PH2OTOGEN

D8.5 – ADVISORY BOARD REPORT (INTERMEDIATE)

WP8 – Task 8.2

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Table of contents

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List of figures

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Summary

This report explains the feedback received during the intermediate Advisory Board meeting held in Month 16 (out of 42) of the PH2OTOGEN project, which aims to produce photocatalytic sheets capable of simultaneous hydrogen production and glycerol oxidation to 1,3-dihydroxyacetone. During the meeting, each of the work packages were presented with Q&A / discussion sessions held after each one. The scientific results presented covered 4 main topics: i. benchmarking of hydrogen evolving particles (HEP) (WP1); ii. benchmarking of oxidising particles (OP) (WP2); iii. preparation of transparent, conductive, porous photocatalyst supports (WP4); iv. System integration through reactor design and modelling (WP5). Furthermore, the plans for integrating the HEP and OP into a tandem system (WP3) later in the project were explained.

Keywords

Photoelectrochemistry, solar to hydrogen, hydrogen evolution reaction, glycerol oxidation reaction, advisory board

Abbreviations and acronyms

Acronym	Description
CAPEX	Capital Expenditure
FTO	Fluorine-doped tin oxide
HEP	Hydrogen Evolving Particle
LCA	Life Cycle Assessment
OP	Oxidizing Particle
TEA	Technoeconomic Analysis
TPCS	Transparent, porous, conductive support
WP	Work Package

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1 Introduction

The PH2OTOGEN project aims to develop photocatalytic sheets capable of producing green hydrogen and 1,3-dihydroxyacetone through the oxidation of glycerol. In the first phase of the project, we have focussed on the benchmarking semiconductors, co-catalysts and charge transport layers for the hydrogen evolving particles (HEP) and oxidising particles (OP) that will carry out the two reactions. These particles have been tested separately in half-cell configurations. However, they will need to be electronically connected in the final device via a transparent, porous, conductive support (TPCS), which is also developed within the scope of the project.

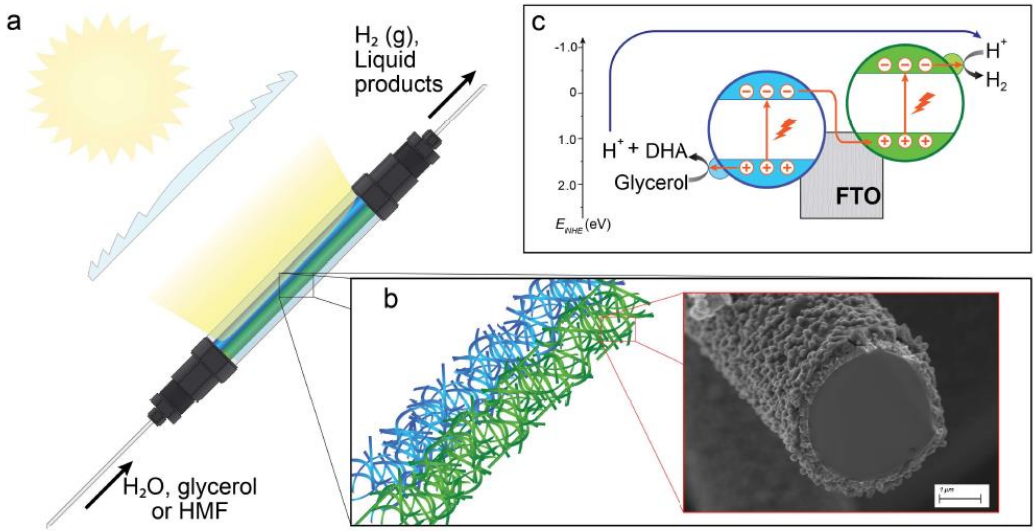

Figure 1: PH2OTOGEN concept: hydrogen evolving particles and oxidising particles deposited on either side of a transparent, conductive support

The primary motivation for organizing the Advisory Board meeting at the intermediate point of the project (16 months after the kick-off of this 42-month initiative) was to ensure that the project's progress and direction are critically evaluated by experts external to the consortium. The selected Advisory Board members are renowned professionals in the field, including university professors whose work closely aligns with the objectives and thematic areas of the project. Their external perspective is essential to validate our progress, provide constructive feedback, and ensure the project remains aligned with scientific, technological, and societal expectations. By presenting the status of each work package and engaging in open discussions, we aimed to benefit from their experience to identify potential risks early, refine our methodologies, and enhance the overall impact and relevance of the project. This kind of structured mid-term evaluation not only adds value in terms of scientific rigor but also reinforces transparency and accountability within the project's management framework.

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2 Composition of the Advisory Board

The Advisory Board was chosen based on recommendations by consortium partners.

2.1 Prof. Francesca Toma (Helmholtz-Zentrum Hereon, Germany)

Prof. Francesca Toma is the Director of the Institute of Functional Materials for Sustainability at Helmholtz Zentrum Hereon with over 120 co-authored publications. Her research is focussed on the synthesis and characterization of sustainable materials for renewable energy applications, especially related to (photo)electrocatalysis. She has extensive research experience on the development of high efficiency photoelectrocatalytic materials and the building of small-scale devices. In particular, her research has included $BiVO_4$ and transition metal dichalcogenides relevant to PH2OTOGEN. Previously, she was as a Staff Scientist at Lawrence Berkeley National Lab, where she served as the Program lead of the Liquid Sunlight Alliance and as the Photoelectrochemistry Technology Lead for HydroGEN.

2.2 Prof. Simelys Hernández (POLITO, Italy)

Simelys Hernández is an Associated Professor at Politecnico di Torino (Polito, Turin, Italy). She is part of CREST (Catalytic Reaction Engineering for Sustainable Technologies) group and is co-author of more than 100 publications. Her work includes the development and scale-up of electrocatalysts, $BiVO_4$-based photoelectrodes and optimization of (photo)-electrochemical devices. She has been involved in several European projects related to photoelectrocatalytic processes, including acting as the technical coordinator of the EU H2020 project SunCoChem and on the scientific team of ArtipHyction, which developed a medium-scale (1 m^2) photoelectrochemical demonstrator for solar water splitting.

2.3 Prof. Hannes Jonsson (University of Iceland, Iceland)

Hannes Jónsson is a renowned theoretical chemist and professor at the University of Iceland, since 2000. He also holds visiting and adjunct roles at institutions such as the Technical University of Denmark, Brown University, Aalto University in Finland, and Stanford University. He is especially known for developing computational methods to model chemical and material processes at the atomic level. His research combines quantum mechanics, particularly density functional theory, with advanced algorithms to study phenomena such as chemical reactions and electrocatalysis—including H_2 production. In recent years, he has also integrated machine learning into these models to improve prediction and efficiency, through national and EU-funded projects.

2.4 Prof. Maria Antonietta Loi (Rijksuniversiteit Groningen, the Netherlands)

Maria Antonietta Loi became assistant professor and Rosalind Franklin Fellow at the Zernike Institute for Advanced Materials of the University of Groningen, The Netherlands in 2006. She is now full professor in the same institution and chair of the Photophysics and OptoElectronics group. She is co-author of more than 300 peer reviewed articles in the photo-physics and optoelectronics of nanomaterials including work on organic semiconductors, as developed in PH2OTOGEN. In 2018 she received the Physicaprijs from the Dutch physics association for

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her outstanding work on organic-inorganic hybrid materials. In 2020 she became fellow of the American Physical Society.

2.5 Dr. Laurent Baraton (ENGIE, France)

Dr. Laurent Baraton is a Senior Research Engineer & Project Manager at ENGIE Lab CRIGEN, working on the assessment and promotion of emerging technologies related to the hydrogen value chain. In particular, he develops technologies to enhance existing industrial process efficiency and the development of new commercial activities in the fields of photoelectrocatalysis and nanomaterials through in-house development. He has also been involved in EU-funded projects, such as CONDOR and Sun-To-X with contributions particularly in scale-up, plant design and device building.

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3 Feedback from the Advisory Board

The discussions following each work package presentation are summarised in the sections below. The comments and questions from the Advisory Board are indicated in italics and the answers from the PH2OTOGEN consortium are given in standard font. Based on the discussions, a series of recommendations to the consortium is presented at the end of each work package summary.

3.1 WP1: Hydrogen Evolving Particle

3.1.1 Semiconductor

FT: *Did you tune the organic semiconductors with the redox potential?* We have a huge bank of organic semiconductors that can be used as donor: acceptor pairs. From the thousands of possible combinations, these were narrowed down to hundreds based on the redox potential.

FT: *What is the stability of the organic semiconductor?* So far we have shown good stabilities but on the order of 15 – 30 minutes. We have cracks in the electron transport layers that allow electrolyte to enter into the organic semiconductor causing degradation. We are now working on ways to prevent / seal these cracks through capping layers.

LB: *Did you try any size selection of WSe2?* We can select the size partially through centrifugation processes. However, this is time-consuming and only gave an incremental improvement in performance. We believe that the exfoliation process should be optimised to allow larger flakes from this point.

LB: *Oxygen can react on the surfaces during the exfoliation processes. Have you tried degassing the solvent during the exfoliation procedure?* No, we haven't tried this but it could be easily implemented.

3.1.2 Co-catalyst

FT: Can the molybdenum sulfide also act as a light absorber? The molybdenum sulfide nanoflakes have a high transparency due to their thickness of approximately 2 nm.

FT: *What is the stability of the co-catalyst?* We have measured a good stability over several hours.

HJ: *Is the size of the flakes important for the activity of the catalyst, since the active sites may be mainly on the edges?* The nanoflakes are amorphous so quite defective (for example, $MoS_{1.5}O_{0.8}W_{0.004}$) with many active sites.

SH: *How is the MoS_x coated onto the semiconductor, have you tried any thermal treatment which would increase interconnection between the layers and improve charge transport?* So far we have deposited the catalyst by spray-coating without thermal treatment. We have used a thermal treatment for the TiO_2 electron transport layer, where a maximum of 100 - 200 °C is possible to avoid damaging the organic semiconductors. We can try the same process for the co-catalyst.

LB: *Which solvent is used in the MoS_x spray coating process? Is it effectively removed before testing?* The MoS_x is dispersed in ethanol for the spray-coating. The solvent is volatile enough that it can be easily removed.

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3.1.3 Measurements

SH: *So far, you have used bias in your half-cell measurements. In the final device do you plan to apply any external bias? The stability will be affected by the applied potential.* We currently need to measure in the half-cell configuration as an intermediate test, however once we start the tandem testing we will start to operate in a bias-free configuration.

3.1.4 Recommendations

- Investigate effect of applied potential on photocatalyst stability
- Ensure a good interconnection between the co-catalyst and photocatalyst or charge transport layer through a mild thermal annealing process – ensuring that the solvent is removed

3.2 WP2: Oxidising Particle

3.2.1 Semi-conductor and co-catalysts

SH: *Did you perform any mechanistic study and/or simulation about the mechanism of the different byproducts obtained from the glycerol oxidation reaction?* Our focus up to now was a purely thermodynamic study to understand the potentials that would lead to a certain product. However, it would also be interesting to do a more mechanistic study covering activation energies and how the surface structure affects the product selectivity.

SH: *Selectivity is strongly influenced by pH and electrolytes; did you consider other conditions in this regard?* We have tested different electrolytes, but no big difference was encountered in terms of selectivity – we did observe a change in the photocurrent, however. We have seen that increasing the surface ratio of Bi:V (i.e. higher Bi) drives selectivity to DHA.

FT: *Ta in not a common dopant for $BiVO_4$, why did you choose it and did you consider other dopants?* Mo and W are commonly used as dopants because they increase conductivity, however selectivity to DHA is also an important parameter for us. Sayama et al. [1] showed a drastic selectivity increase (up to 96% DHA) by Ta doping, where it seats on the V sites (note this is more a modification of the material than doping as the Ta^{5+} is located in the V^{5+} site – same oxidation state). To understand the mechanism of the enhanced selectivity, we are investigating if it is a lattice distortion or related to polaronic conduction. Fom there we can choose other dopants with similar properties to substitute the V^{5+} e.g. Nb and Sb.

HJ: *XRD may not be the best technique to understand the mechanism of the enhanced selectivity as it analyses the bulk and the catalysis is likely to be a surface effect. Can Ta and Nb dopants migrate to the surface? Are there any surface techniques applied in OH_2PERA (parallel EU project) or in Ph2otogen e.g. to check the oxidation state or surface structure?* In OH_2PERA the focus in more at a device level, so surface was deprioritised. For Ph2otogen, we would like to investigate this further, especially now that the $BiVO_4$ has been shown to be highly promising for glycerol oxidation.

3.2.2 Zero-gap membrane-based reactor

FT: *We have some unpublished work where we concluded that the results with two electrode and three electrode set-ups are quite different. What is the configuration you used, and did you see the same?* Yes, we have observed the same. Particularly, when glycerol is in the system the situation is more difficult as crossover can happen, and it may poison the membrane. The conclusion from our side is than two electrode set-up is crucial to understand the system.

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LB: *Is the difference in performance between the two electrode and three electrode set-ups because of ohmic resistance?* This is one contribution, although it may probably not be the main one. We believe the influence lays in the poisoning of the membrane from the cathode side.

3.2.3 Recommendations

- Investigate effect of the lattice distortion, surface structure and polaronic conduction in doped-$BiVO_4$ to understand how these parameters affect the selectivity
- Continue to explore the two-electrode set-ups as these are closer to 'real-life' operation of the device

3.3 WP3: Tandem

3.3.1 Reactor Design

SH: *Will you target a tube or planar design?* Tubular is more complicated as a structure. Planar concept is more straightforward. This should be determined through experiment and modelling. There would be a better distribution of light if a planar device was used, allowing the efficiency to be more uniform. In the case of concentrated light, a Fresnel lens could be used. Concentrated light is used in the project for both accelerated stress testing (high intensity solar simulator at EPFL) and as a way that the hydrogen evolution rate could be increased.

MAL: *How do you avoid the back reaction if you are not using a membrane?* Since we are not producing hydrogen and oxygen in parallel, a membrane is not needed from a safety perspective (i.e. to avoid explosion risk), however there is a possibility that we oxidise glycerol on the oxidising particle and reduce the oxidation product on the hydrogen evolving particle. Literature suggests that the back-reaction is unlikely, however, we are introducing glycerol oxidation products into our half-cell tests in WP1 to confirm this.

MAL: *What electrolyte will be used in the final reactor?* We will use a mixture of glycerol and water so far we have used 0.5 M glycerol in water and the pH is controlled via buffer solutions. Having a not too high concentration of glycerol is important to avoid that the viscosity becomes too high. We are still investigating which pH is the most favourable but pH 2 seems the most promising so far for compatibility between the HEP and OP.

3.3.2 Achieving target efficiency of tandem device

FT: *Considering the previous work in the field, e.g. the water splitting device developed by Prof. Domen (University of Tokyo) that achieved around 1% solar-to-hydrogen efficiency, what are the differences in your device that will allow you to achieve the equivalent of 5% solar-to-hydrogen efficiency?* One key aspect is the alternative oxidation reaction (oxidation of glycerol) which occurs at a lower onset potential than the oxygen evolution reaction. In the half-cell experiments we have already conducted, it is already evident that both the photocurrent and stability are significantly enhanced for glycerol oxidation compared to water splitting. The lower photovoltage required for the reaction also gives a greater choice of suitable semiconducting materials.

FT: *You may have an opportunity in the reactor design to improve the efficiency through optimising the current collection.* Yes, the TPCS will support efficient current collection but as

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a first step we want to ensure that we have sufficient photocurrent for both the HEP and OP at the maximum operating point (likely to be 0.4 – 0.6 V) – a key checkpoint in the project.

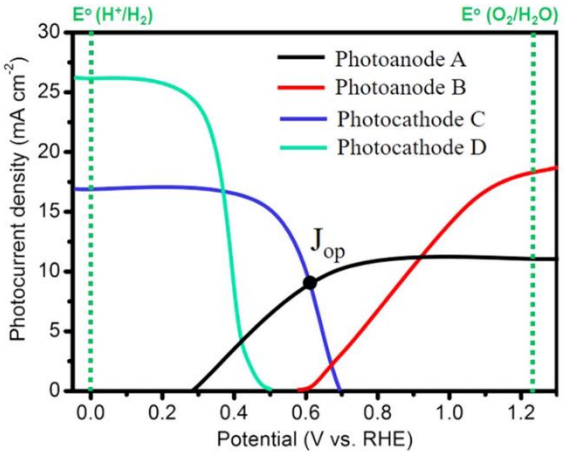

Figure 2: An example of the maximum operating point from the literature [2]

SH: *The position of the curves may be adjusted by the operating conditions not just the material properties.* We can certainly tune the positions with operating conditions but we would like to establish as higher maximum operating photocurrent density with the materials themselves as a strong starting point.

3.3.3 Recommendations

- Once the work package starts, HEP and OP-compatible operating conditions and reactor design should be established as soon as possible to allow sufficient time for optimisation

3.4 WP4: Transparent, Porous, Conductive Support

3.4.1 TPCS

FT: *What is the process involved to moving from circular TPCS to the configuration needed for the reactor?* The TPCS can be cut in any configuration needed after production. For now, two options are considered: two TPCSs (one for the HEP and one for the OP pressed directly together); or three TPCSs (one for the HEP, one uncoated to facilitate electronic conductivity and one for the OP pressed together).

LB: *What are the maximum dimensions of the TPCS that you are aiming at?* Maximum dimensions foreseen are 30 x 30 cm^2, which are sufficient for the 500 cm^2 demonstrator. However, if a larger area is desired in the future, this could be implemented (i.e. with a larger hotplate), as the TPCS manufacturing technique is scalable. The other option is to use TPCS of 30 x 30 cm^2 and connect them together to form a larger structure.

LB: *Is there any plan for commercialisation of the TPCS?* Although we have not planned this yet, it can certainly be considered – noting that Solaronix has experience with commercialisation of other materials developed in the scope of EU-funded projects.

SH: *The performance of TPCS with FTO-coating from Solaronix is enhanced compared to that from EPFL. Is it because of a difference protocol in the process and/or the conditions used?* The process is slightly different as EPFL used a simple atmospheric chemical vapour deposition

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method and Solaronix applies their technology for ultrasonic spray coating which results in a thinner FTO layer. In addition, the temperature used in slightly different. This results in a difference in crystal size, which may lead to the difference in optical, electrical and mechanical properties.

MAL: *The robustness of the TPCS is a big challenge, have you thought about using silver nanowires instead?* It is difficult to make a free-standing structure from only silver nanowires. We have tried in the past to deposit silver nanowires on the transparent porous support as a replacement for FTO but the transmittance is lower due to significant light scattering and the nanowires oxidise easily.

3.4.2 Recommendations

- Identification of differences in process and conditions used to manufacture the TPCS from Solaronix and EPFL to understand key parameters in controlling the characteristics of the TPCS – this may result in opportunities for further improvement.

3.5 WP5: Demonstrator

3.5.1 Bubble Formation

FT: *The models indicate that under realistic assumptions that the target efficiencies can be achieved, which is very encouraging. Did you take account of how bubble formation may affect the efficiency due to light scattering / blocking of active sites). There are several published studies on bubble formation in these types of systems that may be useful as a starting point.* In the 0D model, bubble formation is not taken into account, however, this will be included in the multiscale model which is currently under development in the project. So far, we have experience in modelling bubble formation on flat FTO-coated glass and during PH2OTOGEN, we will expand the model to include the 3D-structure of the TPCS. In the flow reactor configuration, the electrolyte flow should facilitate bubble removal as they are produced. We still need to investigate experimentally and through modelling which type (i.e. parallel to the TPCS substrate or through the TCPS) and rate (i.e. higher rates will facilitate bubble removal, the exact rate required will depend on bubble adherence to the substrate) of flow will be the most effective. We have seen from previous projects, such as Artiphyction, that as the reactor size increases, the bubbles tend to coalesce much more readily than in the small-scale reactors, making them easier to remove.

FT: *If the bubbles coalesce at a particular location on the reactor, this may cause heterogeneity in terms of efficiency and stability. There are already some studies that show that the reactor angle is important in facilitating hydrogen bubble removal. Based on the past studies of the TPCS, do you already have an idea of which flows will be most effective for removing bubbles from the structure?* The previous work, in the Sun-To-X project, focussed mostly on gas-phase hydrogen evolution (where ambient humidity was used as a water source rather than liquid water), so bubble formation was not an issue as everything was in the same phase. However, within the scope of PH2OTOGEN, we have already confirmed that the TPCS can support flow both parallel and through the substrate without any mechanical stability issues. As a first step, optimising flow and reactor angle for bubble removal may be done via a 'dark' process, using the co-catalysts developed in WP1 and 2 on the TPCS under applied bias to reach a similar hydrogen production rate as targeted in PH2OTOGEN (we can also simulate the temperature expected under solar irradiation by heating the electrolyte, as this will also have an effect on bubble adherence).

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3.5.2 Reactor Design

LB: *What is the effect of hydrogen production rate and efficiency depending on the parallel and series reactor configurations modelled?* The series configuration has the OP-coated TPCS positioned above the HEP-coated TPCS, whilst the parallel configuration has the OP-coated TPCS and the HEP-coated TPCS placed side-by-side. The hydrogen production rate is increased in the side-by-side configuration because more light reaches the HEP. However, since the area used is doubled, the overall efficiency is lower.

SH: In the reactor configuration you have now, the HEP and OP are separated spatially. How will you go from this to the final design with one continuous photocatalyst sheet? Since the TPCS is still being scaled up (planned to be ready in M18), we cannot yet assemble the photocatalyst sheet. However, we can use the HEP and OP deposited on FTO glass as an intermediate (wired) configuration for testing. As soon as the TPCS becomes available we can change the sample holder to accommodate the TPCS. In the planned configuration either two (one for the HEP and one for the OP pressed directly together – approximate thickness of 600 µm) or three TPCSs (one for the HEP, one uncoated to facilitate electronic conductivity and one for the OP pressed together – approximate thickness of 900 µm) for will be used.

SH: *The tortuosity and ionic resistance will be important in minimising the Ohmic resistance and resulting efficiency of the system.* From what we have seen in the modelling, the porous nature of the TPCS along allows us to minimise the distance ions have to travel inside the reactor, resulting in a low predicted overall resistance (the conductivity of the electrolyte is sufficient).

3.5.3 Recommendations

- Investigate bubble formation (depending on hydrogen production rate and temperature) and its effect on performance by including it in both the experimental and modelling studies
- Develop mitigation strategies that could facilitate bubble removal (for example, optimising the reactor angle – this may be a compromise as this angle will also affect the incident solar irradiation)
- Consider to minimize distance between electrodes to reduce ohmic losses.

3.6 WP6: Market, technoeconomic and lifecycle assessment

3.6.1 Case study: Medium-scale plant

SH: *The size of the plant study is quite big respect to those existing today, how did you select the size?* The dimensions taken into account for the plant of the study case are based on literature where they propose a medium plant size of 1 ton of hydrogen per day (which corresponds to a 1.1 x 10^5 m^2 plant). Although the scope of this project aims at 500cm^2 device, it is important to already consider scaling to a bigger plant and allow comparison with other technoeconomic studies.

SH: *Considering the data from the scaled-up plant for the TEA and LCA is important. For that, were the data from the lab scaled up linearly to plant dimensions or imagining a scaled-up process for it?* We considered a scaled-up process where recycling, efficient use of chemicals etc. can be included to minimize waste and improve overall efficiency of the plant. For that, we needed to make several assumptions in line with similar studies.

LB: *In the TEA of the scaled-up the plant, did you include components such as heat exchangers, loops to equilibrate pressure drops etc.?* So far, the studies have focussed on the photocatalytic

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sheets themselves and the comparison of materials e.g. for the HEP and OP. The next step will focus on the engineering aspects.

LB: *With respect to the Technoeconomic Analysis, did you consider downstream purification of the oxidation product?* Initially, we thought about including the purification process as part of the demonstrator in the initial proposal. However, the budget required was significant and the call focussed on other aspects which we decided to prioritise. Nevertheless, it will be included in the Technoeconomic Analysis, as the target conversion efficiency of glycerol to 1,3-dihydroxyacetone is 70% (within the project), indicating a need for a purification step. The sensitivity of the cost to conversion efficiency will also be studied to define targets for future plants.

MAL: *Photocatalysis is very challenging. Do you think it's a viable route compared to photovoltaic coupled with electrolyser?* Although photovoltaic coupled with electrolyser has achieved efficiencies of > 20%, the cost is high, > 10 EUR / kg H_2. Studies have shown that photocatalysis may be able to achieve hydrogen costs in the range of 3 – 5 EUR / kg which is much more competitive.

3.6.2 Recommendations

- Envision how the scale up from device level (500 cm^2) to the plant dimensions from an engineering perspective, including heat exchangers, loops to equilibrate pressure and purification in P&ID, as it can have a high impact on CAPEX
- Consideration of sensitivity of cost to plant size i.e. at lower scale which may be more feasible in the short-term

3.7 WP7: Communication and Dissemination

3.7.1 Social Media

FT: *What are your targets for social media engagement? Why was the target set at 350 followers?* We want to engage with our target audiences (scientific community, industry) which are relatively narrow compared to some projects where public engagement is a critical KPI. We set the target based on previous, similar projects, however it seems we had underestimated the interest as we have already achieved our target for followers that we had set for the end of the project. In terms of engagement, we can use our social media presence to further disseminate work done in the project, for example, promoting publications, events organised by PH2OTOGEN etc..

3.7.2 Horizon Results Booster

SH: *Have you used the Horizon Results Booster for the managing the dissemination activities? This can help with organising workshops and other activities, along with networking with other projects.* So far, we have not used the Booster, however, this may become more interesting as our communication and dissemination activities start to increase.

3.7.3 Recommendations

- Investigate the Horizon Results Booster tool to understand if it can support PH2OTOGEN's communication and dissemination activities.

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3.8 WP8: Communication and Dissemination

3.8.1 Management: Project status

The project is overall proving to be well managed, with good partner coordination, and with both Milestones and Deliverables delivered on time and with a good quality, which led to the AB members having no specific question for this Work Package.

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4 Conclusion

Based on the feedback given from the Advisory Board members, we will implement their suggestions to improve the overall outcome of the project. Specifically, we will employ further characterisation to understand the mechanisms behind our results (for example, the selectivity of $BiVO_4$ for DHA and the difference in TPCS properties according to their preparation method). We will also make some changes to the synthesis procedures followed based on their advice (for example, limiting oxygen in the exfoliation process, applying heat to improve adhesion between charge transport / semiconductor / co-catalyst structures). We will also consider the best way to scale-up the reactor from an early stage in the project. In particular, at the demonstrator level, looking at how bubble formation can affect efficiency and the best way to mitigate it and, at the theoretical plant level, how pressure drops and heat management will affect the CAPEX and overall plant efficiency.

Finally, we would like to thank the Advisory Board members for their engagement and positive contribution to the PH2OTOGEN project.

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