

# How much technological progress is needed to make solar hydrogen cost-competitive?

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*Dedicated to Professor Matthias Beller on the occasion of his 60th birthday*

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**Keywords:** Green hydrogen, water splitting, techno-economic analysis, photocatalysis, photovoltaic, electrolysis

## **This file includes:**

Table of contents entry

Abstract

Main text

Figures 1 to 6

Acknowledgements, funding, author contributions, data and code availability, competing interests, correspondence and supplementary materials statements

References

## 25 **Table of Contents Entry**

26 An open-source software and Monte Carlo-based methodology for the analysis of green hydrogen  
27 production are developed. These tools are used to analyze the required technological progress for  
28 cost-competitive hydrogen production via photovoltaic + electrolysis, photoelectrochemical and  
29 photocatalytic water splitting. Based on the results, actionable targets for materials research are  
30 derived.

## 31 **Abstract**

32 Cost-effective production of green hydrogen is a major challenge for global adoption of a hydrogen  
33 economy. Technologies such as photoelectrochemical (PEC) or photocatalytic (PC) water splitting  
34 and photovoltaic + electrolysis (PV+E) allow for sustainable hydrogen production from sunlight and  
35 water, but are not yet competitive with fossil fuel-derived hydrogen. Herein, open-source software  
36 for techno-economic analysis (pyH2A) along with a Monte Carlo-based methodology for modelling  
37 of technological progress are developed. Together, these tools allow for the study of required  
38 technological improvement to reach a competitive target cost. They are applied to PEC, PC and  
39 PV+E to identify required progress for each and derive actionable research targets. For PEC, it is  
40 found that cell lifetime improvements ( $> 2$  years) and operation under high solar concentration ( $>$   
41 50-fold) are crucial, necessitating systems with high space-time yields. In case of PC, solar-to-  
42 hydrogen efficiency has to reach at least 6% and lowering catalyst concentration ( $< 0.2$  g/L) by  
43 improving absorption properties is identified as a promising path to low-cost hydrogen. PV+E  
44 requires ca. 2 or 3-fold capital cost reductions for photovoltaic and electrolyzer components. We  
45 hope that these insights can inform materials research efforts to improve these technologies in the  
46 most impactful ways.

## 47 Main Text

48 Producing green hydrogen at a cost that is competitive with fossil fuel-derived hydrogen is one of the  
49 major challenges for transitioning to a hydrogen economy.<sup>[1]</sup> There are promising technologies for  
50 converting solar energy and water to hydrogen, such as coupling of photovoltaic and electrolysis  
51 (PV+E),<sup>[2]</sup> photoelectrochemical (PEC)<sup>[3,4]</sup> and (particulate) photocatalytic (PC)<sup>[5]</sup> water splitting  
52 (see Figure 1). These technologies, however, cannot currently produce hydrogen at a cost that is  
53 competitive with hydrogen derived from steam reforming.<sup>[6,7]</sup> Hence, the question arises what and  
54 how much technological progress is required to reach a point of competitiveness? Understanding  
55 these requirements can inform (materials) research efforts, focusing them on the areas that are most  
56 impactful for quickly improving green hydrogen production routes.

57 Techno-economic analysis (TEA) is a helpful tool in this regard: it allows for economic modelling of  
58 various (hypothetical) production processes, providing insight into how process parameters affect the  
59 levelized cost of hydrogen (LCOH<sub>2</sub>, herein expressed using the unit \$/kg(H<sub>2</sub>)). In the literature,  
60 various techno-economic studies of hydrogen production from solar energy can be found.<sup>[6–12]</sup>  
61 Broadly speaking, they can be classified into three categories:

- 62 1. Modelling of state-of-the-art technologies to obtain an estimate for the current LCOH<sub>2</sub><sup>[6,11]</sup>
- 63 2. Modelling of hypothetical future technologies to obtain an estimate for a potential future  
64 LCOH<sub>2</sub><sup>[13,14]</sup>
- 65 3. Learning curve analysis based on learning rates to model the decrease of LCOH<sub>2</sub> over  
66 time<sup>[9,10]</sup>

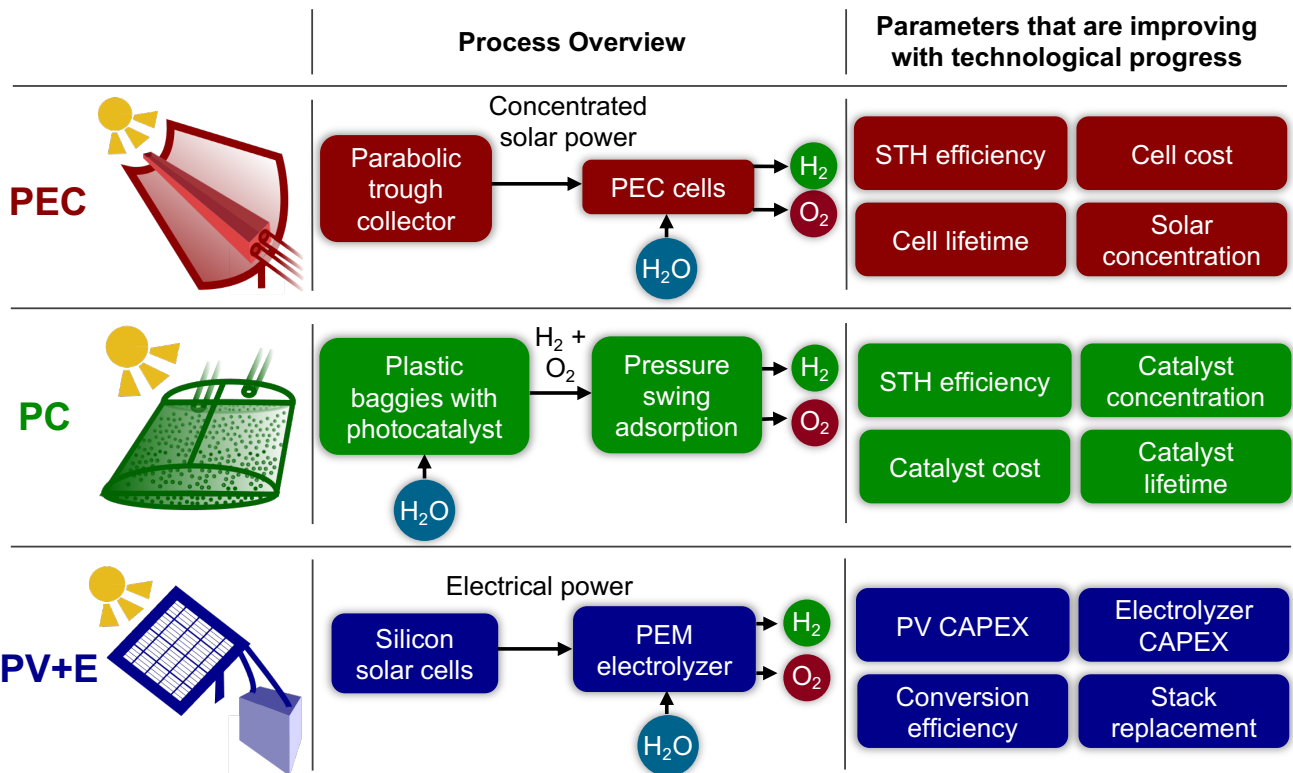
67 Modelling of state-of-the-art or potential future technologies provide valuable single-point cost  
68 estimates and also reveal the impact of individual parameters through sensitivity analysis. However,  
69 they do not capture the trajectory of technological progress. Learning curve analysis does model the  
70 evolution of LCOH<sub>2</sub> over time but it faces two important limitations: firstly, historical data is often  
71 needed to derive reasonable estimates for the learning rates. It is therefore most reliable for mature  
72 technologies and challenging to apply for technologies which have not yet been widely deployed.

73 Secondly, learning curves do not provide straightforward insight into which aspects of technological  
74 progress are actually responsible for the modelled LCOH<sub>2</sub> decrease.

75 Aside from these methodological aspects, there is also a major practical challenge encountered in the  
76 TEA literature: techno-economic models are often implemented in custom environments (e.g. Excel  
77 sheets or programming scripts which are not publicly available) due to the lack of standardized tools.  
78 This leads to reduced transparency and hinders reproduction as well as comparison of literature  
79 results. It also creates overhead effort which goes into creation of these custom environments.

80 Given this backdrop, the present study has three major goals:

- 81 1. Creation of the pyH2A open-source software as a transparent and reproducible tool for  
82 techno-economic modelling. Partly based on the H2A model developed by the U.S.  
83 Department of Energy,<sup>[15]</sup> it allows for flexible modelling of various hydrogen production  
84 pathways.
- 85 2. Development of the Monte Carlo based development distance methodology to capture how  
86 technological progress affects the LCOH<sub>2</sub>. Furthermore, this methodology can be used to  
87 determine which progress is required to reach cost-competitive hydrogen production. It is  
88 inspired by the previous use of Monte Carlo for uncertainty quantification,<sup>[6]</sup> and the use of  
89 contour plots to study how simultaneous change of multiple parameters impacts the  
90 LCOH<sub>2</sub>.<sup>[14]</sup>
- 91 3. Application of this methodology to PV+E, PEC and PC, determining for each how much and  
92 which technological progress is needed produce hydrogen at a cost-competitive level. These  
93 insights are then used to derive actionable research targets for each technology.



94

95 Figure 1 Overview of photovoltaic + electrolysis (PV+E), photoelectrochemical water splitting (PEC) and photocatalytic  
 96 water splitting (PC) for green hydrogen production along with relevant parameters for technological progress.  
 97 Abbreviations: “PEM” proton-exchange membrane, “CAPEX” capital expenditure, “STH” solar-to-hydrogen.

## 98 Methodology

### 99 pyH2A open-source software

100 pyH2A is an extensible framework for techno-economic analysis of hydrogen production,  
 101 implemented in Python. It is open-source, with the source code available on GitHub  
 102 (<https://github.com/jschneidewind/pyH2A>). Input parameters are provided in a plain text file and  
 103 different technologies are modelled by invoking plugins. These feed information into the central  
 104 discounted cash flow calculation, from which the LCOH<sub>2</sub> is obtained. Any given techno-economic  
 105 model can be interfaced with various analysis modules to perform cost breakdown, sensitivity,  
 106 waterfall or Monte Carlo analysis. A detailed description of the general pyH2A methodology is  
 107 provided in SI Section 2.

## Hydrogen production technologies

This study focuses on photophysical/photochemical technologies for converting solar energy and water to hydrogen, namely photovoltaic + electrolysis (PV+E), photoelectrochemical (PEC) and photocatalytic (PC) water splitting. There are other promising solar hydrogen production pathways, such as those based on thermal<sup>[16]</sup> or biological processes for water splitting<sup>[17]</sup> or by utilizing biomass as a feedstock.<sup>[18]</sup> While these routes are outside the scope of the present work, the described methodologies can also be applied to them.

For each selected technology, a hydrogen production plant with a design capacity of ca. 1 metric ton(H<sub>2</sub>)/day was modelled over its entire lifetime, obtaining the LCOH<sub>2</sub>. The financial input parameters shared by all models can be found in SI Section 6.2.

For photoelectrochemical (PEC) water splitting, hydrogen production is achieved by concentrating sunlight using parabolic trough collectors and focusing it on PEC cells, which are in a transparent enclosure with water. Irradiation of the PEC cells leads to hydrogen and oxygen production on opposites sides of cell, so that pure hydrogen can be obtained (see Figure 1, PEC). State-of-the-art properties of the PEC cells are based on devices by Kistler *et al.*<sup>[3]</sup> and Khan *et al.*<sup>[4]</sup> using a III-V absorber. The layout of the hydrogen production plant is based on Pinaud *et al.* (type 4 - PEC).<sup>[13]</sup> A detailed description of the process can be found In SI Section 5.1 and all input parameters are available in SI Section 6.5.

In photocatalytic (PC) water splitting, a particulate photocatalyst is mixed with water and placed in plastic baggie reactors, which are exposed to sunlight.<sup>[13,19,20]</sup> Action of the photocatalyst leads to production of a H<sub>2</sub>/O<sub>2</sub> mixture, which is separated using pressure swing adsorption<sup>[13]</sup> to obtain pure hydrogen (see Figure 1, PC). The CDot/C<sub>3</sub>N<sub>4</sub> photocatalyst reported by Liu *et al.*<sup>[5]</sup> is used as a state-of-the-art reference and the plant layout is based on the “type 1 – single bed” design described by Pinaud *et al.*<sup>[13]</sup> SI Section 4.1 contains a detailed process description and input parameters can be found in SI Section 6.4.

Coupling of silicon solar cells with an off-grid proton-exchange membrane (PEM) electrolyzer is the basis for photovoltaic + electrolysis (PV+E). Electrical power from the solar cells is fed to the electrolyzer to produce pure hydrogen from water (see Figure 1, PV+E). The plant model is based on the one reported by Yates *et al.*<sup>[6]</sup> A process description can be found in SI Section 3.1 and input parameters in SI Section 6.3.

## Monte Carlo/development distance methodology

The aim of the Monte Carlo/development methodology is to model how simultaneous progress for multiple parameters of a technology affects the LCOH<sub>2</sub>. For a given technology, this is accomplished in four steps (see also SI Section 2.4.4):

1. Selection of parameters that improve with technological progress (selected parameters are shown for each technology in Figure 1). For every parameter, a base value, which represents the state-of-the-art, is defined. Furthermore, a limit value is defined, which represents the limit which can possibly be achieved with future progress.
2. A large number (in this case 50,000) of random parameter value combinations are generated. Each parameter value is within its [base, limit] interval. This leads to 50,000 different models, each with random values for the selected parameters.
3. For each model, the normalized distance of its parameter values to the base case is calculated. “Base case” means that all parameter values are equal to their base values (normalized distance is 0), while “limit case” means that all parameter values are equal to their limit value (normalized distance is 1). Details on the distance calculation can be found in SI Section 2.4.4.1. This metric is herein referred to as “development distance”, since it is an indicator for the amount of technological development that is represented by a given model.
4. The full discounted cashflow calculation is performed for every model to obtain the corresponding LCOH<sub>2</sub>.

With this methodology, a dataset of 50,000 models for every technology is obtained. Each model has a unique combination of parameter values, an associated development distance and LCOH<sub>2</sub>.



159 Together, the datapoints map the entire trajectory from the state-of-the-art (base case) to future  
160 technologies (limit case). The Monte Carlo/development distance methodology is implemented in  
161 pyH2A.

162 The tables in Figure 2 show the base and limit values for the selected parameters of each technology.  
163 For PEC the parameters are: STH efficiency, solar concentration factor, cell cost ( $\$/\text{m}^2(\text{PEC cell})$ )  
164 and cell lifetime (in years). For PC, catalyst concentration ( $\text{g}(\text{Catalyst})/\text{L}$ ), catalyst cost  
165 ( $\$/\text{kg}(\text{Catalyst})$ ), STH efficiency and catalyst lifetime (in years) were selected. Selected PV+E  
166 parameters are: PV CAPEX ( $\$/\text{kW}(\text{PV})$ ), electrolyzer CAPEX ( $\$/\text{kW}(\text{Electrolyzer})$ ), conversion  
167 efficiency ( $\text{kg}(\text{H}_2)/\text{kWh}(\text{Electricity})$ ) and stack replacement cost (as a fraction of electrolyzer  
168 CAPEX). In the SI, sources/rationales for each selected base/limit value can be found (PEC: SI  
169 Section 5.1.4, PC: SI Section 4.1.4, PV+E: SI Section 3.1.3).

## 170 **Limitations**

171 There are several limitations for the methodology employed in this study:

- 172 1. The limit values for the Monte Carlo/development distance modelling must be assumed since  
173 it is not possible to know which parameters values will actually be achieved in the future. The  
174 choice of limit values affects the development distance: choosing very optimistic limit values,  
175 for example, makes models with intermediate values appear at shorter development distances.  
176 This means that comparing the development distance values for different technologies is only  
177 valid if the limit values for each are equally “difficult” to achieve. As this notion is  
178 challenging to quantify, the development distance should always be seen in the context of the  
179 underlying base and limit values, especially when comparing technologies. Importantly,  
180 however, the choice of limit values does not affect the analysis of the required parameter  
181 values to achieve a given cost target. In this case, the limit values only determine which part  
182 of the parameter space is explored.
- 183 2. The present models only calculate the cost of hydrogen production, thus the cost for transport  
184 of storage is not considered.

- 185 3. For all calculations, the plant size (1 metric ton H<sub>2</sub>/day) and location (Dagget, CA, USA) are  
186 fixed. Hence, scaling and geographical effects on the LCOH<sub>2</sub> are not considered.
- 187 4. In this study, only a cost analysis of hydrogen production is performed. Other important  
188 aspects, such as modelling of life-cycle greenhouse gas emissions<sup>[21]</sup> and net energy  
189 analysis<sup>[22]</sup> are not included.

## Results and Discussion

### Development distance and LCOH<sub>2</sub>

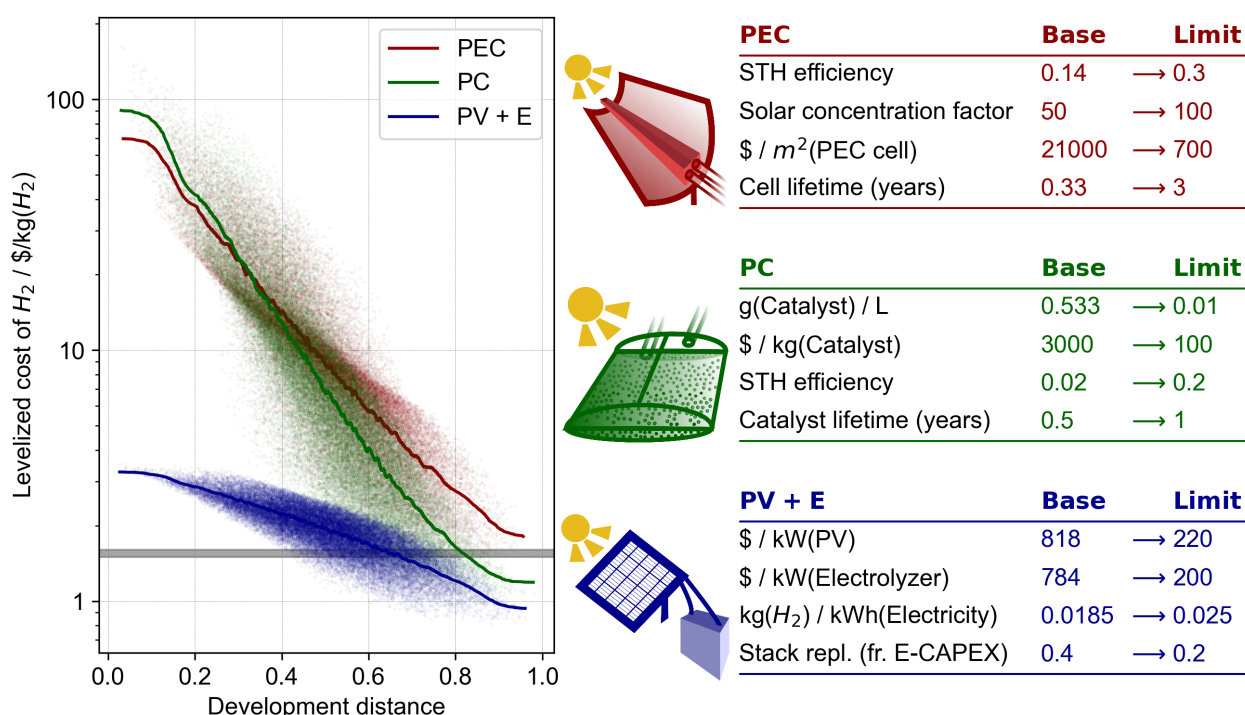


Figure 2 Relationship of development distance and LCOH<sub>2</sub> (log scale) for PEC, PC and PV+E. The grey bar indicates the target cost range (1.5 – 1.6 \$/kg(H<sub>2</sub>)). Savitzky-Golay smoothed trendlines are shown as solid lines. For each technology, parameters that constitute the respective development distance are shown on the right, along with their base and limit values. For details see SI Section 2.4.4.2. “Stack repl. (fr. E-CAPEX)” stands for “Stack replacement cost (fraction of electrolyzer CAPEX)”.

The relationship between development distance and LCOH<sub>2</sub> provides an overview of technological progress’ impact on hydrogen cost. Figure 2 plots the development distance of each random model against its associated LCOH<sub>2</sub>, along with a smoothed Savitzky-Golay trendline for each technology. The shown data reflects the entire trajectory from the current state-of-the-art (base case, development distance of 0) to the limit technologies (development distance of 1).

PEC and PC have a very high LCOH<sub>2</sub> for the base case in excess of 100 \$/kg(H<sub>2</sub>). However, the LCOH<sub>2</sub> for both drops exponentially with increasing development distance, as indicated by the linear trend in the logarithmic plot. Such an exponential decrease points at a strong interaction between the selected parameters, leading to multiplicative effects. In case of PC, for example, improving both the

206 STH efficiency and catalyst concentration produces a multiplicative cost reduction. It can also be  
207 seen that the  $\text{LCOH}_2$  decreases more steeply for PC compared to PEC.  
208 PV+E has a much lower  $\text{LCOH}_2$  of around 3.6  $\$/\text{kg}(\text{H}_2)$  for the base case. Increasing development  
209 distance, however, leads only to a roughly linear cost reduction (sublinear in logarithmic plot),  
210 indicative of weak interactions between selected parameters. In contrast to PEC and PC, parameter  
211 improvements (such as PV or electrolyzer CAPEX reductions) are largely independent of one  
212 another and do not produce multiplicative effects.

### 213 **Models in the target cost range**

214 To be cost-competitive on the global market, solar hydrogen has to reach the cost range of hydrogen  
215 derived from steam methane reforming (SMR), which is currently the dominant hydrogen production  
216 route.<sup>[9]</sup> SMR hydrogen is produced at costs ranging from 1-2  $\$/\text{kg}(\text{H}_2)$ .<sup>[9]</sup> For this study, we  
217 therefore defined the target cost range for cost-competitiveness as 1.5-1.6  $\$/\text{kg}(\text{H}_2)$ , which is  
218 indicated as a grey bar in Figure 2. It can be seen that PV+E crosses into the target cost range at the  
219 shortest development distance. PC also reaches it at somewhat longer distances while PEC seems to  
220 mostly level off above it. To gain insight into the requirements for cost-competitiveness, we turn to  
221 a more detailed analysis of the models for each technology that fall into the target cost range.

222 Figure 3 shows the development distance distribution of all models with a  $\text{LCOH}_2$  in the target cost  
223 range. From this analysis, we can obtain the mean development distances that are required to achieve  
224 cost-competitiveness. As already indicated by Figure 2, PEC displays the longest mean development  
225 distance (0.86, standard deviation: 0.043) and only a very small number of models actually reach the  
226 target cost range (low frequency values on the y axis). The high mean development distance means  
227 that almost all potential for technological improvement has to be exhausted in order to produce  
228 hydrogen at the defined target cost. PC shows a significantly shorter mean development distance of  
229 0.72 with a relatively broad distribution of models from 0.5 to 0.85 (standard deviation: 0.076). This  
230 implies that, while a significant amount of progress is required, the target cost can be achieved  
231 without having to use all of the innovation potential. In case of PV+E, the shortest mean

development distance of 0.61 is observed with an equally broad distribution compared to PC (standard deviation: 0.080). Within the assumptions of this study, the shortest mean development distance indicates that PV+E requires the least amount of technological progress to reach cost-competitiveness.

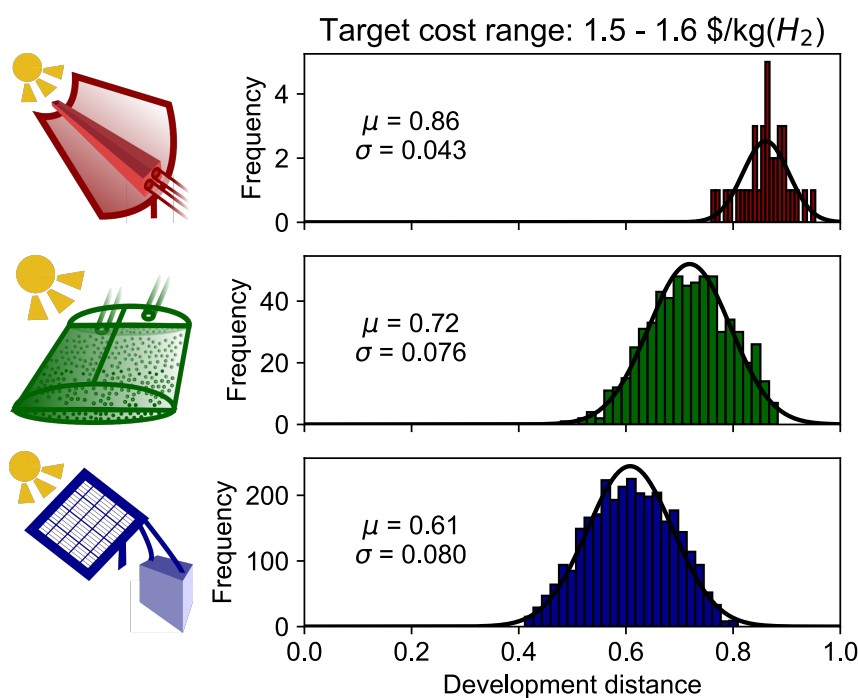


Figure 3 Histograms showing development distance distribution of models within the target cost range for each technology (top: PEC, middle: PC, bottom: PV+E). A fitted and scaled normal distribution is shown for each histogram (black line), with the corresponding mean ( $\mu$ ) and standard deviation ( $\sigma$ ) shown as inlets. For details, see SI Section 2.4.4.3.

## Required progress and research targets

Analysis of the development distances provides on the overall picture of (required) technological progress. To derive actionable insight, especially for informing research and development efforts, it is important to understand how much the underlying technological properties have to advance to achieve cost-competitive hydrogen production. To this end we can analyze the specific parameter values of models which reach the target cost range. In the following, the corresponding data will be visualized using colored scatter plots: each model with an LCOH<sub>2</sub> in the target cost range is shown as a colored dot, with its (x, y) position and color determined by its parameter values (the fourth

parameter which has been varied in the Monte Carlo simulation is not shown). For reference, the base case is also shown as a labelled and colored dot. From this visualization we can see which combinations of parameter values give rise to models with cost-competitive hydrogen production.

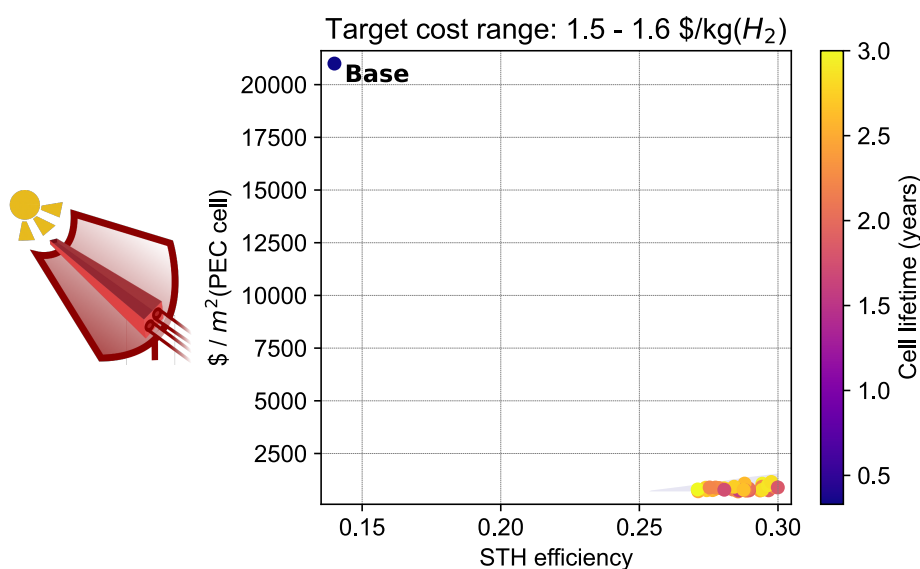
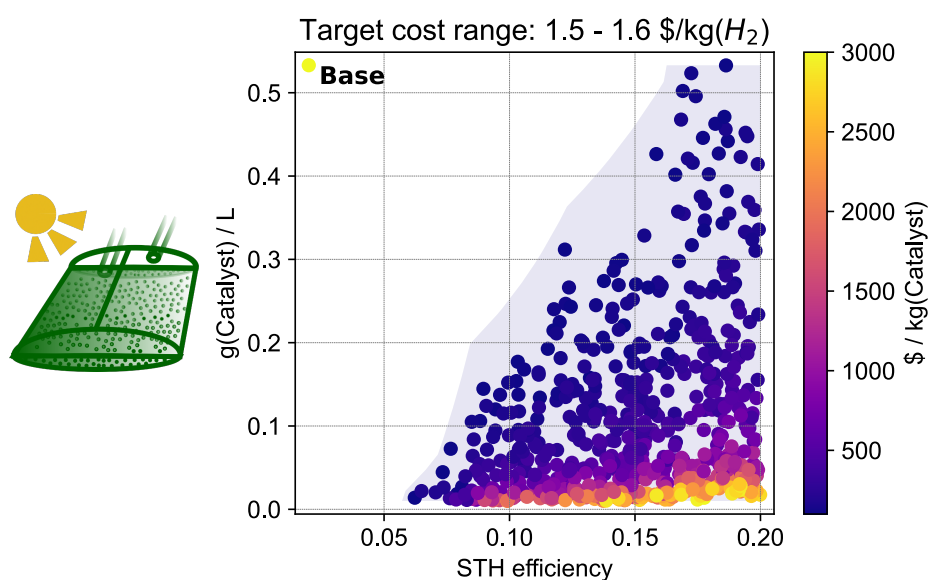


Figure 4 Colored scatter plot showing parameter values of PEC models within target cost range. For reference, the base case is shown in the top left. Light blue area illustrates largest possible region in which models can lie (for details see SI Section 2.4.4.4).

Figure 4 shows the colored scatter plot for PEC. Only a very small region of the parameter space gives rise to models in the target cost range, with this region being at the maximum distance from the base case. STH efficiency has to exceed 26%, cell cost has to be below 1500 \$/m<sup>2</sup>(PEC Cell) and cell lifetime has to exceed 2 years. The central challenge for PEC is that the PEC cells are the most expensive component of the plant for most models (see cost breakdown in SI Figure 5.2-2), but also have a short lifetime (especially compared to solar cells and electrolyzers).<sup>[23]</sup> This is because various components of the cell are exposed to a reactive chemical environment.<sup>[3]</sup> Since PEC cells are by definition highly integrated devices, most components have to be replaced together at the end of their lifetime, leading to high replacement costs (see SI Figure 5.2-1) and thus a high LCOH<sub>2</sub>. Based on our results, only a combination of high efficiency (small area of cells needed for a given H<sub>2</sub> production), low cost and long lifetime can overcome these challenges to reach the target cost range.

267 It should also be noted that solar concentration is very likely necessary for low-cost  $H_2$  production  
 268 using PEC: modelling PEC without solar concentration shows that even for the limit case,  $LCOH_2$   
 269 does not drop below 15  $\$/kg(H_2)$  (see SI Section 5.4). Solar concentrators will likely be significantly  
 270 cheaper than PEC cells (per  $m^2$ ) for the foreseeable future. Hence, replacing PEC cell area with solar  
 271 concentrator area enables effective cost reduction.<sup>[24]</sup> In the limit case, however, solar concentrator  
 272 cost actually becomes the dominant factor in PEC CAPEX (see SI Figure 5.3-2). With respect to  
 273 research targets these results imply the following: the lifetime of PEC cells has to be significantly  
 274 improved (reaching on the order of years) to address the high costs resulting from regular  
 275 replacements. Furthermore, PEC cells should be optimized to operate under high solar concentration  
 276 factors ( $> 50$ ) to reduce the required cell area. This implies that highly active PEC materials  
 277 (absorbers and electrocatalysts) are required which have a sufficient space-time yield to convert the  
 278 high incoming energy flux (peak activity likely has to exceed  $400 \text{ mol } H_2 \text{ h}^{-1} \text{ m}^{-2}(\text{PEC cell})$ ). It is  
 279 uncertain if such progress is realistically achievable, especially to allow PEC to compete with PV+E  
 280 (see below).

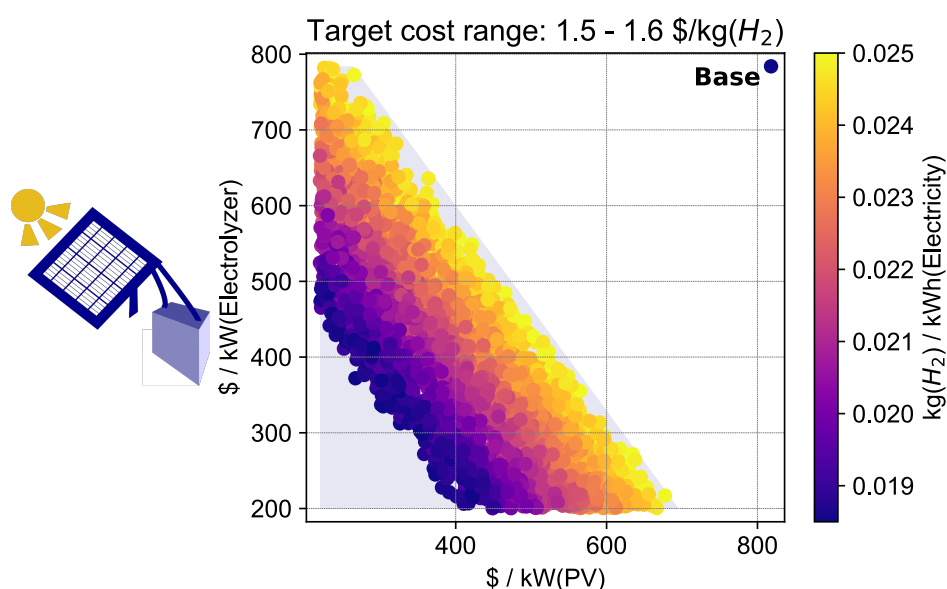


282 Figure 5 Colored scatter plot showing parameter values of PC models within target cost range. For reference, the base  
 283 case is shown in the top left. Light blue area illustrates largest possible region in which models can lie (for details see SI  
 284 Section 2.4.4.4).

For PC, a much larger region of the parameter space gives rise to models in the target cost range (see Figure 5). For cost-competitive hydrogen production, STH efficiency has to be at least 6%. Catalyst concentration can be as high as 0.5 g(Catalyst)/L, but concentrations below 0.2 g(Catalyst)/L open up much more flexibility with regards to efficiency and cost. For most cases, catalyst cost has to be below 1000 \$/kg(Catalyst), except when the catalyst concentration is very low ( $< 0.05$  g(Catalyst)/L). In all cases, the catalyst lifetime is relatively short (between 0.5 and 1 year), which necessitates regular catalyst replacements. In contrast to PEC, however, replacing the catalyst is straightforward because no other components have to be replaced with it: it can be removed from the water/catalyst mixture (e.g. by nanofiltration<sup>[25]</sup>) and new catalyst is added. Looking at research targets, this data suggests that it is crucial to lower the catalyst concentration. Systems with low catalyst concentrations can tolerate lower STH efficiencies and higher catalyst costs, while reduction of the catalyst amount also reduces resource consumption for catalyst production. To achieve lower catalyst concentrations the main consideration is the absorption behavior of the photocatalyst: it needs to have a sufficiently high absorption cross section so that most sunlight is still absorbed even when lower concentrations are employed. The demands for catalytic activity are less stringent to enable low catalyst concentrations. Even for the limit case (highest efficiency, lowest concentration), peak catalytic activity does not have to exceed  $7 \text{ mol H}_2 \text{ g}^{-1} \text{ h}^{-1}$  (activities on the order of  $1 \text{ mol H}_2 \text{ g}^{-1} \text{ h}^{-1}$  have already been achieved<sup>[26]</sup>), which corresponds to a turnover frequency of  $< 1 \text{ s}^{-1}$  for a homogeneous catalyst (assuming a molar mass of 500 g/mol). Hence, light absorption performance is likely more important than highly active catalytic sites for  $\text{H}_2$  and  $\text{O}_2$  evolution. To identify effective paths to a cost-competitive system, it is insightful to look at the parameter values of the model with the shortest development distance that reaches the target cost range: with a distance of 0.48, this model has a STH efficiency of 17.5%, catalyst concentration of 0.01 g(Catalyst)/L, catalyst cost of 2950 \$/kg(Catalyst) and catalyst lifetime of 0.52 years. Hence, high catalyst cost and low lifetime can be tolerated through the combination of high STH efficiency and low catalyst concentration. These characteristics point to the potential of homogenous photocatalysts, which can be used at low



311 concentrations due to high molar absorptivity.<sup>[27]</sup> Furthermore, it was recently shown that it is  
 312 theoretically possible for homogeneous photocatalysts to achieve dual absorber STH efficiencies (>  
 313 20%) with a single catalyst.<sup>[28]</sup> With progress on catalyst concentration and STH efficiency, there is a  
 314 pathway for PC to cost-competitive hydrogen production. Due to the simple plastic baggie reactor  
 315 construction, this approach has a low CAPEX (but rather high OPEX due to catalyst replacements,  
 316 see SI Figures 4.2-1 and 4.3-1), which is complementary to PV+E (high CAPEX, low OPEX, see SI  
 317 Figure 3.2-1) and could allow for easier construction of new plants. Safety issues due to generation  
 318 of a H<sub>2</sub>/O<sub>2</sub> mixture in the reactors have to be considered, but these risks were found to be  
 319 manageable.<sup>[29]</sup>



321 Figure 6 Colored scatter plot showing parameter values of PV+E models within target cost range. For reference, the base  
 322 case is shown in the top right. Light blue area illustrates largest possible region in which models can lie (for details see SI  
 323 Section 2.4.4.4).

324 PV+E shows a well-defined region of the parameter space that gives rise to models with an LCOH<sub>2</sub>  
 325 in the target cost range (Figure 6). The symmetry and gradients indicate that each parameter (PV  
 326 CAPEX, electrolyzer CAPEX, conversion efficiency) has a roughly linear effect on LCOH<sub>2</sub> and  
 327 there are no significant interactions between parameters (which was also shown by the linear  
 328 development distance/LCOH<sub>2</sub> relationship). To reach the target cost range, PV CAPEX has to be

329 below 650 \$/kW(PV) and electrolyzer CAPEX can be as high as 800 \$/kW(Electrolyzer) but only if  
330 the conversion efficiency approaches the theoretical maximum of 0.025 kg(H<sub>2</sub>/kWh(Electricity)).<sup>[6]</sup>  
331 Improving the conversion efficiency in general opens up possibilities to tolerate higher PV and  
332 electrolyzer CAPEX. However, the model with shortest development distance in the target cost range  
333 (distance of 0.41) has the base case conversion efficiency and stack replacement cost (0.0185  
334 kg(H<sub>2</sub>)/kWh(Electricity) and 40% of electrolyzer CAPEX), PV CAPEX of 300 \$/kW(PV) and  
335 electrolyzer CAPEX of 330 \$/kW(Electrolyzer). Hence, even without other improvements, it is  
336 possible to enable hydrogen production at the target cost by reducing PV and electrolyzer CAPEX 2  
337 or 3-fold each. The implication for research and development targets is that cost reductions are key,  
338 and efficiency improvements are not strictly necessary but open up possibilities to enable cost-  
339 competitive H<sub>2</sub> production even with more expensive components.

## Conclusion

In summary, an open-source tool for transparent and reproducible techno-economic modelling of hydrogen production, called pyH2A, has been developed. Using pyH2A, a novel Monte Carlo-based methodology was conceived and implemented, which enables the study of how technological progress impacts the LCOH<sub>2</sub> using the concept of “development distance”. With this methodology it is also possible to dissect the influence of specific technological parameters and determine how much each has to advance to reach a defined target cost range.

The Monte Carlo/development distance method was then applied to the study of three solar hydrogen production routes: photoelectrochemical (PEC) and photocatalytic (PC) water splitting as well as photovoltaic + electrolysis (PV+E). For each, it was determined how much and which technological progress is needed to produce hydrogen at a cost level of 1.5-1.6 \$/kg(H<sub>2</sub>) and the results were used to derive appropriate research targets.

For PEC, significant progress with respect to STH efficiency (> 26%) and PEC cell stability is required, as lifetimes of at least 2 years are needed to alleviate the high costs resulting from cell replacements. Furthermore, solar concentration is a crucial component to enable low-cost hydrogen production using PEC and cells should be optimized to operate with high solar concentration factors (> 50), necessitating highly absorbent semiconductors and highly active electrocatalysts.

For PC, STH efficiency has to exceed 6% and it is important to lower the catalyst concentration (< 0.2 g(Catalyst)/L) by developing catalysts with large absorption cross sections. With a sufficiently high STH efficiency and low catalysts concentration, high catalyst cost (> 2000 \$/kg(Catalyst)) and a short lifetime (ca. 0.5 years) can be tolerated, pointing towards the potential utility of homogeneous photocatalysts. Improvements of the photocatalyst open a path to cost-competitive H<sub>2</sub> production using PC, which could be a complementary technology to PV+E due to the low CAPEX of the plastic baggie reactor construction.

For PV+E, CAPEX reductions for both the photovoltaic and electrolyzer components are needed. The target cost can be reached by a 2 or 3-fold cost reduction for each (300 \$/kW(PV) and 330

366 \$/kW(Electrolyzer) even without other technological improvements. Increasing the conversion  
367 efficiency, however, opens up more flexibility for the cost of PV and electrolyzer systems.  
368 It is our hope that these techno-economic insights inform materials research in the area of solar  
369 hydrogen production, so that research efforts can be directed to improve these technologies in the  
370 most impactful ways. Ultimately, these efforts will hopefully allow us to transition solar hydrogen  
371 into large scale applications, providing affordable green hydrogen on a global scale.

372 **Acknowledgments:** Hrishi Olickel is gratefully acknowledged for insightful discussions. Prof.  
373 Walter Leitner, Dr. Markus Hölscher and Dr. Giancarlo Franciò (RWTH Aachen University) as well  
374 as Prof. Matthias Beller and Dr. Henrik Junge (Leibniz-Institute for Catalysis) are acknowledged for  
375 supporting the research activities.

376 **Funding:** Financial support by Fonds der Chemischen Industrie (Liebig-Stipendium for J.S.) and the  
377 Landesförderinstitut Mecklenburg-Vorpommern (LFI-MV) (Project number 20-0001) is gratefully  
378 acknowledged.

379 **Author contributions:** J. S. conceived and coordinated the project, developed the software,  
380 performed techno-economic modelling and data analysis, wrote the manuscript and curated the  
381 results for the supporting information and public repository.

382 **Data availability:** Original data supporting the results of this study is available at:  
383 <https://github.com/jschneidewind/pyH2A>

384 **Code availability:** Code developed for this study is available at:  
385 <https://github.com/jschneidewind/pyH2A>

386 **Competing interests:** The author has no competing interests.

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## 389 **Supplementary Materials**

390 Methods and Parameters

391 SI Figures 3.1-1 to 5.4-3

392 SI Tables 2.4-1 to 6.1-1

393 Original data and code: <https://github.com/jschneidewind/pyH2A>

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