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# MODELLING BASED DESIGN OF INTEGRATED PHOTOELECTROCHEMICAL DEVICES WORKING UNDER CONCENTRATED IRRADIATION


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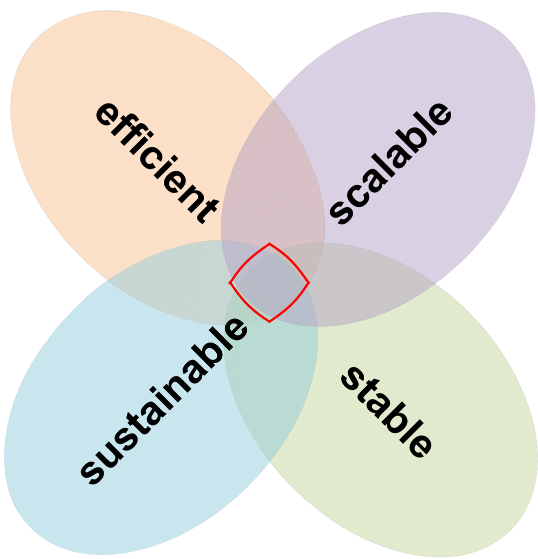
## Introduction

Photo-electrochemical water-splitting has the potential to significantly contribute to a future, sustainable energy economy if its technological implementation *simultaneously* meets four requirements:

1) High efficiency
2) Low cost
3) Stable long-term performance
4) Low environmental footprint

We coupled a 0D performance model, incorporating degradation, to economic and sustainability inventories in order to provide *holistic* design guidelines.




Integrated PEC devices, composed of an integrated photovoltaics (PV) component and an electrolyzer (EC) component, allow to circumvent some of the challenges imposed by solid-liquid interfaces in traditional PEC devices, and operate at higher efficiencies than externally wired (non-integrated) PV-EC devices. To make the device cost competitive, concentrated irradiation is employed. We utilize *multi-physics modeling* to propose a novel integrated design, shown in Fig. 1.

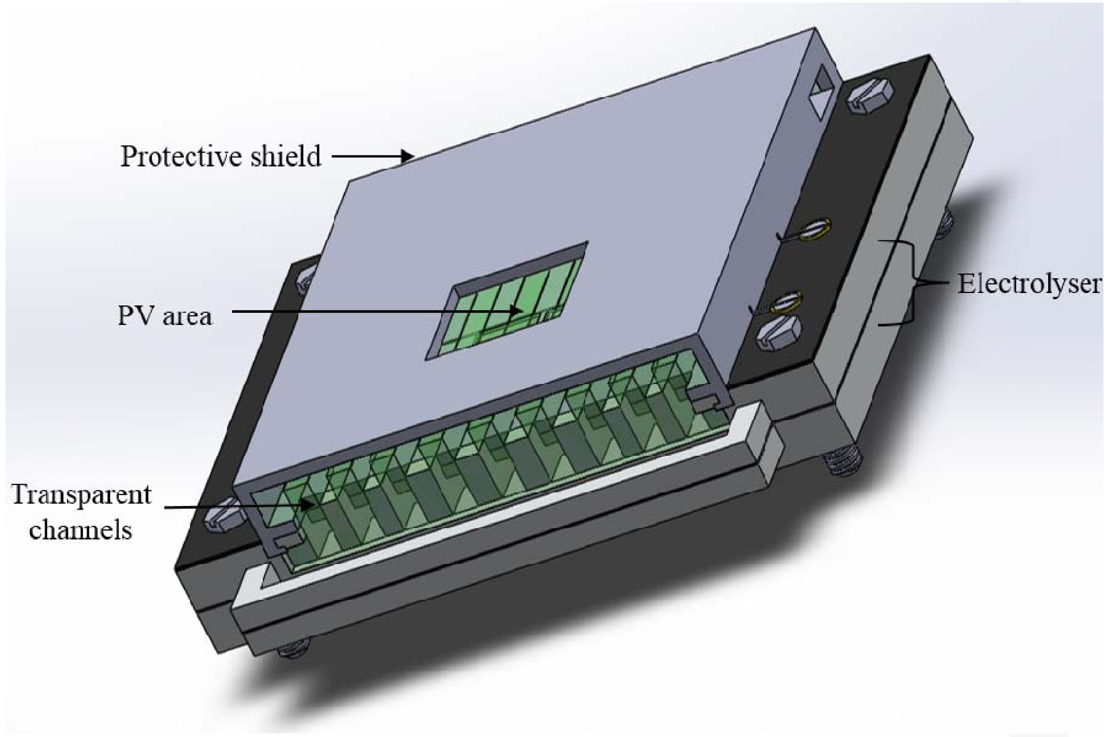



**Fig. 1** *Schematic of integrated PEC demonstrator device.*

## Results – Holistic design guidelines

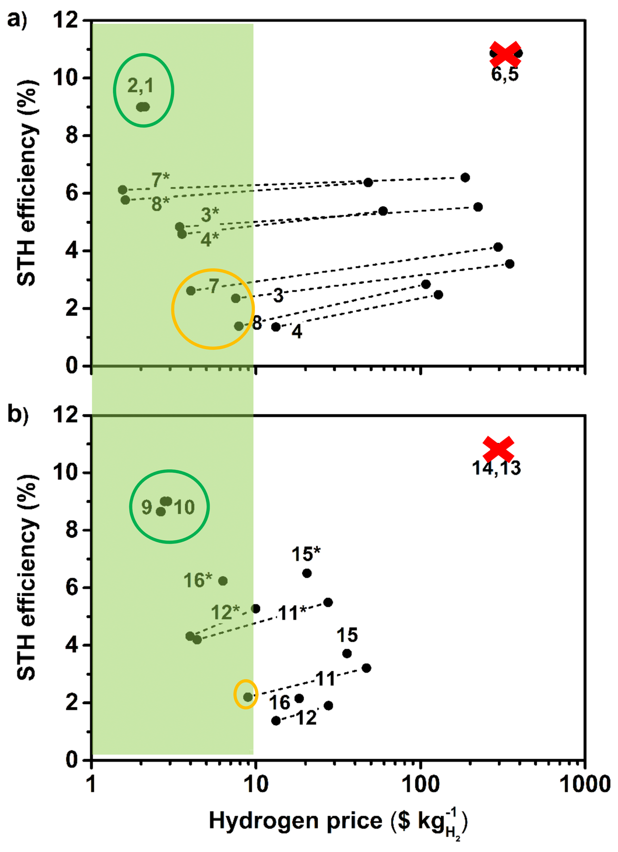



**Fig. 2** *Hydrogen price and STH range for devices 1 to 16. Devices with (*) subscript have a $V_{OC}$ of 2.5V.*

III-V PV-based devices (no. 1+2) have a global optimum in which efficiency, price and energy demand are simultaneously optimized. Proper thermal management allows III-V based device to achieve best performance and lowest price under concentrated irradiation.

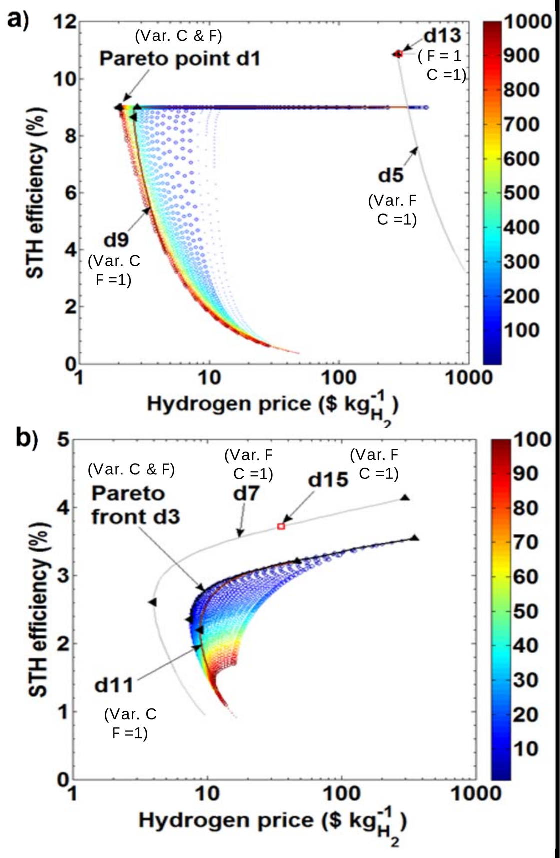



**Fig. 3** *Pareto plots for efficiency and price optimization for PV material made of (a) III-V, or (b) thin film Si.*

**Devices studied (number code used):**

| Concentrator | PV cell | Varying F - Catalysts | | F = 1 - Catalysts | |
|---|---|---|---|---|---|
| | | $RuO_2$/Pt | $Co_3O_4$/Ni | $RuO_2$/Pt | $Co_3O_4$/Ni |
| Yes | III-V | 1 | 2 | 9 | 10 |
| (varying C) | Silicon | 3 | 4 | 11 | 12 |
| No | III-V | 5 | 6 | 13 | 14 |
| (C = 1) | Silicon | 7 | 8 | 15 | 16 |

## Results – Multi-physics modeling

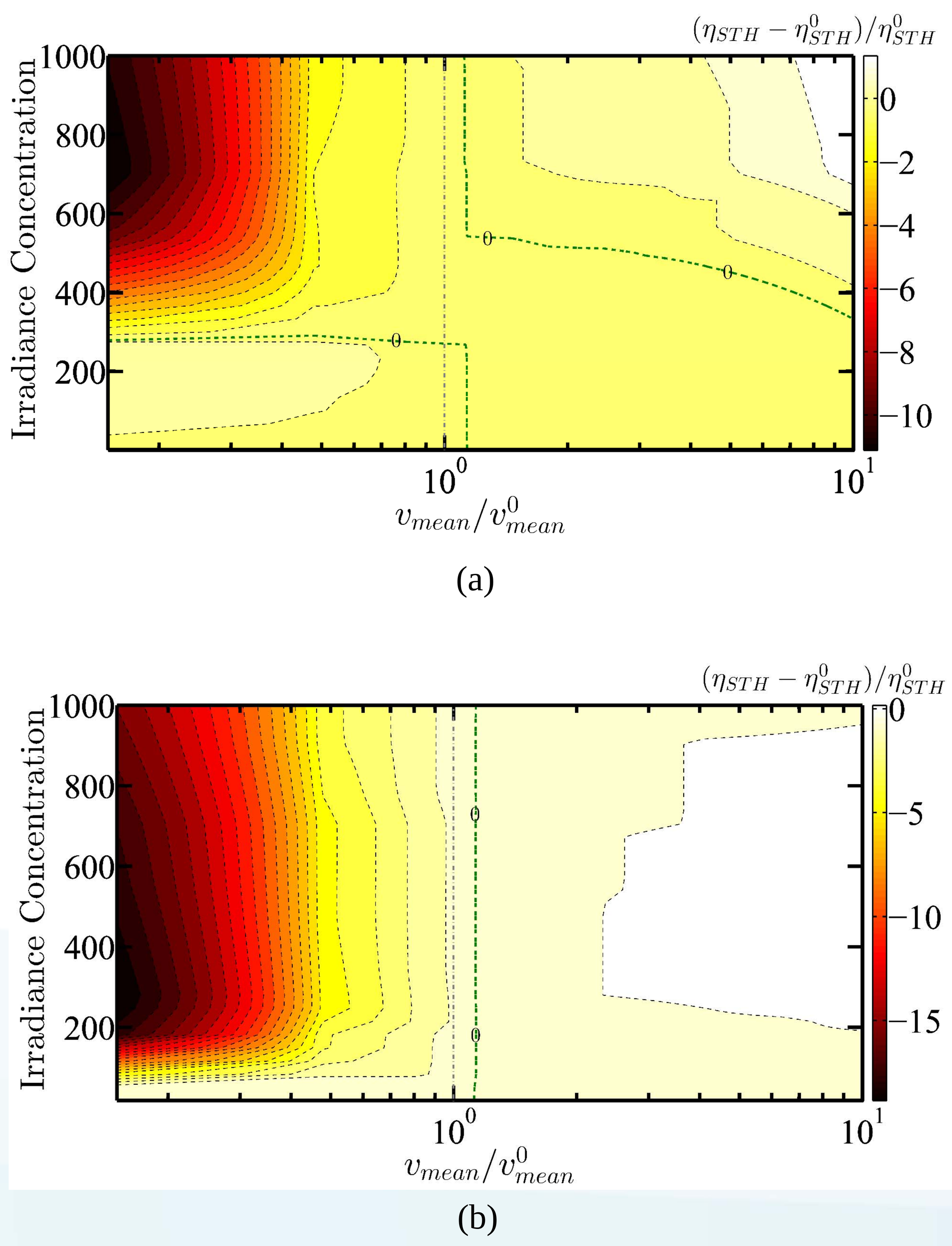
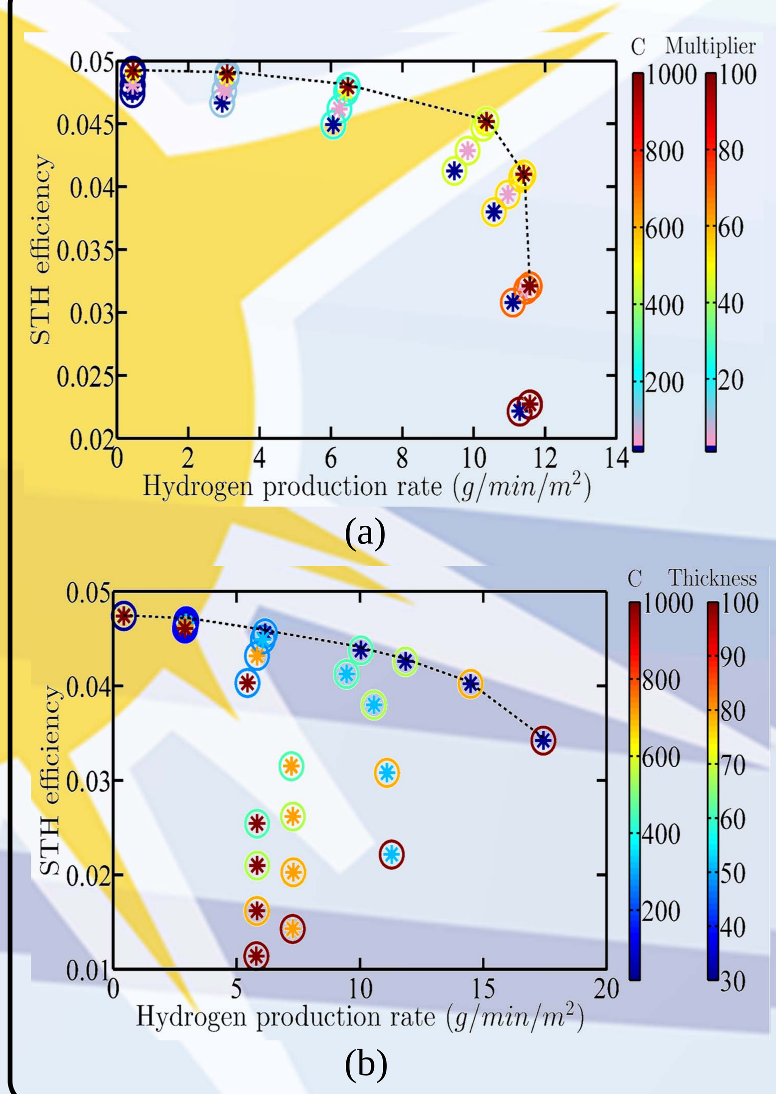



**Fig. 4** *Contour plots showing STH efficiency degradation/enhancement w.r.t the reference case for (a) aSi-ucSi-ucSi thin film triple junction and (b) $Ga_{0.51}In_{0.49}P$-GaAs dual junction solar cell based device. The reference velocity, $v^0_{mean}$, is 0.2m/s.*

The mass flow rate plays an integral role in thermal management in the integrated device. The integrated PEC can be operated without significant decrease in performance, even at very high concentrations, provided the water flow velocity in the cooling channel is at least 0.2 m/s.



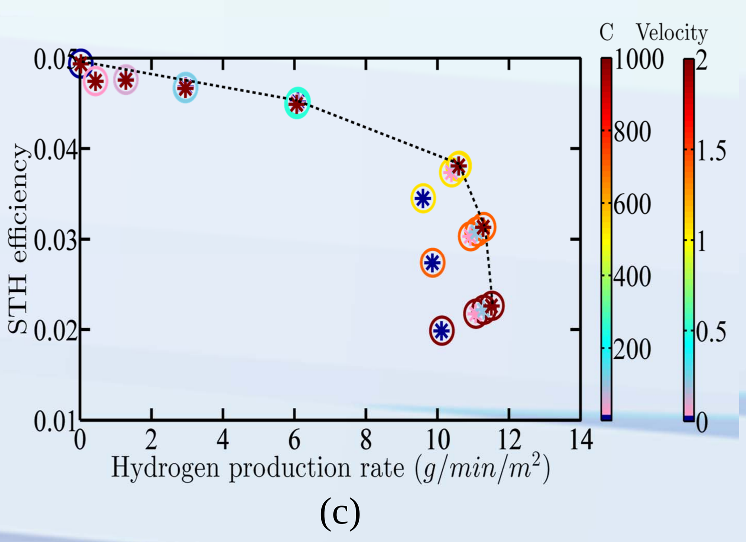
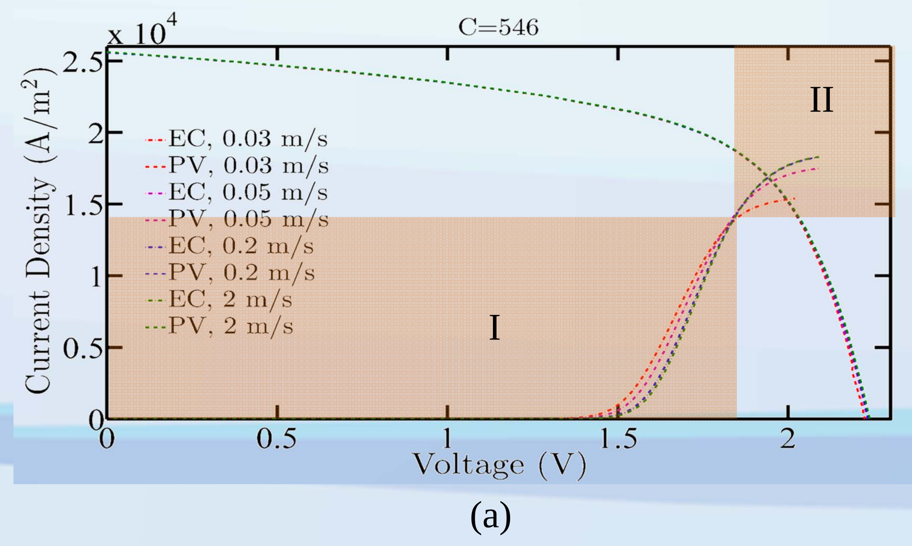




**Fig. 5** *Pareto fronts showing semi-optimal efficiencies for (a) exchange current density (b) Nafion membrane thickness, and (c) mass flow rate analysis. The* **circles** *represents C and* **stars** *represents (a) exchange current multiplier, (b) membrane thickness in um, and (c) mean flow velocity in m/s.*

Aim = Efficiency increased Hydrogen production

High irradiation concentration operated with $v_{mean}$ = 0.2 m/s

Nafion thickness = 30um
Cat. thickness = 200nm
GDL thickness = 300um
ASSA= $10^5$ m$^{-1}$



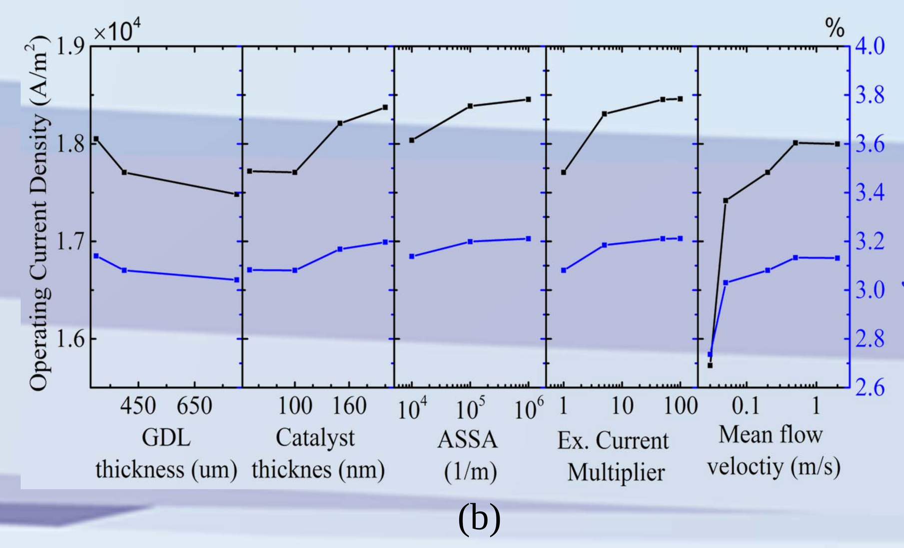




**Fig. 6** *(a) J-V curves for C = 546 showing formation of characteristic operation regions I and II. (b) Operating current density and STH efficiency variations with various operational, dimensional, and material parameters.*

Region I is characterized by temperature effects and region II by mass transport limitations. The objective functions show a saturating trend for various parameters.

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## References


[1] S. Tembhurne et al., 15th International Heat Transfer Conference, Kyoto, Japan, 2014. [2] M. Dumortier et al., Energy and Environmental Science, 2015 .


## Conclusion

Devices using concentrators and III-V based PV cells show the best tradeoff between profitability, sustainability, and efficiency.

When operating in region II, the mass flow rate allows for controlling of the operating point and acts as a controlling parameter to counteract degradation effects. Smart thermal management - which is possible due to the integrated nature of our device design - helps significantly in designing a system with a stabilized and high performance for an elongated fraction of the system lifetime.