GUIDING PRACTICAL PATHWAYS FOR SOLAR-DRIVEN ELECTROCHEMICAL HYDROGEN GENERATION

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Abstract

Photo-electrochemical electrolysis of water provides a direct pathway for the conversion of solar energy into an energy-dense, storable and transportable fuel. The practical implementation of photoelectrochemical approaches requires focusing simultaneously on four key developmental concerns: device and system *i)* efficiency, *ii)* durability and reliability, *iii)* environmental sustainability, and *iv)* scalability with economic viability.

We developed a techno-economic model and coupled it to a life cycle assessment (LCA) in order to jointly assess efficiency, hydrogen cost, energy input, and lifetime/degradation of photo-electrochemical devices. The general input and output of the model platform is depicted in figure 1.a. The model we used accounted for optical losses in the concentrator, recombination and resistive losses in the photoabsorbers, overpotentials in the electrocatalysts (including mass transport limitations, relevant at high irradiation concentrations), as well as photoabsorber and electrocatalytic degradation. The sustainability assessment accounted for the energy input required for material mining and manufacturing of the device components, as well as operation. The cost assessment accounted for material and component cost and manufacturing. The model was used to investigate and compare a class of 16 devices: combinations of devices using *i)* concentrated or non-concentrated irradiation (irradiation concentration, C), *ii)* low quality Si-based or high quality III-V-based photoabsorbers, *iii)* earth abundant or rare electrocatalysts, and *iv)* integrated photoabsorber and electrocatalyst with the same or different absorber and electrolysis area (current concentration, F).

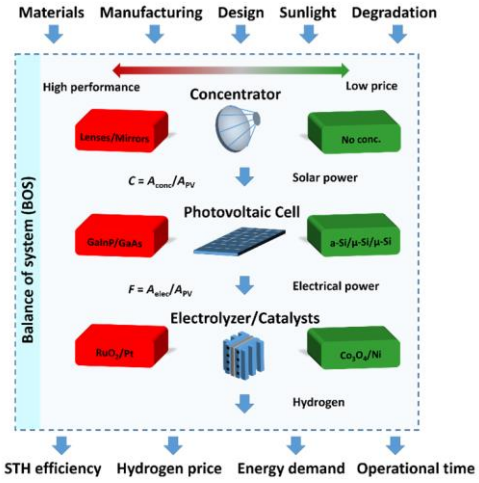

Figure 1 (a): Schematic representation of device component choices with inputs and outputs of this study.

		With current concentration (variable F)		No current concentration ($F = 1$)	
		High quality catalyst (RuO_2/Pt)	Low price catalyst (Co_3O_4/Ni)	High quality catalyst (RuO_2/Pt)	Low price catalyst (Co_3O_4/Ni)
With concentrator (variable C)	High quality photoabsorber (III-V)	1	2	9	10
	Low price photoabsorber (Si)	3	4	11	12
No concentrator (C=1)	High quality photoabsorber (III-V)	5	6	13	14
	Low price photoabsorber (Si)	7	8	15	16

Figure 1 (b): Device combinations and numbers.

The choice between advantageous performance or cost for the concentrator, the PV cell, and the PEMEC results in 8 possible device solutions, which are extended by considering current concentration for each case (F≠1), resulting in 16 device types investigated. For the concentrator, low price technology implies no concentration. b) Number coding of device types investigated according to PV cell and the PEMEC component choice, with (C≠1) or without (C=1) concentrated irradiation, and with (F≠1, decoupled) or without (F=1, closely integrated) current concentration.

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The results predict that maximum efficiency does not guarantee minimum hydrogen price or minimum energy demand, as depicted in figure 2 for a selection of devices. Devices using large irradiation concentration and III-V-based photoabsorbers (designs 1, 2, 5, 6, 9, 10, 13, and 14) showed low hydrogen prices and best efficiencies while non-concentrating devices using Si-based photoabsorbers and rare electrocatalysts (designs 3, 7, 11, and 15) showed slightly higher energy demand and hydrogen price. An increase in the component's lifetime was generally beneficial to efficiency, cost, and energy demand. Degradation significantly influenced all three characteristics, and the calculations provided guidance for the most suitable exchange time of individual components – keeping overall device efficiency high while reducing energy and cost resulting from component exchange – during the lifetime of the complete device.

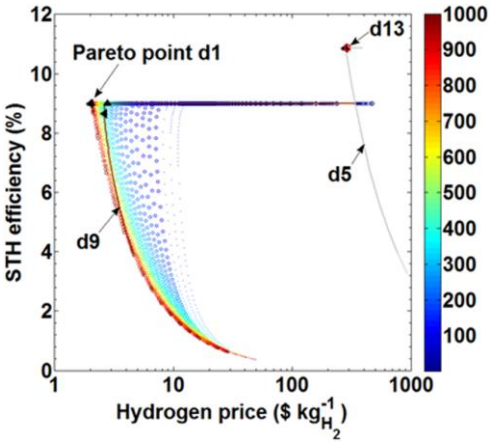

Figure 2 (a): STH efficiency as a function of energy demand.

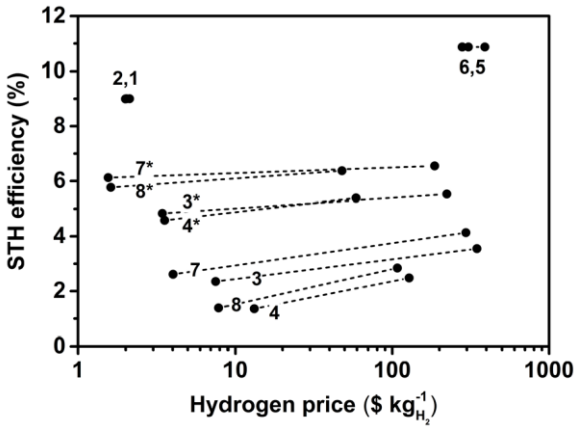

Figure 2 (b): STH efficiency as a function of hydrogen cost, for devices using concentrated irradiation (no. 1-8) or not (no. 9-16), using Si-based cells (no. 3, 4, 7, 8, 11, 12, 15, 16) or III-V cells (no. 1, 2, 5, 6, 9, 10, 13, 14), and using rare catalysts no. 1, 2, 5, 6, 9, 10 ,13, 14) or earthabundant catalysts (no. 3, 4, 7, 8, 11, 12, 15, 16). No. 7* and 8* are Si-based cells with an additional junction.

The variations for the individual design results from variations in irradiation concentration (C) or current concentration (F). For the first time reported, we provide evidence that tailored device designs can significantly reduce hydrogen cost while ensuring high efficiency and low manufacturing and operation energy input.

We predict that devices utilizing extremely expensive components can operate cost competitively and efficiently if irradiation and current concentration is employed. Further, we demonstrate that not all device designs incorporating various material choices exhibit a global optimum, but rather, a set of partially optimal designs are found (a Pareto front) requiring a tradeoff and the prioritization of one of the four indicators (efficiency, cost, sustainability, lifetime). Finally, the influence of component degradation on the four indicators is quantified and strategies for device operation and component replacement are described. An accessible web-based form of the platform was developed and is accessible to the community.

Our model provides holistic design guidelines for integrated photo-electrochemical hydrogen generation accounting simultaneously for the four pillars of a practical and competitive future technology: efficiency, cost, sustainability, and lifetime. The results identify knowledge gaps that warrant further research on photo-electrochemical water splitting. The framework and findings presented here support the decision-making process for an integral and practical approach to competitive solar hydrogen production in the future.