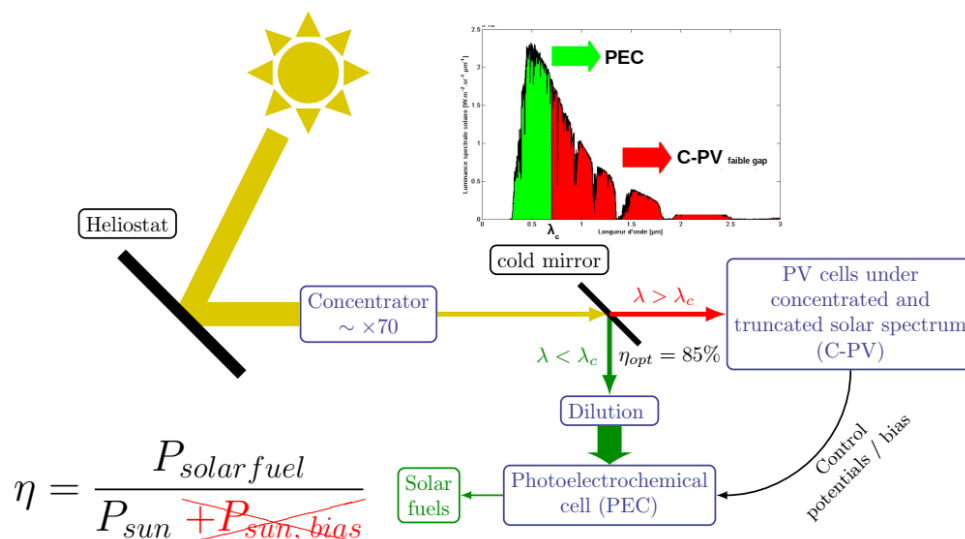


Figure 1 – Schematic diagram of a hybrid photovoltaic/photoelectrochemical system for the production of solar fuels



Objectives of the internship

Despite its potential, this hybrid approach remains understudied and raises several fundamental questions:

- What efficiency gains can be expected from PEC/PV hybridisation?
- Which material combinations offer the best performance?
- How do real non-idealities (recombination, resistive losses, heating) influence achievable yields?

In order to answer these questions, the internship will aim to develop a physical model based on the detailed balance formalism, which is also widely used for modelling conventional photovoltaic cells[2]. This formalism will enable the maximum solar-to-hydrogen conversion performance to be calculated using a radiative and energy exchange model incorporating a limited number of physical parameters.

The main stages of the work will be:

1. **Ideal modelling:**

1-a- In the first phase, based on the literature, we will seek to gain an in-depth understanding of the concept of detailed balance as applied to PV cells[3]. The principle of detailed balance makes it possible to link the overall behaviour of a thermodynamic system to the reversibilities of the properties describing the interactions within it, at the molecular level (in this case, the light/matter interactions leading to the generation of charges), and the interaction of these charges in electrostatic and electrochemical potential fields.

1-b- The in-depth understanding that will result from this first stage should then enable the method to be transposed, applied for the first time to a photoelectrochemical cell (the area of expertise of the supervisors at the Pascal Institute). This work will enable an assessment of the theoretical maximum performance of the hybrid system as a function of the bandwidths of the PEC and PV cells and the illumination conditions.

- #### 2. **Taking non-idealities into account:** the aim here will be to bring the model closer to the actual behaviour of PEC and PV cells observed experimentally by integrating real losses (resistive, non-radiative, thermal) in order to estimate the yields achievable under realistic conditions (based on a demonstrator currently being developed at the Pascal Institute).
- #### 3. **Sensitivity analysis and optimisation:** if time permits, the final model will be used to identify the critical parameters and most promising configurations for maximising the overall efficiency of the hybrid system.

Environment:

The internship will take place at the PROMES-CNRS laboratory in Odeillo (Font-Romeu), in the French Pyrenees, at high altitude (1,600 m), combining a unique mountain setting with world-class solar research infrastructure. PROMES is home to one of the largest solar facilities in the world, including a 1 MW solar furnace and a 6 kW solar concentrator for laboratory-scale experiments. Expect clear skies, abundant sunshine and immediate access to outdoor activities (hiking, skiing, climbing), while conducting cutting-edge research on high-temperature energy.

This internship is part of a close collaboration with academic partners at the Institut Pascal in Clermont-Ferrand (Jérémi Dauchet, Thomas Vourc'h, Jean-François Cornet) and LAAS-CNRS in Toulouse (Rodolphe Vaillon). It will involve regular scientific exchanges, follow-up meetings and active participation in inter-laboratory discussions, offering the intern a hands-on immersion in a collaborative research network.



Required profile

Master's level student (thermodynamics, statistical physics) or engineering school student, with:

- a solid background in physics, energy or thermodynamics, with an interest in modelling,
- a keen interest in renewable energies and photovoltaic conversion,
- good coding skills (Matlab/Python).

This internship is for a candidate who is motivated by research and wishes to contribute to the development of new high-efficiency solar conversion technologies at the interface between photochemistry, photonics and thermodynamics.

How to apply:

Send a CV and a cover letter explaining your interest in this internship to:

- **Alexis Vossier:** alexis.vossier@promes.cnrs.fr
- **Jérémi Dauchet:** jeremi.dauchet@sigma-clermont.fr

References:

- [1] T. Bak, J. Nowotny, M. Rekas, and C. C. Sorrell, "Photo-electrochemical hydrogen generation from water using solar energy. Materials-related aspects," *International Journal of Hydrogen Energy*, vol. 27, ^{no.} 10, pp. 991-doi:
- [2] W. Shockley and H. J. Queisser, « Balance Limit of Efficiency of p-n Junction Solar Cells », *Appl. Phys.*, vol. 32, ^{no.} 3, pp. 510-doi: 10.1063/1.1736034.
- [3] A. Vossier, F. Gualdi, A. Dollet, R. Ares, and V. Aimez, "Approaching the Shockley-Queisser limit: General assessment of the main limiting mechanisms in photovoltaic cells », *J. Appl. Phys.*, vol. 117, ^{no.} 1, p. 015102, Jan. 2015, doi: 10.1063/1.4905277.