Modelling, experimentation and scaling of solar hydrogen generation devices

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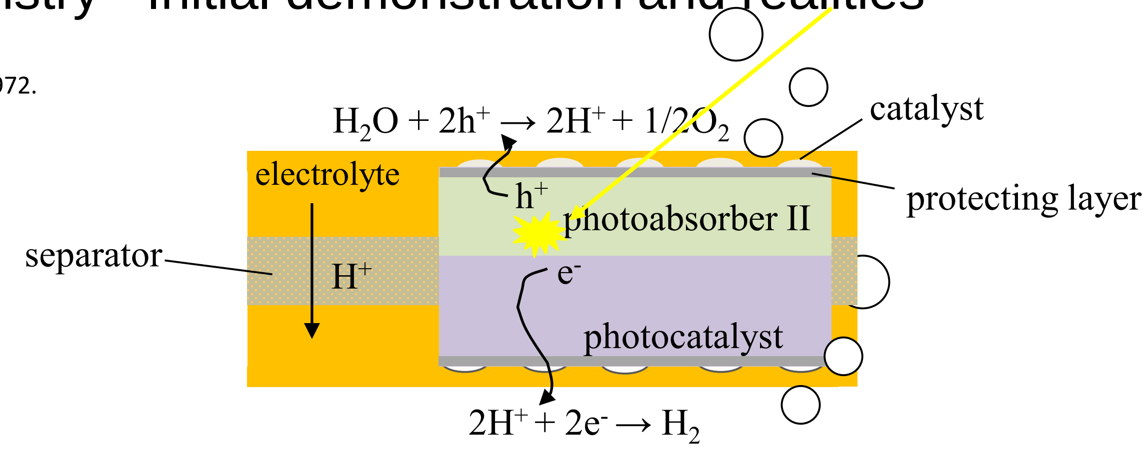
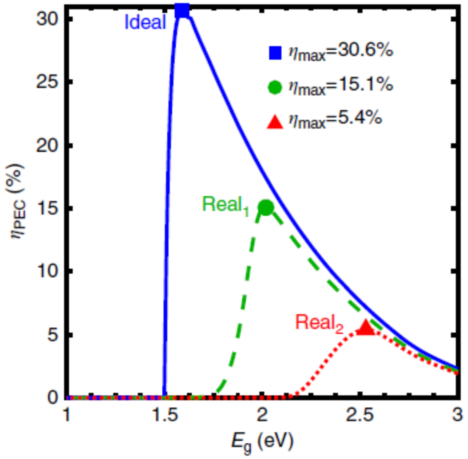
Photo-Electrochemical Approach

- Photoelectrochemistry - Initial demonstration and realities

Fujishima et al., *Nature*, 238, 1972.

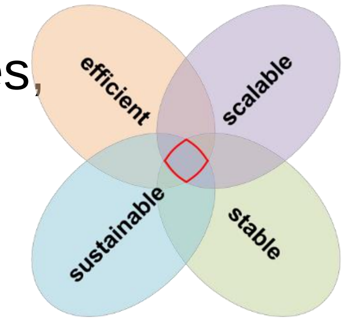


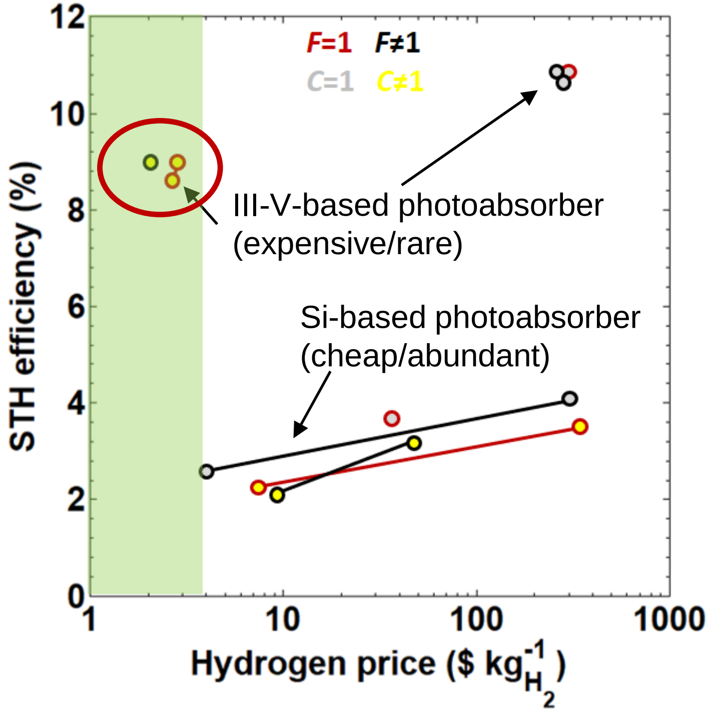


Fountaine et al., *Nature Com.*, 7, 2016

- Stringent material requirements hinder implementation
→ Functional decoupling into multiple materials

- Challenges: Component integration for practical devices, few successful implementations





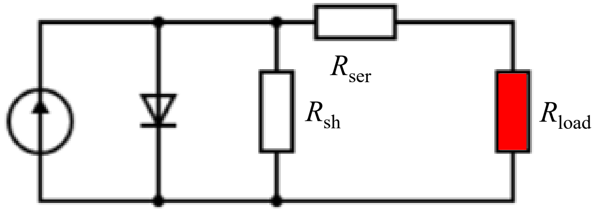
- Economic driver: Requires ***high power density***
→ Achieved through irradiation concentration
→ Thermal management critical

Dumortier, Tembhurne, Haussener, *Energy Environ Sci*, 8, 2015; http://specdo.epfl.ch

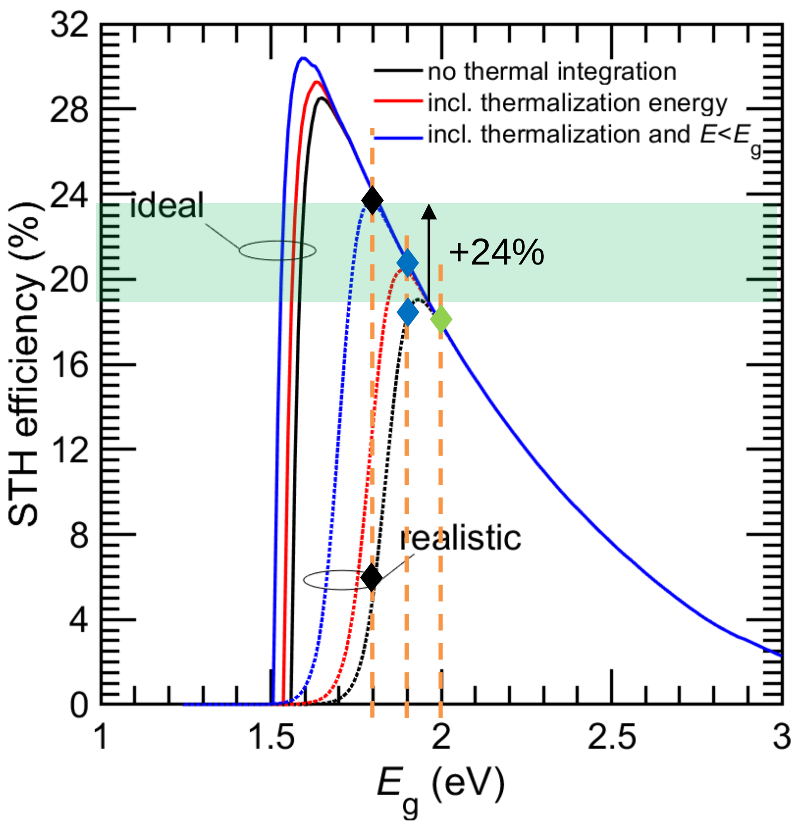
Thermal Integration

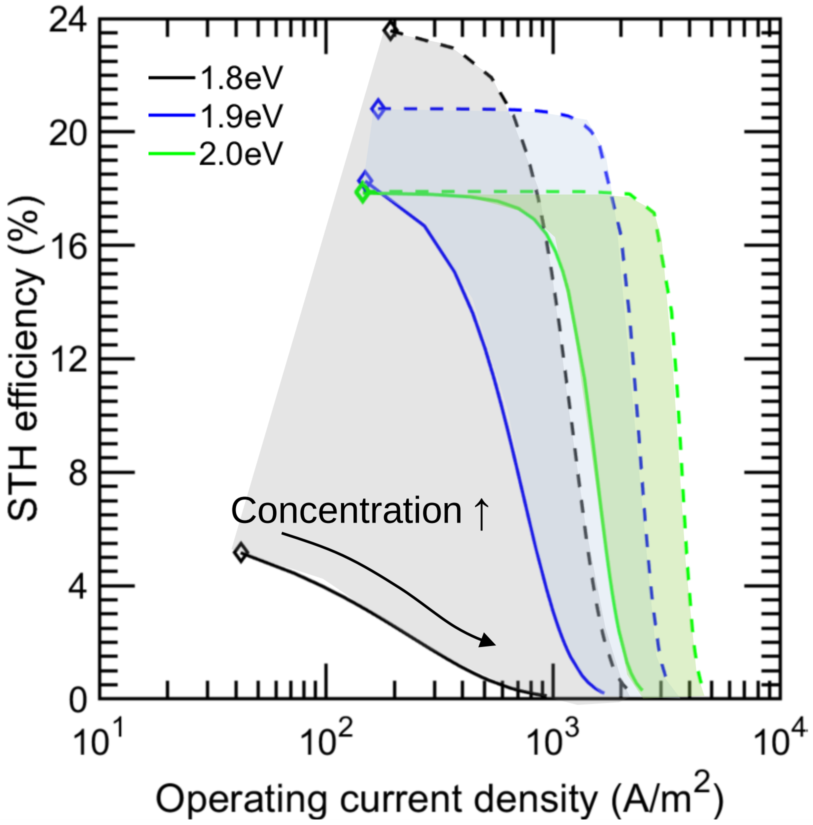
- Engineering to go beyond the perceived limits:

Tembhurne, Nandjou, Haussener, *Nature Energy*, doi: 10.1038/s41560-019-0373-7, 2019



Solid lines: no thermal integration
Dashed lines: with thermal integration

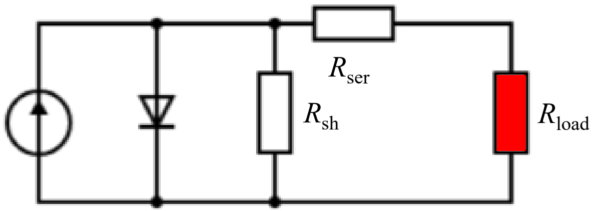




High electrochemical and power densities enabled by thermal integration

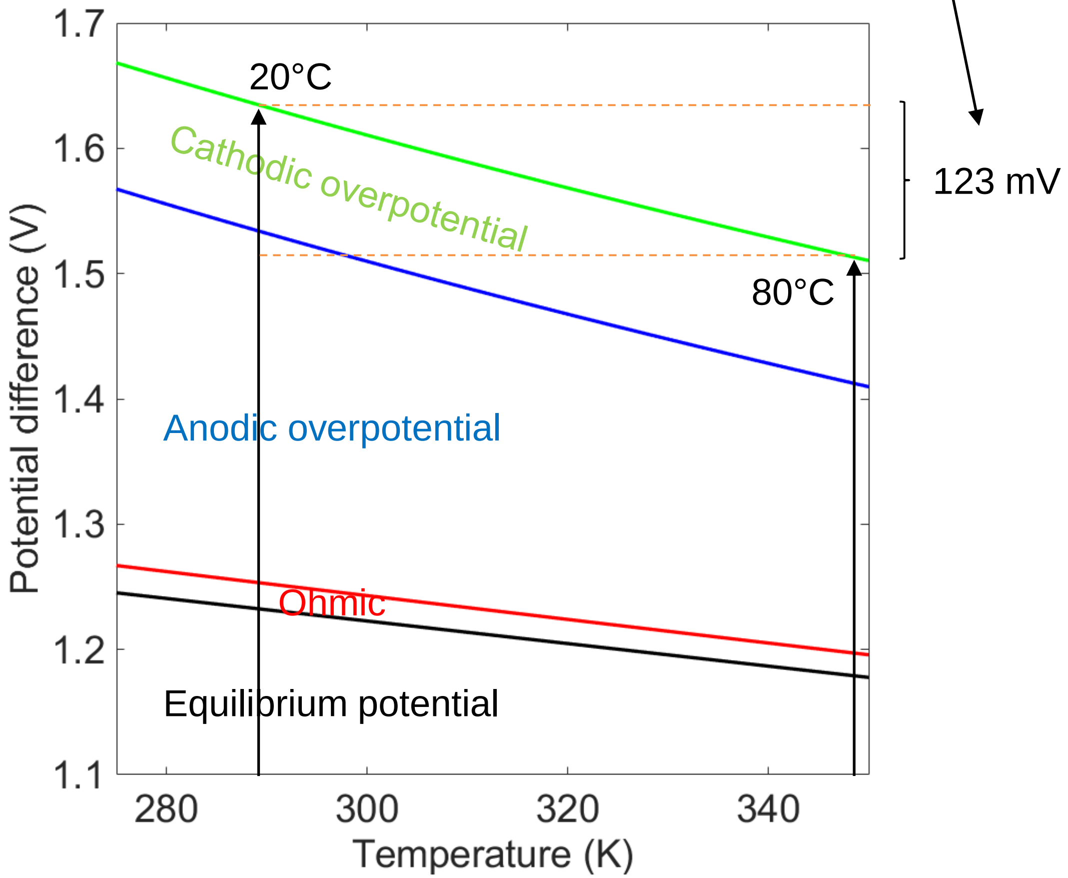
Thermal Integration

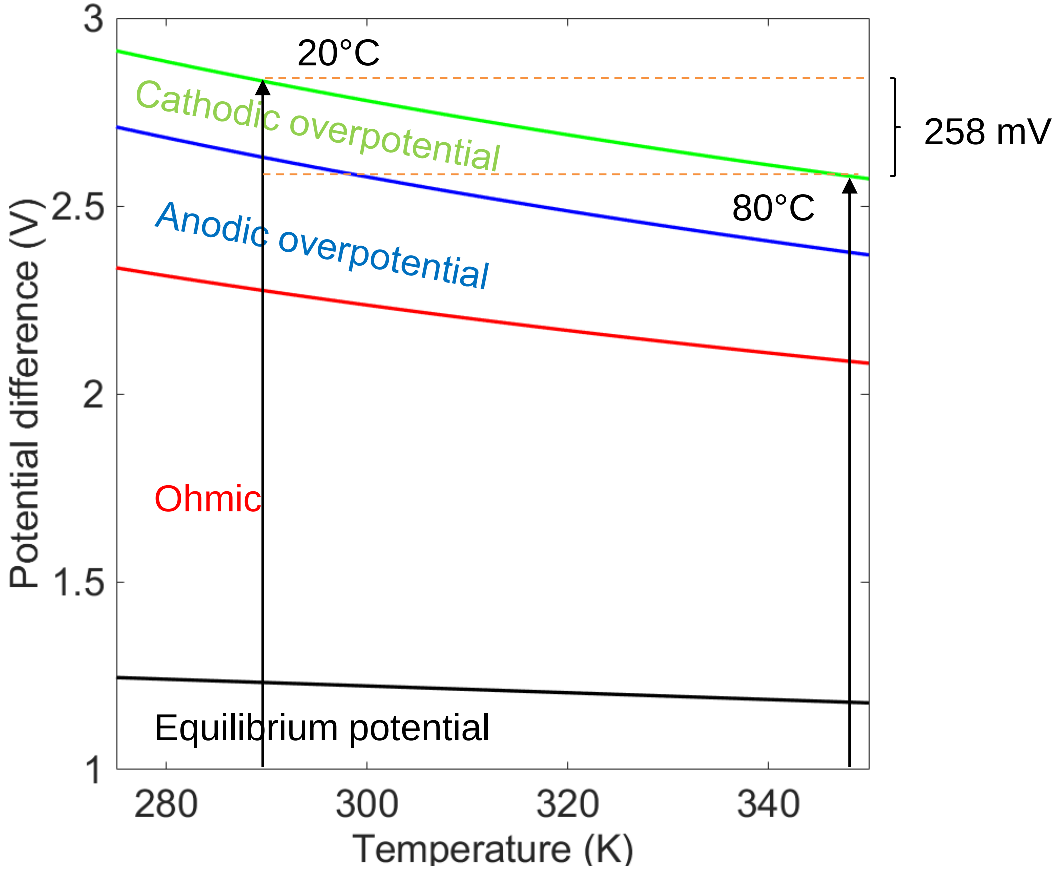
- Thermal benefit



@ 20 mA/cm^2

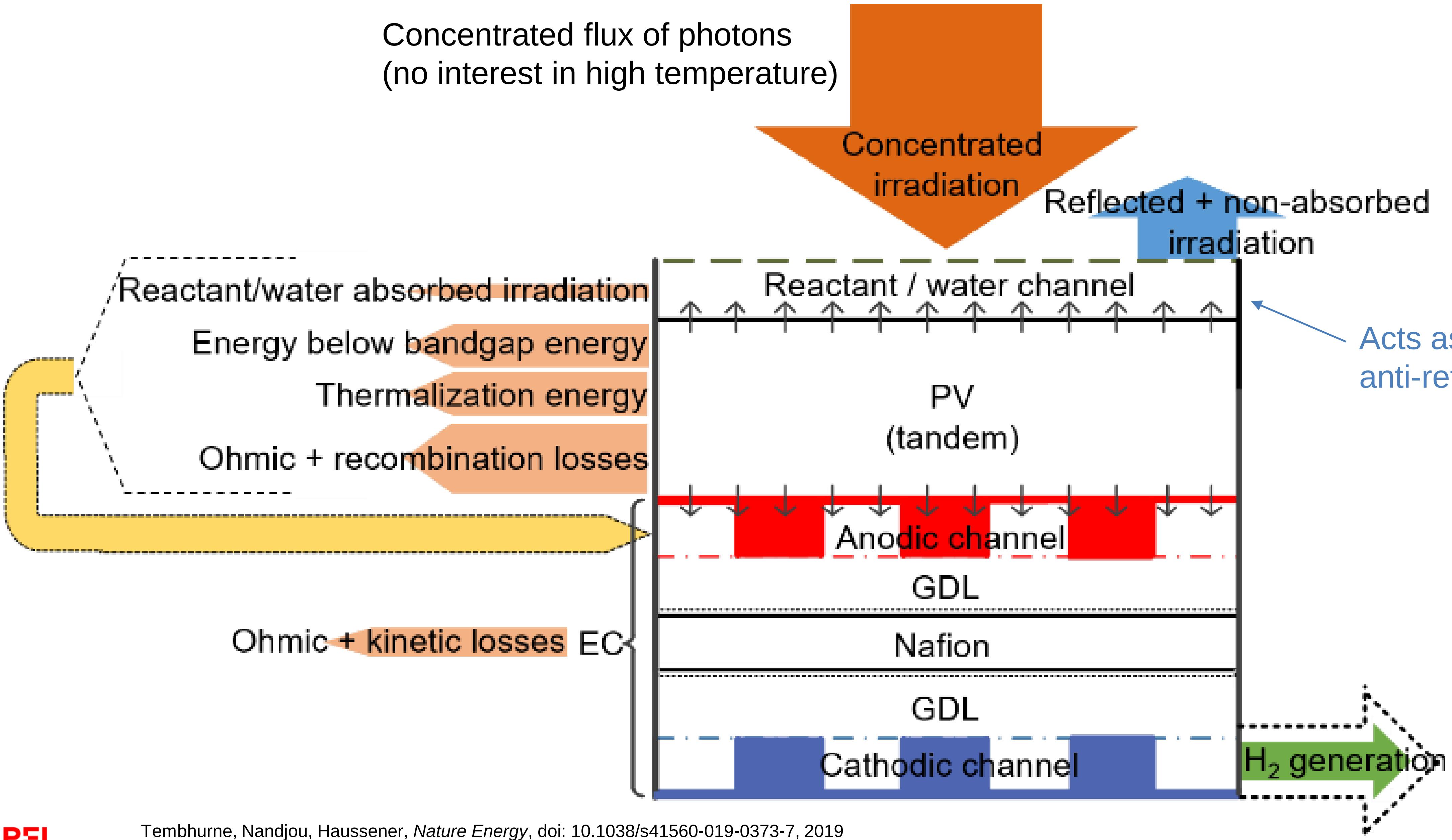
A decade of catalysis research





Conceptual Device Design

Concentrated flux of photons
(no interest in high temperature)



Acts as
anti-reflection coating

Tembhurne, Nandjou, Haussener, *Nature Energy*, doi: 10.1038/s41560-019-0373-7, 2019

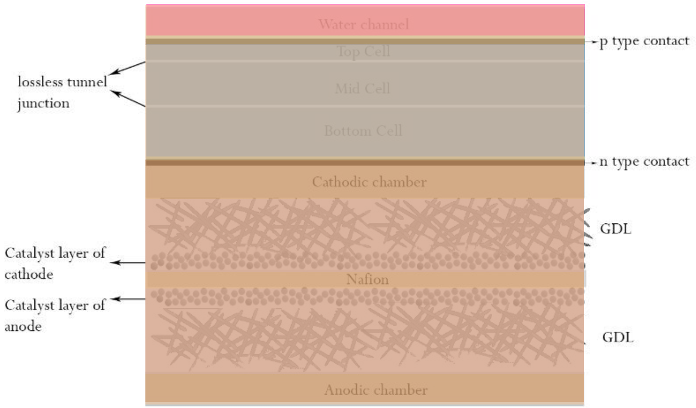
2D Modeling

- How to design a device that has never been considered before?
  → Coupled multi-physics simulations

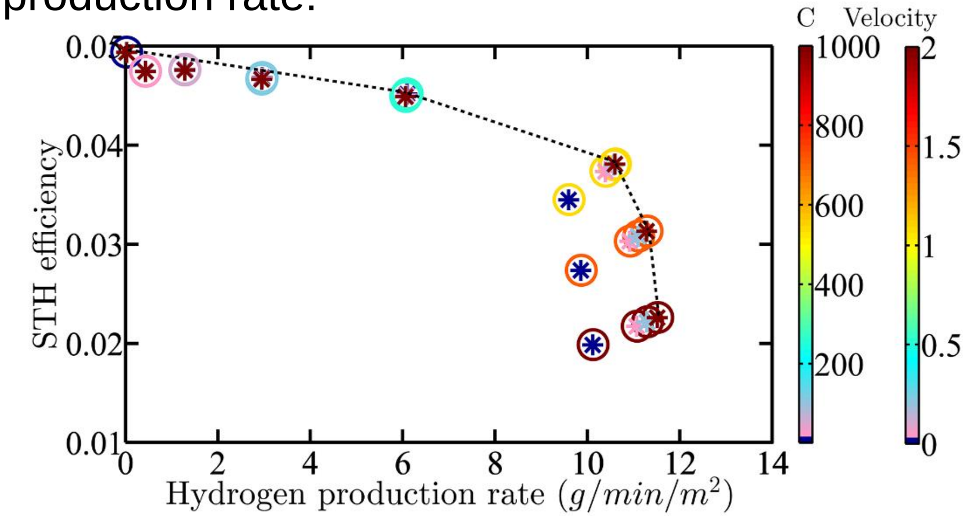
Electromagnetic wave propagation
Semiconductor charge conservation / transfer
Electrodes/electrolyte charge conservation / transfer
(Reactive) fluid flow
Energy conservation / heat transfer

$$\rho C_p \mathbf{u} \cdot \nabla T = \nabla \cdot (k_{th} \nabla T) + Q$$

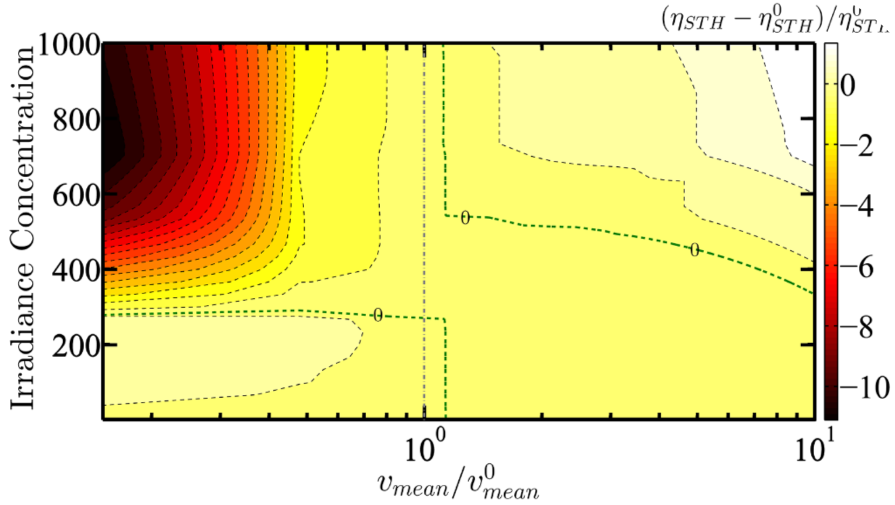
$$Q = Q_W + Q_{TH} + Q_R + Q_M + Q_{PV} + Q_{EC}$$



Efficiency vs. production rate:



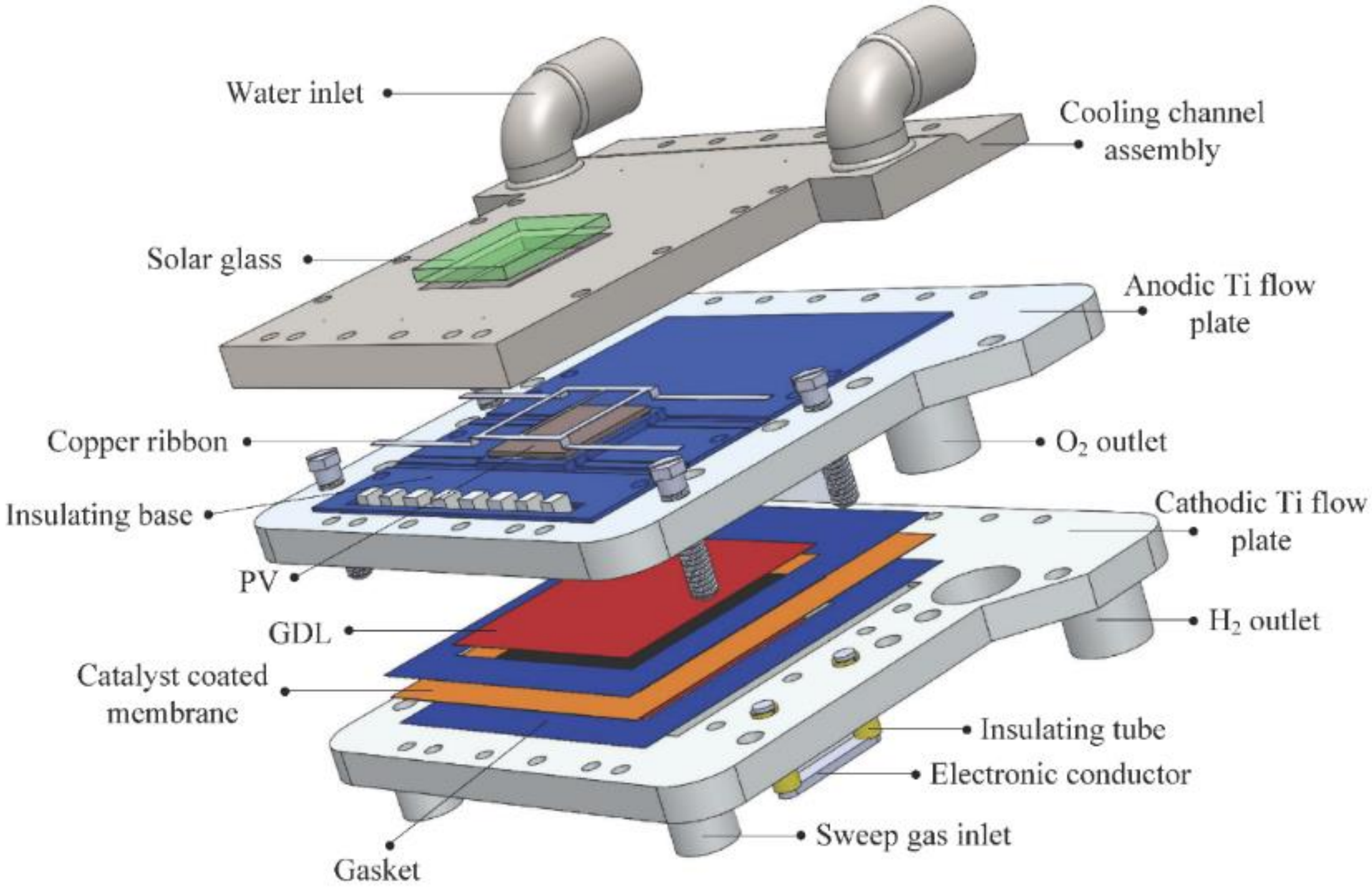
Efficiency improvement for varying operating conditions:

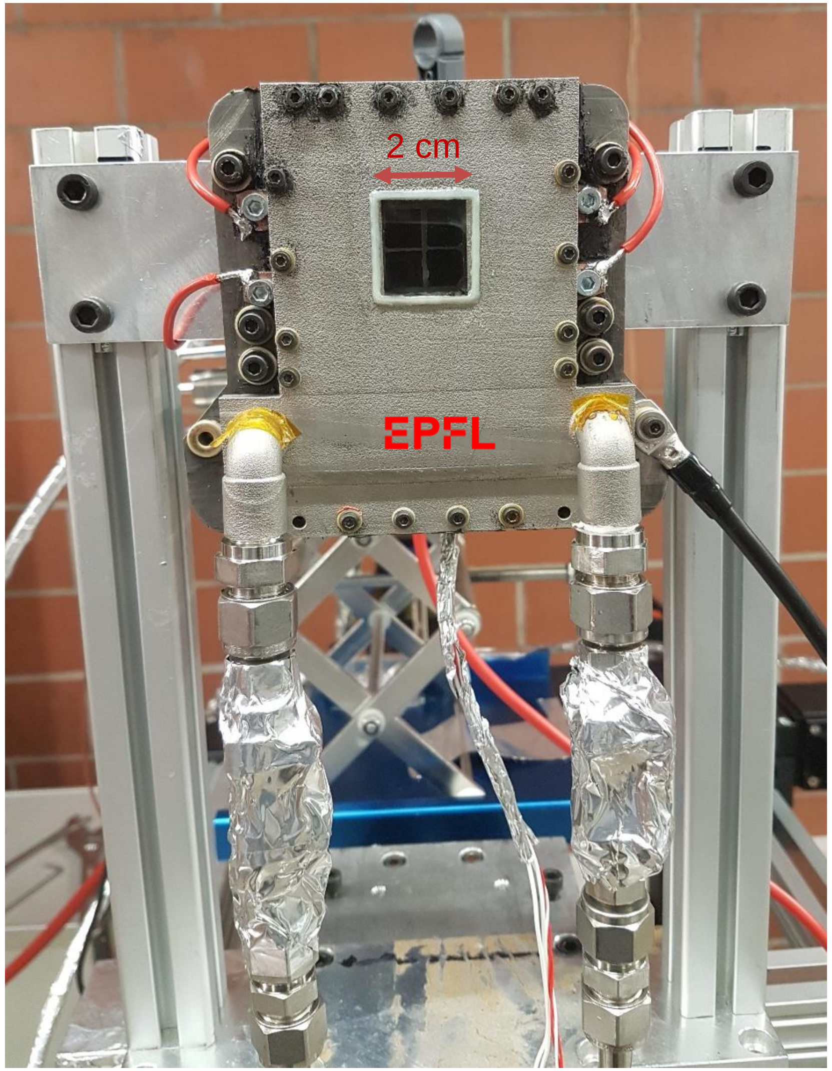


Tembhurne, Haussener, *JECS*, 163, 2016

CPEC Design

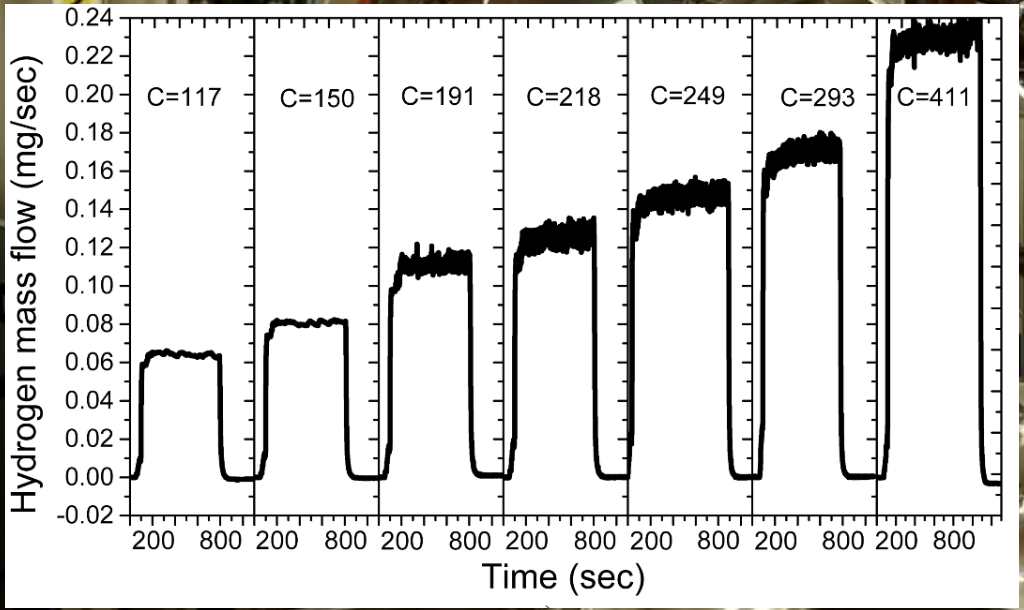
- Implementation:





US Patent 62/376923
EP Patent 16020308.9

Tembhurne, Nandjou, Haussener, *Nature Energy*, doi: 10.1038/s41560-019-0373-7, 2019



Output power of PEC at 474 kW/m^2: 27 W

Current density in electrolyzer component: 0.88 A/cm^2

Current density in photoabsorber component: 6.04 A/cm^2

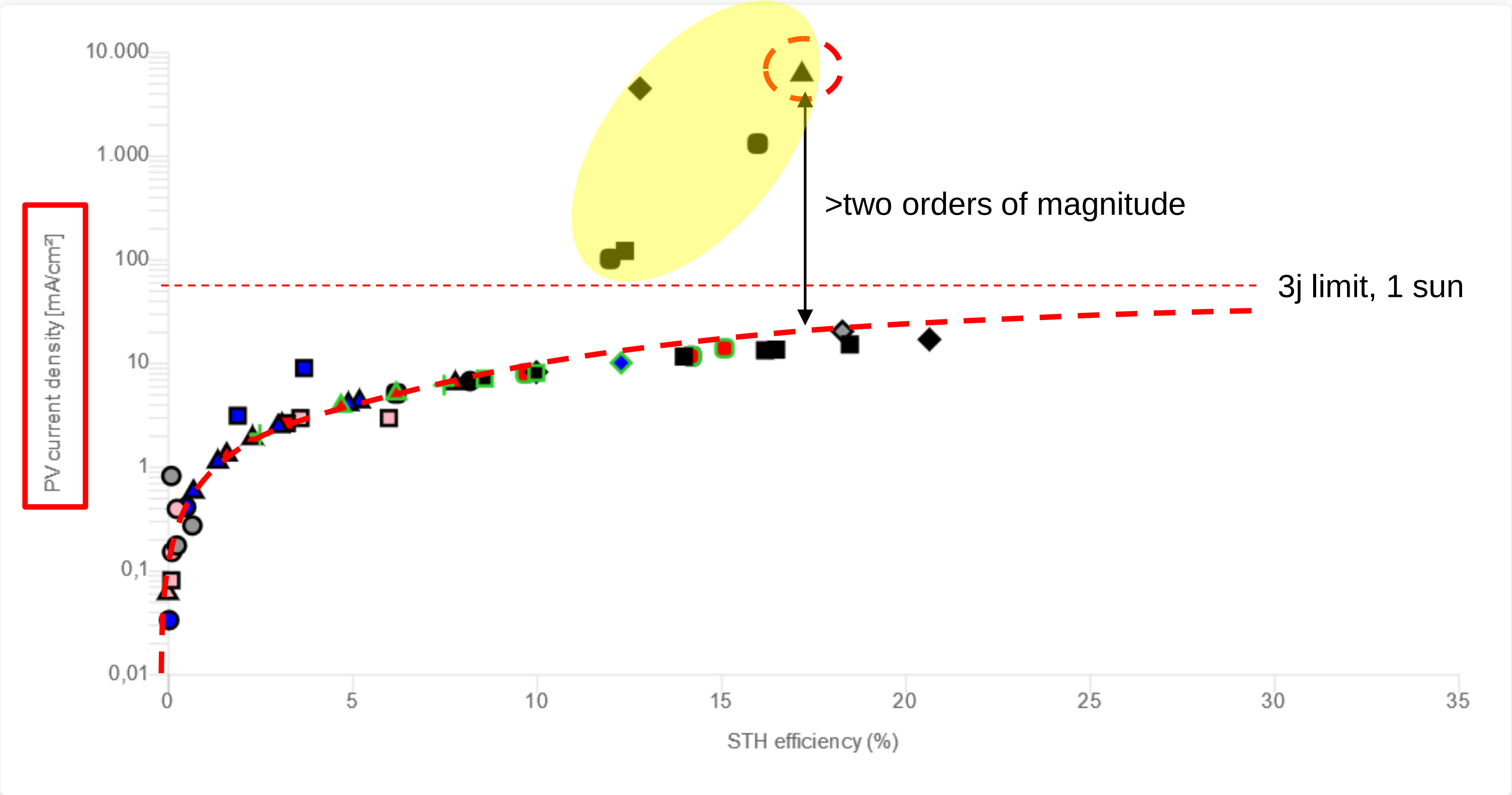
Efficiency: 17.1% solar-to-fuel

Tembhurne, Nandjou, Haussener, *Nature Energy*, doi: 10.1038/s41560-019-0373-7, 2019

Leveque, Bader, Lipinski, Haussener, *Optics Express*, 24, 2016

Comparison

- Dynamic and online tool: – http://specdc.epfl.ch/



w/o multi-module demonstrations
w/o multiple electrolyzer demonstrations

LEGEND

Fill color - PV / photoabsorber material	Boundary color - EC material	Symbol shape - PV / photoabsorber and EC configuration	
All III-V	Rare metal-based (expensive)	○ 2J, integrated PVs and catalyst	+ 3J, integrated PVs and catalyst
Partial III-V	Abundant (cheap)	□ 2J, integrated PVs, wired catalyst	△ 3J, integrated PVs, wired catalyst
All Si		◇ 2J, non-integrated PVs or catalyst	O 3J, non-integrated PVs or catalyst
Partial Si			
Oxides and others			

EPFL

Tembhurne, Nandjou, Haussener, *Nature Energy*, doi: 10.1038/s41560-019-0373-7, 2019

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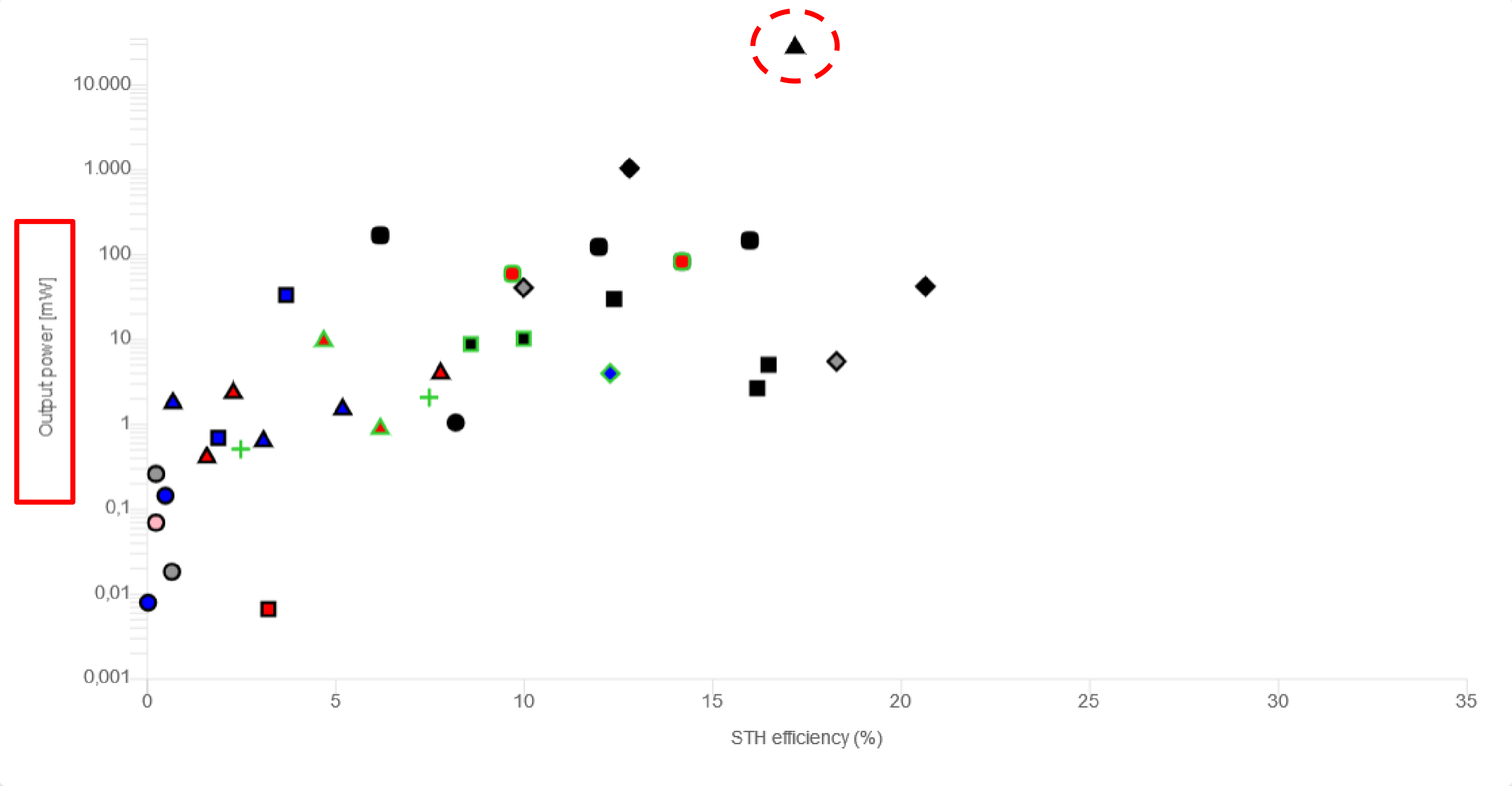

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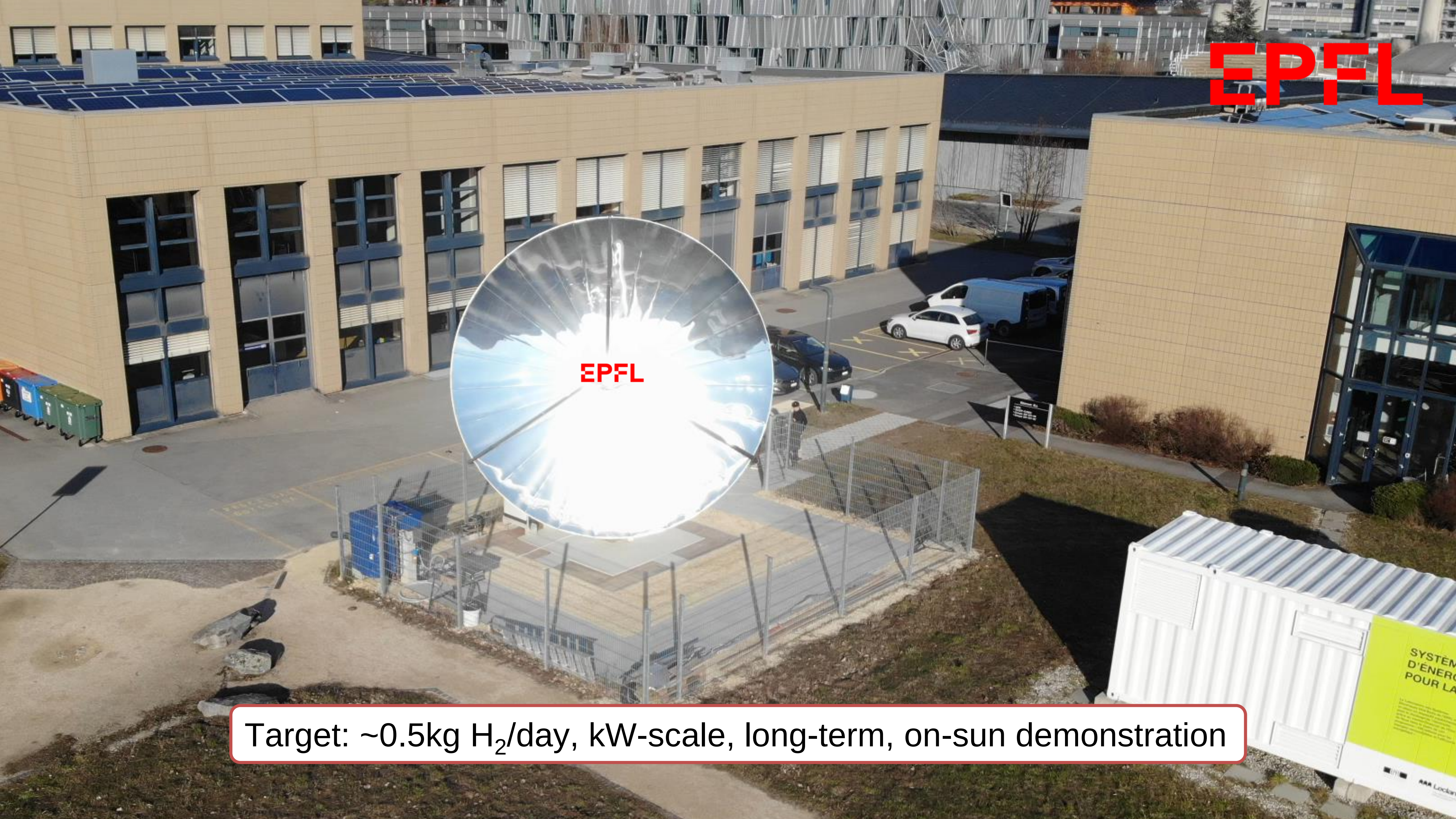
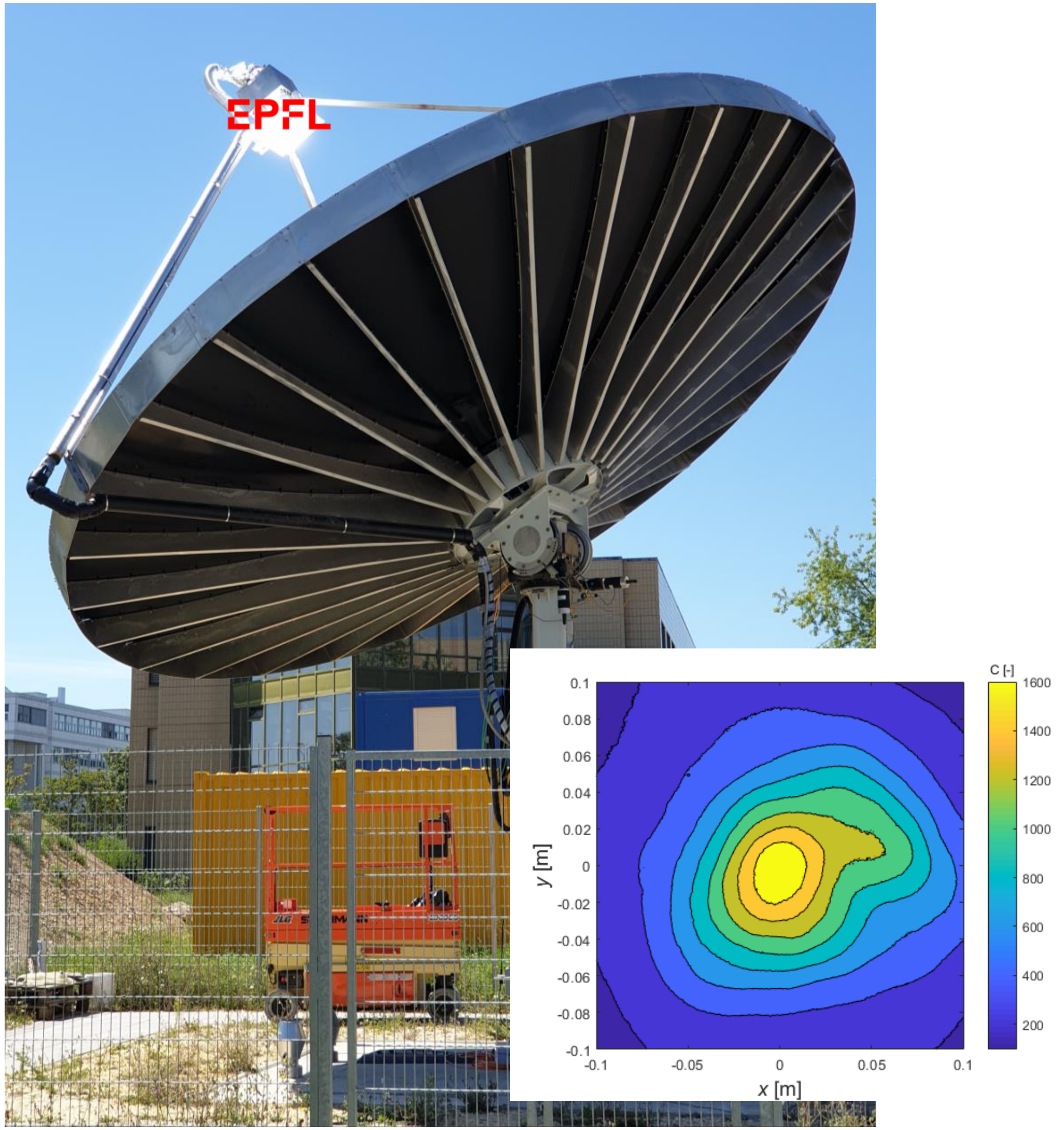


Target: ~0.5kg H_2/day, kW-scale, long-term, on-sun demonstration

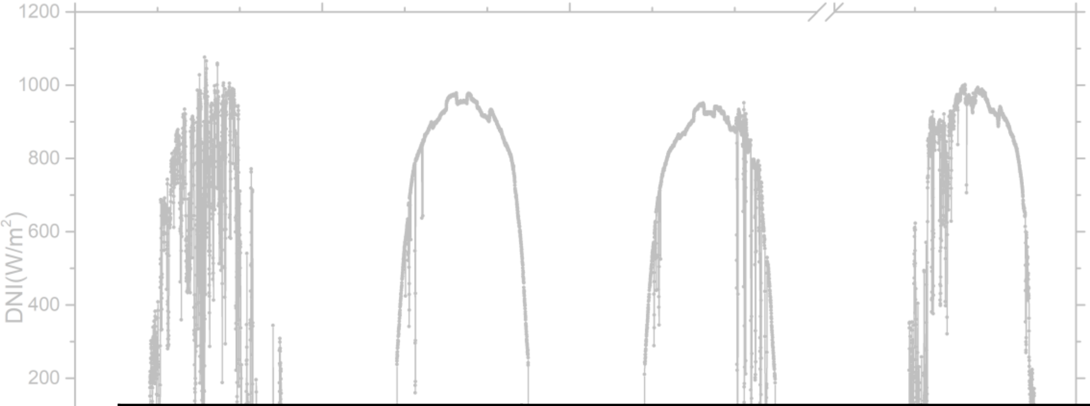
Reactor and System in Operation

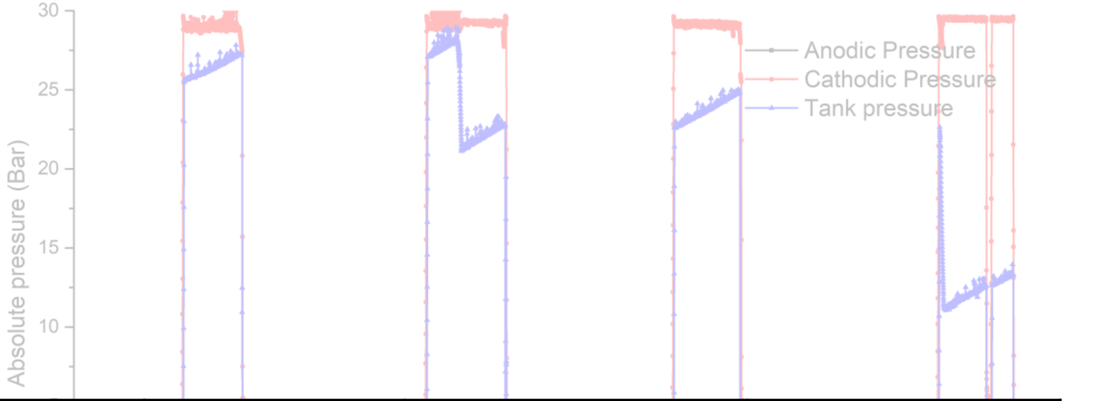


Tembhurne, Holmes-Gentle, Suter, Haussener, in preparation, 2020

Integrated System Test

- Full operation over multiple days in varying meteorological conditions





Date	Average DNI [W/m²]	Operational time [h]	m_{H_2} [kg]	V_{H_2} STP [NL]	Peak rates [NL/min]
19/08/2020	716	5.48	0.24	2940	13.8
20/08/2020	932	7.77	0.46	5680	13.6
21/08/2020	894	6.49	0.36	4510	13.2
24/08/2020	924	7.50	0.44	5450	13.9

Tembhurne, Holmes-Gentle, Suter, Haussener, in preparation, 2020

Dynamic Process Model

- Generic system model developed in gPROMS ModelBuilder, parameters inspired by our installation

Electrolyser stack

$$\eta_{\text{kinetic}} = \frac{RT_{\text{EC}}}{\alpha_{\text{ano}} n_e F} \ln\left(\frac{i_{\text{cell}}}{i_{\text{o,ano}}}\right) + \frac{RT_{\text{EC}}}{\alpha_{\text{cat}} n_e F} \ln\left(\frac{i_{\text{cell}}}{i_{\text{o,cat}}}\right)$$

$$\sigma_{\text{m}} = (0.00514\lambda_{\text{m}} - 0.00326) \exp\left(1268\left(\frac{1}{303} - \frac{1}{T_{\text{EC}}}\right)\right)$$

$$C_{\text{EC}} \frac{dT_{\text{EC}}}{dt} = Q_{\text{gen}} - Q_{\text{loss}} - Q_{\text{fluid,a}} - Q_{\text{fluid,c}}$$

$$\frac{dM_i}{dt} = x_{\text{inlet},i}\dot{m}_{\text{inlet}} - x_{\text{outlet},i}\dot{m}_{\text{outlet}} + M_{w,i}\nu_i R_{\text{rxn}}$$

$$\Delta P = K_{\text{flow}} \left(\frac{Q_L}{N_{\text{EC},s}}\right)^{a_{\text{flow}}}$$

Solar dish

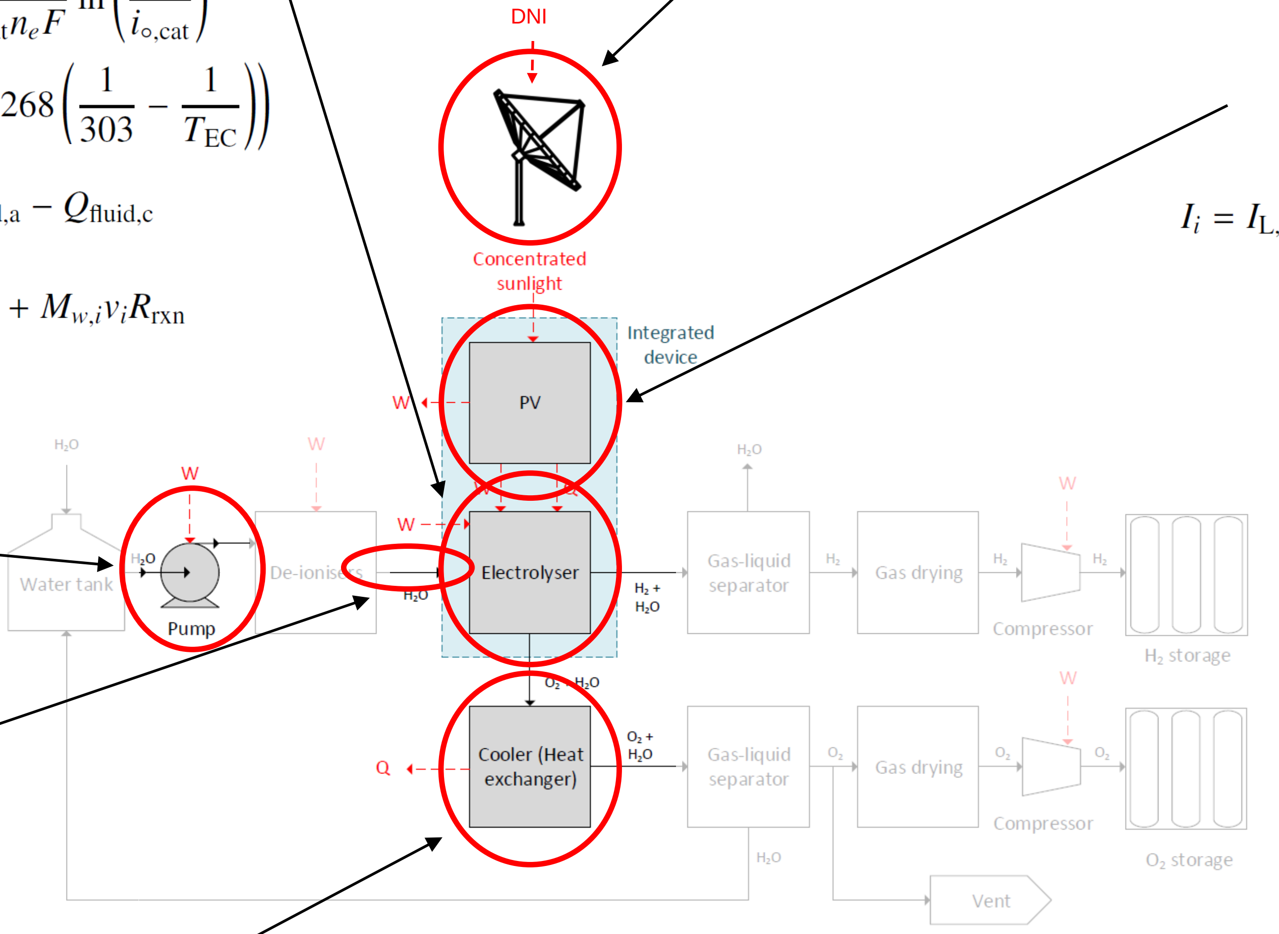
$$Q_{\text{solar}\to\text{CPV}} = \overbrace{\rho_{\text{s}}\gamma_{\text{dish}}\eta_{\text{clean}}}^{\eta_{\text{opt}}} A_{\text{dish}} \times \text{DNI}$$

CPV module

$$I_i = I_{\text{L},i} - I_{o,i}\left[\exp\left(\frac{q(V_i + I_i R_{\text{s},i})}{n_i k_{\text{B}} T_{\text{PV}}}\right) - 1\right] - \frac{V_i + I_i R_{\text{s},i}}{R_{\text{sh},i}}$$

$$0 = f_{\text{abs}} P_{\text{total}} - V_{\text{PV}} I_{\text{PV}} - Q_{\text{PV}\to\text{HS}}$$

$$C_{\text{HS}} \frac{dT_{\text{HS}}}{dt} = Q_{\text{PV}\to\text{HS}} - Q_{\text{HS}\to\text{CW}} - Q_{\text{HS}\to\text{amb}}$$



Pump

$$P_{\text{pump}} = \frac{\Delta P_{\text{sys}} F_{\text{pump}}}{\eta_{\text{pump}}}$$

Pipes

Heat exchanger

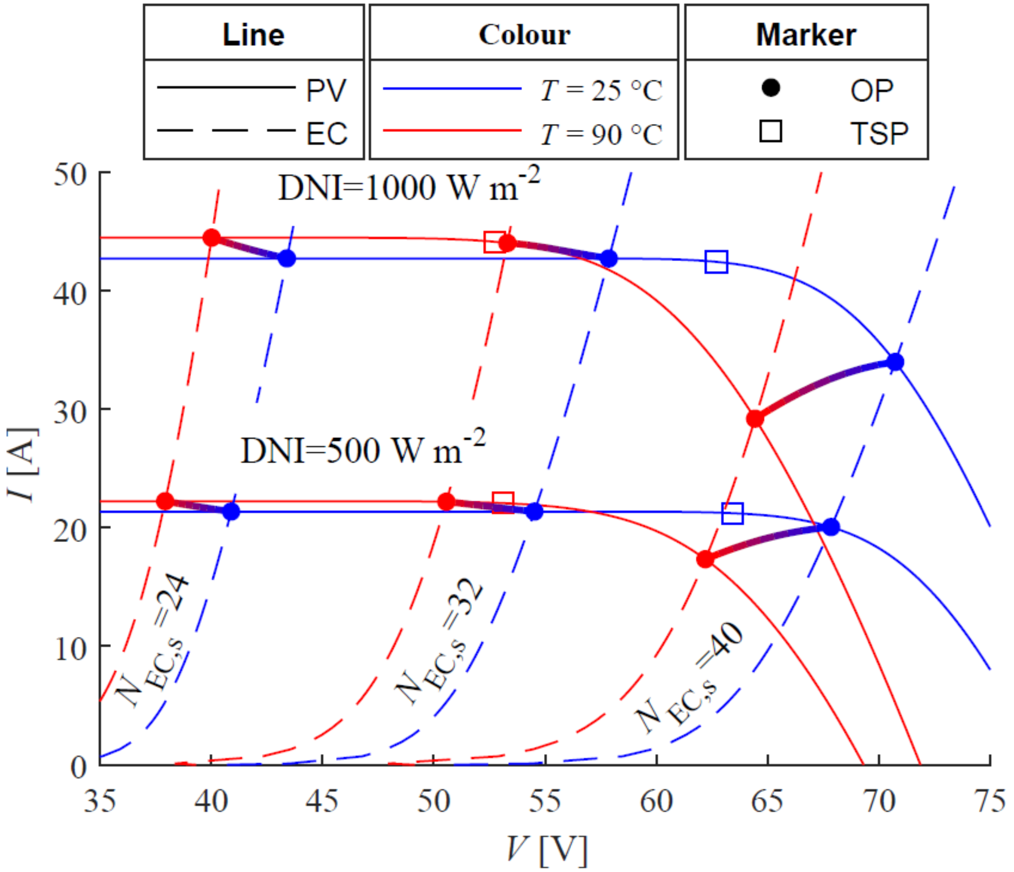
$$\text{NTU} = \frac{\eta_{\text{o}} U_{\text{HS}\to\text{CW}} A_{\text{HS}}}{c_{p,\text{CW}} \dot{m}_{\text{CW}}}$$

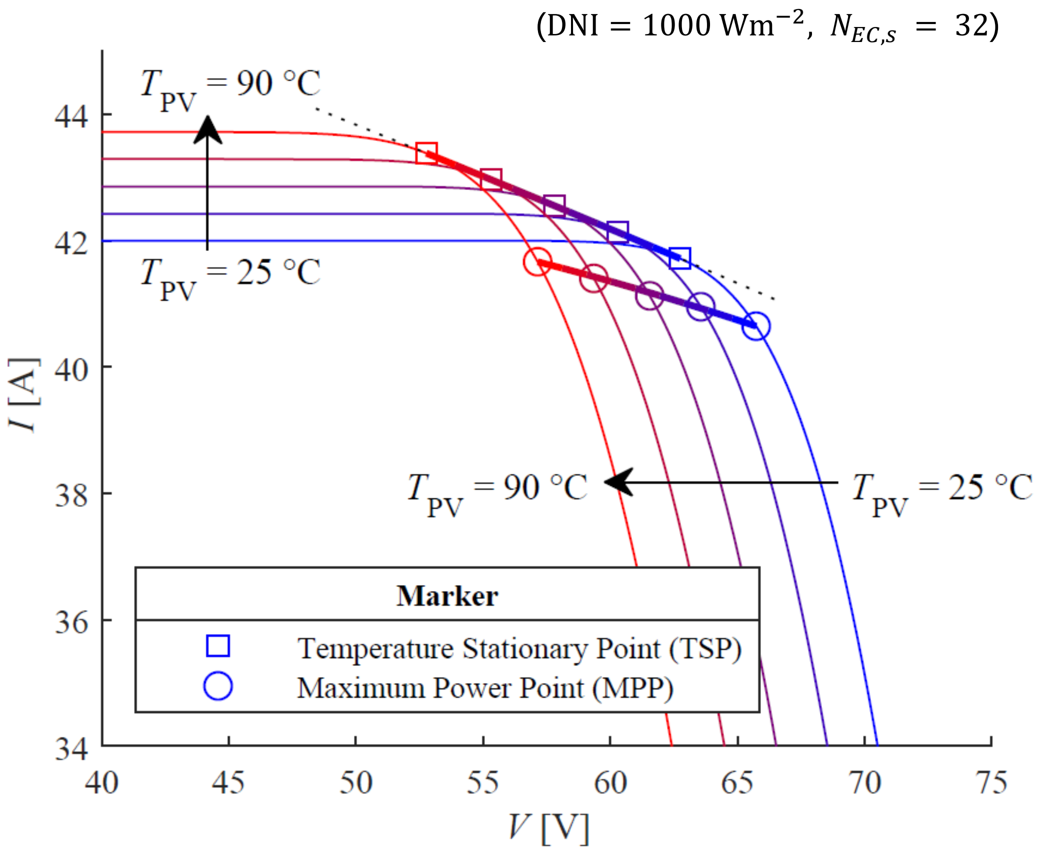
$$\Delta P = f_D \frac{L\rho v^2}{2D_{\text{h}}}$$

Tembhurne, Holmes-Gentle, Suter, Haussener, submitted, 2020

Temperature Dependence of Electrical Models

- Position of operating point heavily dependent on operating temperature (here shown for isothermal case)
- Behavior dependent on position of operating point relative to what we define as the "Temperature Stable Point" of the PV: $\left(\frac{dI_{PV}}{dT_{PV}} = 0\right)$

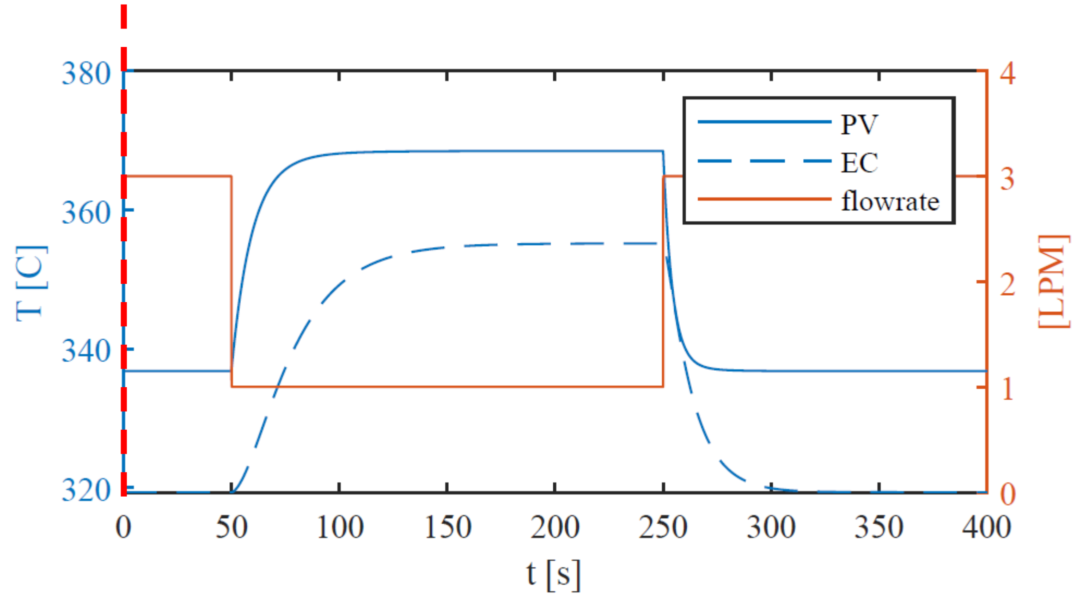


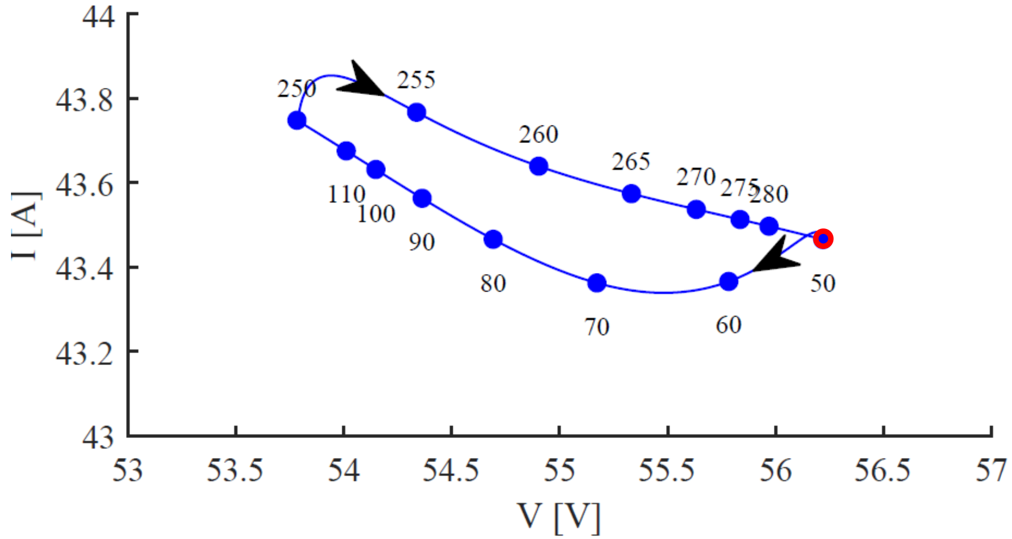


System Dynamics to Step Changes

- Dynamics in the electrical performance of the CPV and the EC originates from the changes in their operating temperatures
- Leads to non-linear behaviour – operating point hysteresis

- Step change in flowrate ($3 \rightarrow 1$ L min^{-1}):





EPFL

SoHHytec
Solar Fuel, the smarter way.

http:\\www.sohhytec.com

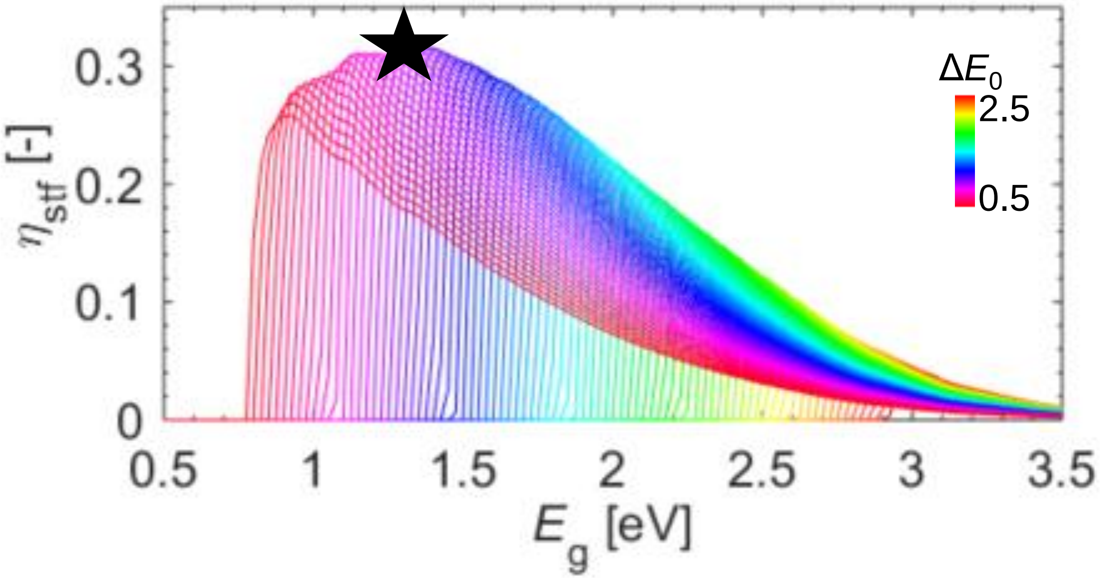
Industry
Steel production
Fertilizer production

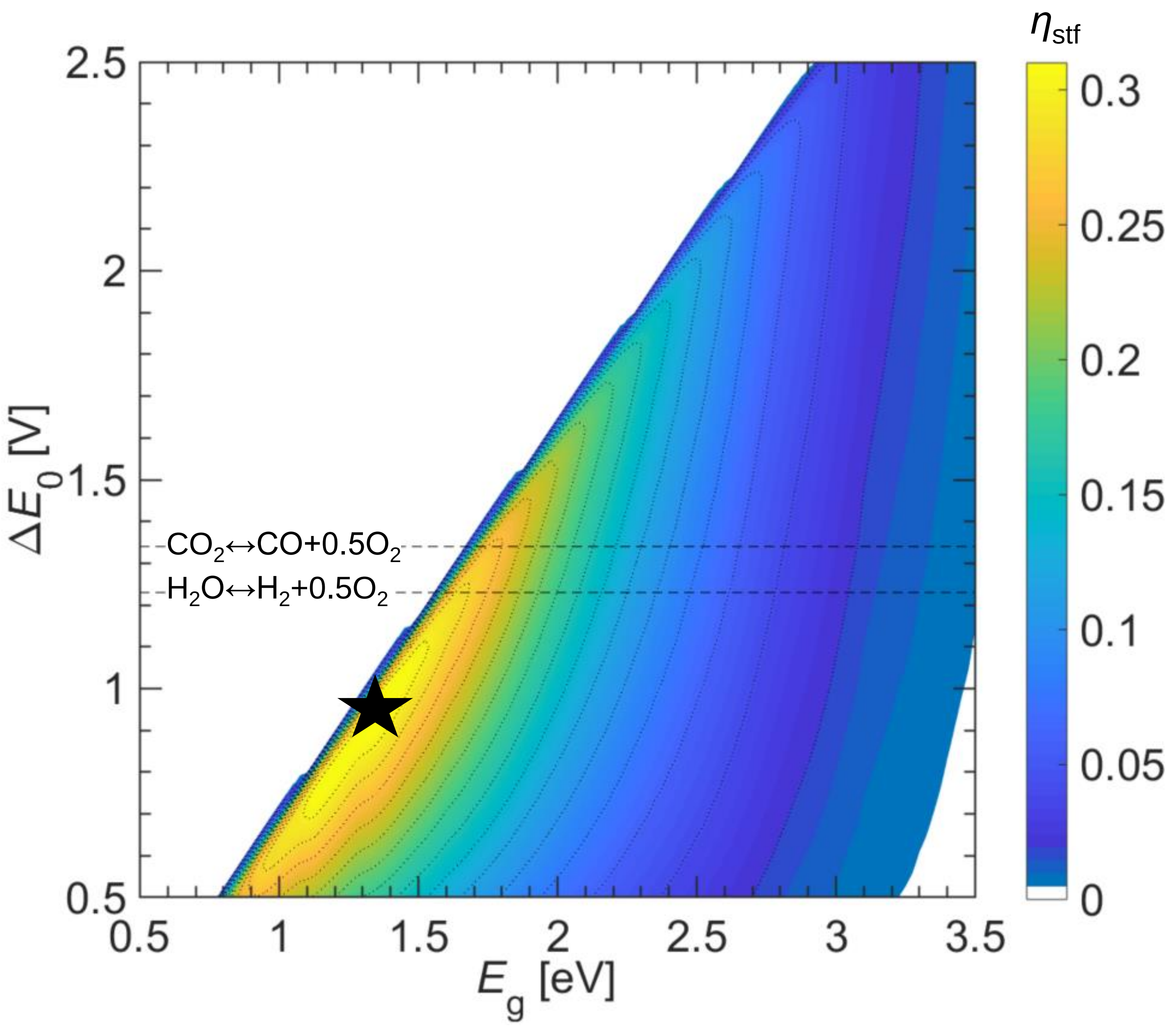
Fuel/Mobility

Electricity/(Seasonal) storage

Beyond water splitting

- Which reactions are interesting?
- Limiting efficiencies:





Global maxima:
η_{STF} = 32% at E_g=1.35eV and ΔE_0=0.96V

Haussener, Suter, Gutierrez Perez, Solar fuel devices: Multi-scale modeling and device design guidelines, Chapter, Springer, 2020

Acknowledgements

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