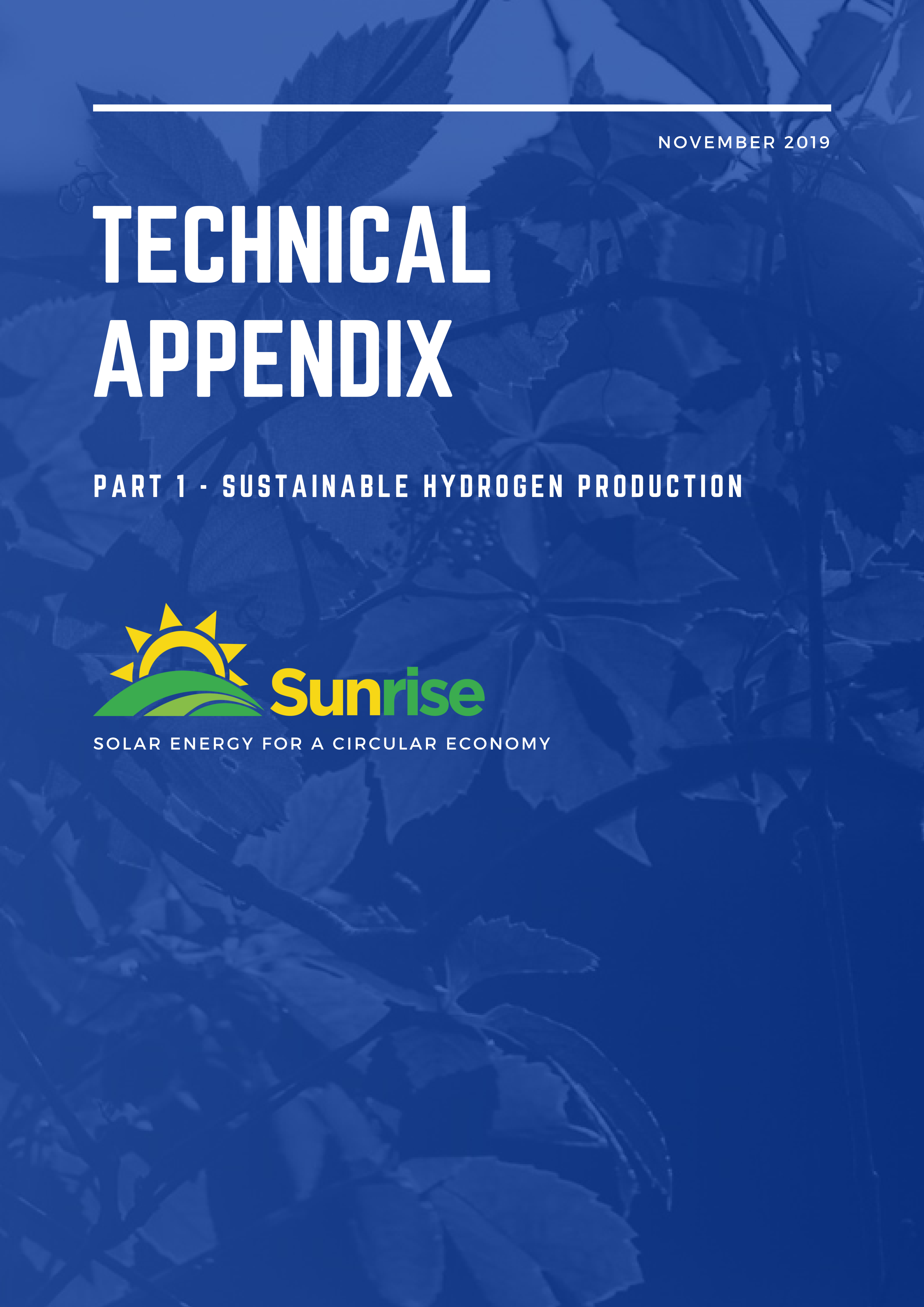


NOVEMBER 2019

TECHNICAL APPENDIX

PART 1 - SUSTAINABLE HYDROGEN PRODUCTION

Sunrise

SOLAR ENERGY FOR A CIRCULAR ECONOMY

SUNRISE

Solar Energy for a Circular Economy

Technological Roadmap

Technical Appendix

Part 1 - Sustainable Hydrogen Production

November 2019

Authors: Carina Faber (UCLouvain), Yagut Allahverdiyeva-Rinne (University of Turku), Vincent Artero (CEA), Laurent Baraton (Engie), Andrea Barbieri (CNR), Hervé Bercegol (CEA), Maximilian Fleischer (Siemens), Han Huynhthi (Engie), Joanna Kargul (Warsaw University), Hélène Lepaumier (Engie), Laura Lopez (ICIQ), Ann Magnuson (Uppsala University), Arne Roth (Fraunhofer)

Contributors: Nicola Armaroli (CNR), Eva-Mari Aro (University of Turku), Stefan Baumann (FZ Jülich), Artur Braun (EMPA), Stefano Cucurachi (Leiden University) James Durrant (Imperial College), Huub de Groot (Leiden University), Leif Hammarström (Uppsala University), Juliette Jouhet (CEA & CNRS), Henrik Koch (NTNU), Jan Mertens (Engie), Marcel Meeus (EMIRI), Robert Potter (Johnson Matthey), Martin Roeb (DLR), Anita Schneider (EERA), Antonin Vlcek (Heyrovsky Institute)

Development of new methods and software tools for early quantitative sustainability assessment of emerging SUNRISE technologies: bridging environmental, economic and social impacts

Redesigning photosynthesis for the biocatalytic production of chemicals and fuels

Synthetic Biology

Bottom-up chemical engineering of bioinspired artificial photosynthesis reactor materials and cascades

Upscaling artificial photosynthesis systems for a sustainable larger scale production of energy carriers

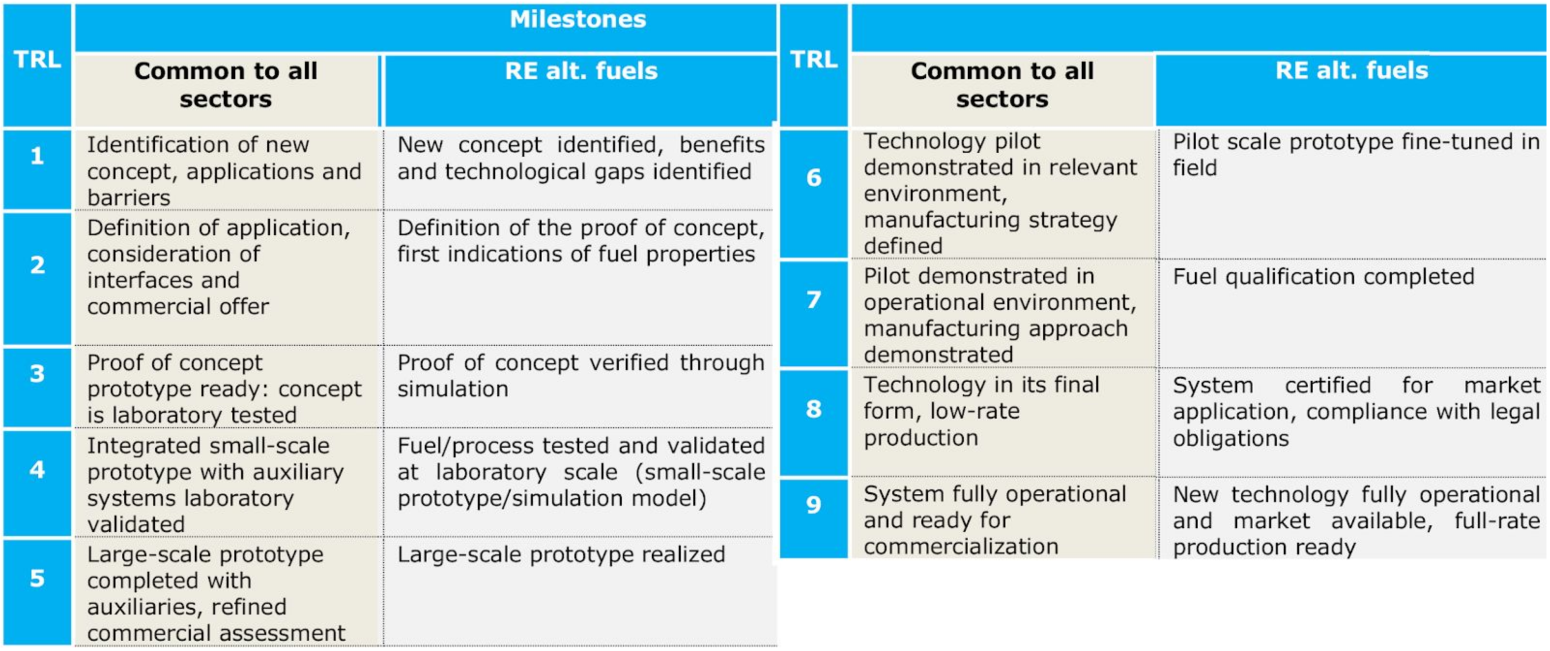
Oxygen evolution (Water oxidation)

Definitions

Energy: specific energy consumption (**SEC**) in GJ/t is the amount of energy that an average plant requires to produce a specific product. It includes net electricity and fuel consumption to provide heat, hence processes generating electricity or supplying excess steam are accounted for in the SEC. The **total energy demand** in addition to the SEC contributions also includes the energy required to produce the feedstock used in the process and the energy content of the feedstock which is built in the product.

Carbon footprint: Emissions during synthesis of the target product comprise energy related emissions (i.e. heat and electricity) and process related emissions (e.g. CO2 generated in ammonia synthesis), i.e. **cradle to gate** contributions (Production of methanol from hydrogen and CO2 includes the supply of electricity for electrolysis of water to produce hydrogen, the electrolysis process itself, capture and supply of CO2 and subsequent methanol synthesis).

Technology Readiness Level (TRL):



TRL	Milestones	
	Common to all sectors	RE alt. fuels
1	Identification of new concept, applications and barriers	New concept identified, benefits and technological gaps identified
2	Definition of application, consideration of interfaces and commercial offer	Definition of the proof of concept, first indications of fuel properties
3	Proof of concept prototype ready: concept is laboratory tested	Proof of concept verified through simulation
4	Integrated small-scale prototype with auxiliary systems laboratory validated	Fuel/process tested and validated at laboratory scale (small-scale prototype/simulation model)
5	Large-scale prototype completed with auxiliaries, refined commercial assessment	Large-scale prototype realized
6	Technology pilot demonstrated in relevant environment, manufacturing strategy defined	Pilot scale prototype fine-tuned in field
7	Pilot demonstrated in operational environment, manufacturing approach demonstrated	Fuel qualification completed
8	Technology in its final form, low-rate production	System certified for market application, compliance with legal obligations
9	System fully operational and ready for commercialization	New technology fully operational and market available, full-rate production ready

TRL: based on *Technology Readiness Level: Guidance Principles for Renewable Energy technologies*, DG RTD 2017;

Sustainable hydrogen production

Conventional process data

Conventional fossil-based process	**Steam-reforming of natural gas**
Global annual production volume	70 Mt (total production) < 0.1% from electrolysis of water (IEA 2019)
Total energy demand [GJ/t]	165 GJ/t
Energy feedstock [GJ/t]	Natural gas (methane): 205 billion m^3 Coal: 107 Mt
Fuel demand [GJ/t]	
Steam balance [GJ/t]	
Electricity [GJ/t]	
Air separation unit	
Compressors	
CO_2 emissions [tCO2 eq/t] (cradle-to-gate, including feedstock production)	12 t CO_2/t H_2 net emissions (not including feedstock production) Up to 9% higher emissions due to source leakage
Water consumption per t product	6.6 m^3/t
Current TRL	9
Current cost per t product	1000 USD (1 $/kg), with no CCUS Approx 2000 – 2500 USD (2-2.5$/kg) with CCUS
DOI References	“The future of hydrogen”, IEA 2019. The report was prepared as an input for the 2019 G20 Osaka Summit, and is an IEA contribution. The report lays out where things stand now; the ways in which hydrogen can help to achieve a clean, secure and affordable energy future; and how governments and industry can go about realising its potential. Together with other related information, the report can be found at the IEA hydrogen web portal at https://www.iea.org/topics/hydrogen/.

SUNRISE technologies

Large-Scale hydrogen production using PEM electrolysis

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</table>
</td></tr>
<tr><td>Who are the main actors? Who has to be involved?</td><td>
SIEMENS
NEL
ITM
Hydrogenics (acquired by Cummins)
AREVA H2Gen
…

Missing R&D and academics working on :
- Precious-metal free catalysts
- Stable anionic membranes
- Process engineering of PEM electrolysers (stack lifetime/heat management)

Institut Européen des Membranes
Institut Charles Gerhardt
Mines ParisTech
China
US DoE
e-conversion Cluster of Excellence in Germany (DFG-funded for 2019-2026) https://www.e-conversion.de/
</td></tr>
</table>

* key enabler: fundamental for diverse technological approaches ° TRL: see Annex

Contributors	Various
Affiliation	Various

1. Short description of the proposed technological solution

Main technological elements, working principle (max. 5 lines, for scientists not expert in the field)	Low-temperature PEM electrolysis uses proton-conducting polymer membranes between the two classical electrodes where water splitting and hydrogen formation take place. The main advantages of this technology are: improved yields, higher flexibility toward electrical input (better suited for RES), safer operation due to the absence of corrosive electrolyte compared to alkaline electrolyzers.
Why is this technology not commercially available right now? (major challenges)	Mid-scale (20 MW) PEM electrolyser are already commercial. Large-scale PEM electrolyser using current technology would be limited to 1 GW/yr due to the use of critical materials such as iridium. Cost of PEM stacks is a second bottleneck mainly due to the lack of automated manufacturing chains. Finally, current stacks last around 45000h, which leads to high maintenance costs.
What does it take to make it happen? (in short)	On the catalyst aspect, membranes using lower loading of iridium and platinum would unlock large-scale PEM electrolysis. Alternative pathways would be (i) to develop precious-metal free catalysts (ii) to develop stable anionic membranes that would allow the get rid of iridium-based catalysts. On the engineering aspects, modular, compact electrolysers designs are required as well as longer stack lifetime. On the manufacturing aspects, the setup of dedicated, automated production lines will be needed to leverage costs issue. This would also benefit to fuel-cells industry. Alternative pathway could be the development of new cationic membrane to substitute Nafion (sulfonate based, one single supplier).
What is the benefit for society? (in short)	Access to low-cost green hydrogen. Easier implementation of RES seasonal storage.

2. Existing R&I projects

Existing national/EU project	Final objective	TRL	Run-time	Funding Instrument
FCH-JU	Implement hydrogen economy	1-9	-	FCH-JU

3. State-of-the-Art: where are we now?

Technological solution to be developed in SUNRISE	**Electrochemical H2 production from solar electricity at large scale**
TRL	7 - 9
Cost	1000 €/KWh □ 100 € kW for electrolyzer at scale
Energetic conversion yield	65% □ 75%(higher heating value)
Stability	Years
Product separation yield	OK, few O2 residues in H2 can be easily removed
Total energy demand [GJ/t]	
Electricity needs [GJ/t]	
Energy demand utilities [GJ/t]	
Steam balance [GJ/t]	
CO_2 emissions [tCO2 eq/t] (cradle-to-gate, including feedstock production)	
Water consumption	Given by chemical reaction: 9 l water per kg H2
Air separation unit	
Compressors	Dependent on application setting, sometimes close to atmospheric, sometimes 20-30 bar
Resources	Current technology uses Iridium catalyst for O2 evolution thst needs to be replaced by another material
DOI References	

4. Available techno-economical analysis:

DOI Reference	doi.org/10.1038/s41560-019-0326-1
Summary	G. Glenk & S. Reichelstein (2019) “Economics of converting renewable power to hydrogen” Nature Energy 4, 216-222.

	The paper describes a model of a hybrid energy system that combines renewable power with an efficiently sized power-to-gas facility. The available capacity can be optimized in real time to take advantage of fluctuations in electricity prices and intermittent renewable power generation. The model was applied to the current environment in both Germany and Texas. A key finding is that renewable hydrogen is cost competitive in niche applications, although not yet for industrial-scale supply.

5. Deliverables, milestones

Milestones for the short, medium and long terms are given in separate tables below

Timescale: short-/medium-/long-term	**Short term**
Deliverable, milestone	Dilution of Iridium for oxygen evolution (OER)
Solved Challenges / Lifted barrier (in bullet points)	● Ir is scarce, develop technologies to reduce from 2 mg/cm2 to 0,2 mg/cms
What was necessary to solve the challenge? Did it depend on advances in other fields?	Develop new nanostructured catalyst mix materials like core.shell structures, Ir dilution in alloys
TRL	6
Stability	10000h
Energetic conversion efficiency	70%
Scale	MW
DOI Reference	

Timescale: short-/medium-/long-term	**Medium term**
Deliverable, milestone	Replacement of Iridium for oxygen evolution (OER)
Solved Challenges / Lifted barrier (in bullet points)	● Ir is scarce, develop technologies that use abundant materials that have similar robustness and overpotentials

What was necessary to solve the challenge? Did it depend on advances in other fields?	● Develop new nanostructured compounds (e.g. PolyMetalOxalats POM, Metal Oxide Frameworks MOFS) that contain no Iridium
TRL	6
Stability	10000h
Energetic conversion efficiency	70%
Scale	MW

Timescale short-/medium-/long-term	**Medium term**
Deliverable, milestone	Develop Anion Exchange Membranes (AEM), which are OH- conducting and allow the use of alkaline electrolytes
Solved Challenges / Lifted barrier (in bullet points)	Using alkaline electrolyte would release the burden to replace Iridium since several OER catalysts are available in the alkaline regime
What was necessary to solve the challenge?	General advances in membrane technologies
TRL	6
Stability	1 year at least
Energetic conversion efficiency	70%+
Scale	MW
DOI Reference	

Timescale: short-/medium-/long-term	**Long-term**
Deliverable, milestone	Automated and optimized manufacturing technologies for PEM electrolysers
Solved Challenges / Lifted barrier (in bullet points)	Bring down bill of materials (BOM) and manufacturing price (labour) by automatisation Price target < 100€/kW including balance of system at scale

What was necessary to solve the challenge?	Use advanced industrial manufacturing technologies, cheaper power electronics
TRL	9
Stability	Electrolyser has 20 years lifetime with yearly maintenance
Energetic conversion efficiency	75%
Scale	GW

Link to TRL level

At TRL 5-6: See TRL 7-8

At TRL 7-8:

Production volume	50 000 t/yr (= current production volume from pure electrolysis)
Light harvesting area needed per t/product	Assuming 1000 W/m^2 At 10-15% STH efficiency: 35-55 m^2 /t H_2 (1 t/day production) For northern European insolation: ~175-275 m^2/t (Ref: James et al. (2009) "Technoeconomic Analysis of Photoelectrochemical (PEC) Hydrogen Production" https://www.energy.gov/sites/prod/files/2014/03/f12/pec_technoeconomic_analysis.pdf)
Political/societal barriers to be overcome	Subsidies for hydrogen infrastructure (storage, transport, fuelling stations), to aid pilot plants and community-based testbed installments. European-wide outreach to boost public acceptance.
Market barriers to be overcome	Interest in H2 as fuel must be raised, e.g. Industry need to increase volumes in the fuel cell vehicle segment.

At TRL 9:

Production volume	70 Mt/yr (= current global production from steam reforming)

Light harvesting area needed per t/product	Assuming 1000 W/m^2 At 30% STH efficiency: 10-20 m^2 /t H$_2$ (1 t/day) (see above) For northern European insolation, area increases to ~50-100 m^2/t
Political/societal barriers to be overcome for market introduction	CO2-tax on artificial fertilizers from traditional fossil fuel-dense production. Tax alleviations for fuel-cell car owners.
Market barriers to be overcome	Switch from production from fossil sources must not only be economically feasible, but also bring additional value to producers. New opportunities for producers with no previous investments in fossil technology is necessary.

6. Opportunity criteria

The potential opportunity is scored from 0 (very low) to 12 (very high).

Opportunity criteria	**Individual Score**
Scalability, from individual house to communal small-scale and large-scale facilities	12
End-user price-tag on installment, competitive to other solutions	12
End-user (prosumer) access to renewable hydrogen at own property/compound	6
Customization of design and connection to other processes	10

7. Feasibility criteria

Feasibility criteria	**Individual Score**
Ease of installment	10
Scalability	12
Management cost (time and monetary)	7
Price-tag on installment	6 (depends on available subsidies)

	12 Without subsidies
Recyclability on de-comissioning	5
Lifetime (stability) of installment	10
Large-scale production necessitating new infrastructure	10

8. Key learning points

Decision points	Current PEM electrolysers can be used to start and implement demonstrators, but cannot be used for the energy transition at scale (TW) with reasonable pricing
Knowledge gaps	
Risks	When no Iridium replacement is found (or AEM membranes) the required scale cannot be achieved

Resources

Resource	**Comment**
Critical, rare elements	Non-noble metals are desirable, but materials using abundant metals need to be developed.
Non-fluctuating energy sources	
Hydrogen storage	Engineering and technological development which entails more investments rather than research.
CO2 storage	-
Water purification	Current technologies such as electrolysis (approach 1) have a great need for pure water. However, this does not have to be a limitation in future solutions. Some proof-of-principle devices are robust in impure water. More research Is needed to find this out.
CO2 from the atmosphere	-
Concentrated, pure CO2	-
Specific, new infrastructures	

Low-cost, low-carbon electricity	-
Renewable energy	
Renewable heat	

Breakthroughs in key enabling disciplines

Scale-Up	
System integration	Inherent to the technology
Novel reactor designs	Reactor/device design is a fundamental part of the development of this technology.
Novel catalyst materials: earth-abundant, non-toxic, efficient, stable	
Novel absorber materials: earth-abundant, non-toxic, efficient, stable	See above
Standardized life-cycle assessment methodologies	This will be needed on a long-term basis, but should be developed now.

Hydrogen production using photo-electrochemical cell devices

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Engie
Fraunhofer inst. for solar energy systems
EPFL
Helmholtz Center Berlin
Imperial (mekanismer)
NREL
JCAP
Siemens
E-conversion Cluster of Excellence in Germany https://www.e-conversion.de/

<u>Dye-Sensitized PEC (DS-PEC):</u>
Swedish CAP (center at Uppsala university):
Royal Swedish Technological university (KTH)
EPFL
Univ Grenoble Alpes/CNRS/CEA
Univ Cambridge
Japan: Tokyo Tech
USA: Univ North Carolina Chapel Hill</td></tr>
</table>

* key enabler: fundamental for diverse technological approaches ° TRL: see Annex

Contributors	Vincent Artero, Murielle Chavarot-Kerlidou (CEA, Univ. Grenoble Alpes), Leif Hammarström (Uppsala), Tobias Gärtner (Fraunhofer), Artur Braun (Empa), Gustav Berggren (Uppsala), Johannes Messinger (Uppsala), Andreas Kafizas (Imperial), Thomas Soller (Siemens), Laurent Baraton (Engie)

1. Short description of the proposed technological solution

Main technological elements, working principle (max. 5 lines, for scientists not expert in the field)	**Photoelectrochemical cells (PECs and DS-PECs)** A single, integrated device based on abundantly available, non-toxic and cheap materials. It directly splits water into hydrogen and oxygen, where the needed energy is provided by sunlight. In a PEC device, the same surfaces are active in charge separation and catalysis, and there are no ohmic contacts to catalysts. **Solid state PEC** Solar energy is harvested by photoelectrodes composed of metal oxide and/or semiconductor photoelectrodes. Common materials include TiO_2, $CuCrO_2$). Photoanode and photocathode can be the same or separate (Back-to-back, or separated by a membrane). **Dye-sensitized PEC** Solar energy is harvested and converted on transparent electrodes which are functionalized with multicomponent photocatalytic molecular systems, combining dyes and catalysts in a way that the natural photosynthetic process is reproduced (a.k.a. Artificial photosynthesis). The used electrode materials are commonly nanostructured metal oxides (TiO_2, NiO, $CuGaO_2$, $CuCrO_2$…) and today's most efficient dyes include organic and metallo-organic pigments while catalysts are based on Co, Mn and Ni based. Mixed Solid state and Dye sensitized PEC systems can be developed
Why is this technology not commercially available right now? (major challenges)	**PEC** To date, PEC tandem cell prototypes have shown low overall solar-to-hydrogen efficiencies (up to ~1 %). Thus far, prototypes have been on a very small scale, with low TRL levels (3 - 4). High performance materials are often susceptible to corrosion (e.g. c-Si), and is not straightforward to prevent. Intrinsically stable materials (e.g. transition metal oxides) show lower performance, mostly due to lower light absorption, and often limits the theoretical maximum efficiency to < 10%, but are promisingly simple to fabricate at scale. Suitable OER and HER co-catalysts are to some extent lacking. In the case of functional catalysts, the challenge is the creation of stable configurations of semiconductors and catalysts, stabilized in the liquid phase (electrolyte). Suitable OER and HER catalysts need to have

	low overpotential (efficient), and be based on abundant, non-platinum group elements (sustainable). **Dye-sensitized PEC** Efficiencies of DS-PEC devices for water splitting are very low (0.05% solar-to-hydrogen conversion yield). Improving it by 2 to 3 orders of magnitude is the major challenge. However, one has to bare in mind that this represents a very young and emerging field with the first operating device reported only in 2012. Stability has only been granted for a few hours and is another challenge to address.
What does it take to make it happen? (in short)	**PEC** Developing novel and scalable coatings that can passivate high performance materials (e.g. c-Si) that are susceptible to corrosion, or, improving the performance of intrinsically stable materials (e.g. transition metal oxides). Demonstrating larger prototypes of promising architectures, in particular, PEC + PV hybrids. Identification of candidate materials through combinatorial exploration or computational modelling, followed by their synthesis, testing and optimization to develop new light absorber materials and surface co-catalysts. Solving stability issues at the semiconductor/liquid interface. Creation of standard devices for testing combinations of semiconductors and surface co-catalysts (which may otherwise yield different results than from isolated materials). **DS-PEC** The multiple interfaces between electrode supports, dyes and catalysts play a crucial role in these devices, and control the efficiency of light absorption, energy conversion and catalytic processes that do not take place at the same timescales. It is crucial to control the assembly of the molecules at the interface, i.e. to reproduce in a human-made system the optimized machinery of natural photosynthesis. For this, advances in understanding and controlling the light-driven electron-transfer processes at the interfaces are needed and molecular technology has to be explored to prepare more efficient photocatalytic systems that self-assemble and possibly self-repair; it also relies on progress in the finding of better semiconducting transparent materials.

	A safer by design approach should be used during its development phase.
What is the benefit for society? (in short)	Sustainable H2 production in scalable systems, for implementation in any desirable or necessary scale. A major advantage is the potential low cost of materials and processing. In particular molecular catalysts (DS-PEC) will allow avoiding noble metals and toxic materials. Decentralisation of production of H2 as fuel. Energy independence on local, regional and global level.

2. Existing R&I projects

Existing national/EU project	**Final objective**	**TRL**	**Run-time**	**Funding Instrument**
NANOPEC (Nanostructured Photoelectrodes for Energy Conversion) https://cordis.europa.eu/project/rcn/89410/reporting/en			3 years (ended Dec 2011)	EU ~€3.6 M
SOLAR FUEL BY III-VS https://cordis.europa.eu/project/rcn/102899/reporting/en			3 years (ended July 2015)	EU ~€0.25 M
ARTIPHYCTION (Fully artificial photo-electrochemical device for low temperature hydrogen production) https://cordis.europa.eu/project/rcn/104284/reporting/en			3 years (ended Oct 2015)	EU ~€3.6 M
SOLAROGENIX (Visible-Light Active Metal Oxide Nano-catalysts for Sustainable Solar Hydrogen Production) https://cordis.europa.eu/project/rcn/106812/reporting/en			3 years (ended Jan 2016)	EU ~€3.9 M
HETMAT (Heterostructure Nanomaterials for Water Splitting) https://cordis.europa.eu/project/rcn/104906/reporting/en			3 years (ended Oct 2016)	EU ~€0.1 M
PECDEMO (Photoelectrochemical			3 years	EU

Demonstrator Device for Solar Hydrogen Generation) https://cordis.europa.eu/project/rcn/185723/reporting/en			(ended Mar 2017)	~€3.3 M
photocatH2ode https://cordis.europa.eu/project/rcn/104489/factsheet/en			3 years (ended Nov 2017)	EU ~€1.5 M
ETASECS (Extremely Thin Absorbers for Solar Energy Conversion and Storage) https://cordis.europa.eu/project/rcn/185663/reporting/en			3 years (ends in Aug 2019)	EU ~€2.15 M
a-leaf http://www.a-leaf.eu/project/	Demonstrate integrated prototype	3 - 5	2017.2020	EU/ H2020 FET Open
UK 1. Nanocrystalline Water Splitting Photodiodes II 2. Nanocrystalline Photodiodes 3.Spectroscopic studies of water splitting photocatalysis Solar Optofluidics (SOLO) 4. Feasibility study of growth by MBE of As doped GaN layers for photoanode applications in hydrogen production by photoelectrochemical water splitting 5. Nanocrystalline Water Splitting Photodiodes 6. Energy and the Physical Sciences: Hydrogen Production using a Proton Electron Buffer 7. NanoEC	1.Device Engineering, Integration and Scale-up 2. Novel Devices for Water Splitting 3.Water Splitting beyond the 1.23 eV Thermodynamic con-straints 7. Towards a Parameter-Free Theory for Electro-chemical Phenomena at the Nanoscale		Funding between 2011 up to 2022	EPSRC UK ~£6.1 M

DS-PEC				
Molecular-Semiconductor hybrid cells	Order of magnitude higher yield and stability compared to SOTA	3	2017-2019	Swedish Energy Agency
p-type	Finding p-type materials for DS-PEC photocathode	3	2017-2023	EC
https://www.e-conversion.de/	Cluster of Excellence e-conversion		2019-2026	DFG

3. State-of-the-Art: where are we now?

	PEC and DS-PEC devices for direct, photoelectrochemical H_2 production from solar energy
TRL	3
Cost	Cheap (2 €/kg H_2 projected)
Energetic conversion yield	PEC: 1%; DS-PEC: 0.03% Projected: 27% (Total system energy cost not included) https://doi.org/10.1038/316495a0
Stability	Few hours
Product separation yield	Due to separation of the HER and OER reactions in PEC tandem devices (with use of an appropriate membrane), the product separation can be made feasible. This is not realized yet, but should not be an issue with a membrane.
Total energy demand [GJ/t]	124 PJ for total construction of a 1GW annual plant, producing 610 tonnes per day. Calculated EROI (Energy Return On Energy Investment) 2,7:1 at 20% STH efficiency (R. Sathre 2014) Possibly EROI 3,5:1 at 30% efficiency.
Electricity needs [GJ/t]	For the central processes (i.e. photocatalysis): 0 For PEC systems, utility systems need 7-15 GJ/t (As a comparison, pure electrolysis, regardless of power source, demands ~190 – 290 GJ/t (50-80 MWh/t) depending on electrolyser efficiency.)

Energy demand utilities [GJ/t]	7-15 GJ/t
Steam balance [GJ/t]	
CO_2 emissions [tCO2 eq/t] (cradle-to-gate, including feedstock production)	This must be determined later, as it depends on the energy input. TEA analysis is somewhat limited by the lack of larger scale prototype development, but some have estimated that GWP will range between ~0.4 and 2.6 t CO2/ t H2 produced (see Technoeconomic Analysis of PEC Water Splitting at Various Scales, https://doi.org/10.1039/9781782629863-00266). CO_2 emissions will also depend on which materials are chosen for the device, both the active catalyst materials, as well as the frame and glass panel.
Water consumption	Water is required as substrate (i.e. raw material), but also as electrolyte (i.e. process support). Approximately 9 m^3 water is needed to produce 1 ton of H_2
Air separation unit	Monolithic **PEC** device configurations need separation of output gases. **DS-PEC** devices are most often tandem cells, which means that gases are produced in separate compartments, hence not needing any separation unit.
Compressors	250-470 MJ/t for compressor at 300 psi or in some cases the direct output from the device is at 300 psi (DOE 2009; Pinaud et al. 2013) The final pressure for H_2 to be used as fuel needs to be 700 bar (~1000 psi)
DOI References	B.A. Pinaud et al. (2013) Energy Environ. Sci. 6, 1983. **DOI: 10.1039/c3ee40831k** R. Sathre et al. (2014) Energy Environ. Sci. 7, 3264. **DOI: 10.1039/c4ee01019a** M.R. Shaner et al. (2016) Energy Environ.Sci. 9, 2354. **DOI: 10.1039/c5ee02573g** "The future of hydrogen", IEA 2019. https://www.iea.org/topics/hydrogen/

4. Available techno-economical analysis:

DOI Reference	1. James et al. (2009) "Technoeconomic Analysis of Photoelectrochemical (PEC) Hydrogen Production" https://www.energy.gov/sites/prod/files/2014/03/f12/pec_technoeconomic_analysis.pdf 2. Pinaud et al (2013) *Energy Environ. Sci.* 6, 1983. DOI: 10.1039/c3ee40831k

	3. Shaner et al. (2016) *Energy Environ. Sci.* 9, 2354. DOI: 10.1039/c5ee02573g 4. “The future of hydrogen”, IEA 2019. https://www.iea.org/topics/hydrogen/ 5. A. Maljusch and M. Wullenkord (2018), “Technoeconomic Analysis of PEC Water Splitting at Various Scales” https://doi.org/10.1039/9781782629863-00266 6. Architectures for scalable integrated photo driven catalytic devices-A concept study, R. van de Rol et al., (2016) International journal of hydrogen energy, 41, 20823 DOI:10.1016/j.ijhydene.2016.05.088
Summary	

5. Deliverables, milestones

Define a set of deliverables that provide a series of stepping stones from the current state to the future application/vision.

Define time: **short-term**	**2023**
Deliverable, milestone	Improving efficiency and stability of light-absorbing materials and catalysts. - A review and analysis of the materials applied, and performances found, in PEC devices to date – to guide future prototype development to be applied at TRL 5 and 6 (i.e. pilot and large scale). - Review and analysis of light absorbing semiconductor materials and other materials (e.g. ternary metal oxides etc) and co-catalysts that have been applied in PEC water splitting devices, with the use of key performance parameters (e.g. light absorption capability, stability, cost and scope for upscalable production).
Solved Challenges / Lifted barrier (in bullet points)	● Several metal oxides with OER activity at relatively low overpotential are available and have been tested in proof-of concepts devices with PV and Pt-based HER electrodes (e.g. WO3, BiVO4, α-Fe2O3) ● Remaining challenge: Molecular OER catalysts that are stable and efficient are still lacking for nano-particle and/or dye-sensitized systems
What was necessary to solve the challenge? Did it depend on advances in other fields?	To date, more than 130 semiconductors have been investigated for PEC water splitting. A greater focus on key materials that have shown some promise. In order to further

	develop prototypes, key materials of interest should to be identified through a thorough assessment of the literature. **DS-PEC:** Find more efficient substrate materials Graft more molecular species on the surface Optimize the interaction between grafted photosensitizer and catalysts
TRL	3 – 4 (*i.e.* bench scale)
Stability	Depends on the materials chosen, but often losses in performance show within a few days of operation.
Energetic conversion efficiency	Solar-to-hydrogen conversion efficiencies of above 1 % in PEC or DS-PEC cells .
Scale	Bench-top prototypes > 50 cm^2
DOI Reference	10.1039/C5RA20115B 10.1038/ncomms3195 10.1002/aenm.201801403 10.1021/acsnano.5b03859

Define time: **medium-term**	**2030**
Deliverable, milestone	● Artificial quantasome realized. ● HER catalysts from abundant, non-platinum group metals working at medium/low overpotential. Either metal oxides (for hybrid or buried junction devices), or molecular catalysts (for liquid phase dye-sensitized devices). ● Improved STH conversion efficiency of inherently stable PEC materials (*e.g.* transition metal oxides) to ~10% and producing demonstrators at a higher TRL level (meter square scale, TRL 5 to 6).
Solved Challenges / Lifted barrier (in bullet points)	To date, PEC tandem prototypes have only achieved STH efficiencies of up to ~1%, and DS-PEC at 0.03%. A key challenge is to improve the STH efficiencies of both PEC and DS-PEC prototypes, and scale-up to TRL 5 (i.e. demonstrator scale). Medium-time frame milestones are:

	● Demonstration of operation with solid (membrane) electrolyte for solid state PEC cells ● Implementation of a water vapor absorber with the photoanode ● Self-organization fully mastered to avoid recombination. ● **Improved photocathodes for PEC cells**. Their improvement may be achieved by optimizing existing materials (*e.g.* Cu_2O) of promise or developing alternative materials (*e.g.* $CuFeO_2$). ● **Scale-up and demonstration of larger prototypes** - Unity ultra-bandgap, light conversion efficiency, and stability for several weeks, should be incorporated within larger prototypes. This may require the translation of synthetic methods used in the lab, to those more compatible with industry methods used to grow materials at scale. Moreover, attention should be given to the additional challenges that are faced, when fabricating efficient prototypes on the m^2 scale (*e.g.* the effect of pH and ionic conductivity, electrode resistance *etc*). ● **Guidance from TEA & LCA analysis** - to date, few TEA & LCA have been carried out on PEC water splitting devices. TEA & LCA analysis should be developed, and applied more rigorously to promising prototype architectures.
What was necessary to solve the challenge? Did it depend on advances in other fields?	To solve this challenge requires collaborative research efforts between those who work in the areas of materials science (materials development), chemical engineering (prototype development) and TEA & LCA (economical evaluation).
TRL	5 – 6 (*i.e.* demonstrator scale)
Stability	Several months
Energetic conversion efficiency	Target ~10 % STH efficiency (more modest than targets for traditional PV materials given the lower light absorption found in such inherently stable materials yet favorably lower production cost)
Scale	Demonstrate >1 m^2 scale prototypes
DOI Reference	10.1002/aenm.201801403 10.1038/srep11141

	10.1038/s41560-017-0057-0 10.1039/C6EE03036J 10.1038/NPHOTON.2012.265 DOI: 10.1021/ar900110c DOI: 10.1039/c7cc00022g DOI: 10.1021/jacs.6b03889 DOI: 10.1039/c4cs00448e

Define time: **long-term**	**2050**
Deliverable, milestone	Maintaining high STH conversion efficiency at between ~15 to 20%. Demonstrators at a higher TRL level (meter square scale, TRL 6-7). Developed membrane-based devices able to take H2O from the air
Solved Challenges / Lifted barrier (in bullet points)	● Demonstration of operation with solid (membrane) electrolyte ● Implementation of a water vapor absorber with the photoanode ● Efficient and stable photoelectrodes in PEC devices, based on abundant, non-platinum group metals working at low overpotential. Either metal oxides (for PEC devices), or molecular catalysts (for DS-PEC devices).
What was necessary to solve the challenge? Did it depend on advances in other fields?	Discovery of catalytic materials and molecules, made from abundant elements. Some are known today but require further fundamental research. Possible advancements in coating science (*e.g.* atomic layer deposition, chemical vapour deposition *etc*) may better enable the development of scalable protection methods of such materials.
TRL	6-7 (i.e. demonstrator scale pilot)
Stability	Several months with less than 20% loss in efficiency
Energetic conversion efficiency	Target between ~15 and 20% STH (higher than inherently stable materials)

Scale	In situ prototypes
DOI Reference	10.1039/C6EE03036J 10.1021/cr1002326 10.1038/nenergy.2017.28

Link to TRL level

At TRL 5-6:

Production volume	
Light harvesting area needed per t/product	
Political/societal barriers to be overcome	
Market barriers to be overcome	

At TRL 7-8:

Production volume	50 000 t/yr (= current production volume from pure electrolysis)
Light harvesting area needed per t/product	Assuming 1000 W/m^2 At 10-15% STH efficiency: 35-55 m^2 /t H_2 (1 t/day production) For northern European insolation: ~175-275 m^2/t (Ref: James et al. (2009) “Technoeconomic Analysis of Photoelectrochemical (PEC) Hydrogen Production” https://www.energy.gov/sites/prod/files/2014/03/f12/pec_technoeconomic_analysis.pdf)
Political/societal barriers to be overcome	Subsidies for hydrogen infrastructure (storage, transport, fuelling stations), to aid pilot plants and community-based testbed installments. European-wide outreach to boost public acceptance.
Market barriers to be overcome	Interest in H2 as fuel must be raised, e.g. Industry need to increase volumes in the fuel cell vehicle segment.

At TRL 9:

Production volume	70 Mt/yr (= current global production from steam reforming)

Light harvesting area needed per t/product	Assuming 1000 W/m^2 At 30% STH efficiency: 10-20 m^2 /t H_2 (1 t/day) (see above) For northern European insolation, area increases to ~50-100 m^2/t
Political/societal barriers to be overcome for market introduction	CO_2-tax on artificial fertilizers from traditional fossil fuel-dense production. Tax alleviations for fuel-cell car owners.
Market barriers to be overcome	Switch from production from fossil sources must not only be economically feasible, but also bring additional value to producers. New opportunities for producers with no previous investments in fossil technology is necessary.

6. Opportunity criteria

What are the criteria that make this technology an opportunity when ready?
Score the potential opportunity from 0 (very low) to 12 (very high).
Each contributor provides an individual score (we average afterwards).

Opportunity criteria	**Individual Score**
Scalability, from individual house to communal small-scale and large-scale facilities	12
End-user price-tag on installment, competitive to other solutions	10
End-user (prosumer) access to renewable hydrogen at own property/compound	12
Customization of design and connection to other processes	

7. Feasibility criteria

What factors determine the feasibility of the final application?
Score the potential feasibility from 0 (very low) to 12 (very high).
Each contributor provides an individual score (we average afterwards).

Feasibility criteria	**Individual Score**
Ease of installment	10
Scalability	12
Management cost (time and monetary)	7
Price-tag on installment	6 (depends on available subsidies)
Recyclability on decommissioning	5
Lifetime (stability) of installment	10
Large-scale production necessitating new infrastructure	10

8. Key learning points

From the exploration of the selected topic, what are the key learning points?
(Resources, enablers, barriers, decision points, knowledge gaps, risks)

Decision points	
Knowledge gaps	
Risks	

Resources

Suggestion	**Please detail**
Critical, rare elements	Non-noble metals are desirable, but materials using abundant metals need to be developed.
Non-fluctuating energy sources	Dye-sensitized solar fuels devices may be more tolerant towards intermittent energy sources, but this needs to be investigated.
Hydrogen storage	Engineering and technological development which entails more investments rather than research.
CO2 storage	-
Water purification	Current technologies such as electrolysis (approach 1) have a great need for pure water. However, this does not have to be a limitation in future solutions. Some proof-of-principle devices are robust in impure

	water. More research Is needed to find this out.
CO2 from the atmosphere	-
Concentrated, pure CO2	-
Specific, new infrastructures	
Low-cost, low-carbon electricity	-
Renewable energy	
Renewable heat	Solar heat can be utilized in conjunction with flat panel solar fuel devices.

Breakthroughs in key enabling disciplines

Scale-Up	Present SOTA is very small lab-scale devices. Scale-up must be part of research and development to reach further than TRL3.
System integration	Inherent to the technology.
Novel reactor designs	Reactor/device design is a fundamental part of the development of this technology.
Novel catalyst materials: earth-abundant, non-toxic, efficient, stable	This is where most of the break-throughs must be in the nearest future (~5 yrs)
Novel absorber materials: earth-abundant, non-toxic, efficient, stable	See above.
Standardized life-cycle assessment methodologies	This will be needed on a long-term basis, but should be developed now.
Further developments in quantitative sustainability analysis	

Hydrogen via buried-junction photoelectrochemical cells

Technology	**PEC Buried Junction**

Targeted product	H_2	NH_3	CH_3OH	EtOH	CH_4	Jet fuel	CO_2	Other
	X							

Nature of active material	X	Solid-state Inorganic		Molecular		Biomolecular		Biological (living cells)
Sunrise approach		PV-powered electrocatalysis	X	Photoelectrochemical direct conversion		biological and biohybrid direct conversion		Key enabler*, Other
Device category		Electrolyzer	X	Photo(bio)electrolyzer		Photo(bio)reactor		fermentors, thermocatalytic reactors

Contribution to SUNRISE goals (what?)		
	X	Sustainable low-carbon production of carbon-based fuels with high efficiency and competitive costs
	X	Sustainable low-carbon production of carbon-based commodity chemicals with high efficiency and competitive costs
	X	Sustainable low-carbon production of ammonia with high efficiency and competitive costs
	X	Sustainable low-carbon production of hydrogen with high efficiency and competitive costs
		CO_2 as a valuable feedstock
		Sustainable building materials, mineralization, long-lasting C-based materials

Sustainability criteria		
		Carbon capture from the atmosphere
		Carbon capture from point sources/ flue gas
		Exclusive use of abundantly available, non-toxic and non-critical elements
	X	Sunlight as the primary energy source
		Low resource consumption
	X	Solar to products yields tenfold to hundredfold higher than current biomass practice

Envisaged production system	X	Decentralized, local production at small scale (households, niche applications)				
		Large-scale production using existing centralized infrastructure				
	X	Large-scale production necessitating new centralized infrastructure				
Rough timeline (when?)	Short term (2020-25)		Medium term (2025–30)		Long term (2030–50)	
	TRL°	3-5	TRL°	5-7	TRL°	7-8
Who are the main actors? Who has to be involved?	Harvard JCAP EPFL ICIQ Forsch.Julich Helmholtz Berlin + Many more in the EU					

* key enabler: fundamental for diverse technological approaches ° TRL: see Annex

Please indicate who gave concrete input; this is **optional**, but allows us to quantify the reach of the proposed technological solution.

Contributors	Vincent Artero (CEA), Leif Hammarström (Uppsala), Tobias Gärtner (Fraunhofer), Artur Braun (Empa), Gustav Berggren (Uppsala), Johannes Messinger (Uppsala), Andreas Kafizas (Imperial), Thomas Soller (Siemens), Laurent Baraton (Engie)
Affiliation	

1. Short description of the proposed technological solution

Main technological elements, working principle (max. 5 lines)	A PV material is protected from solution by a cover layer, that works as an ohmic contact to catalyst layers on the surface, forming a stand-alone “artificial leaf”. It can be viewed as an integrated PV-electrolysis device where the ohmic contact layers are nm-sized “wires”. High STH efficiency (19%) and relatively long-term stability (several days) has been achieved.
Why is this technology not commercially available right now? What are the major challenges?	Very new development. Too expensive to manufacture. Lack of demand for renewable H2. Products not separated.

What does it take to make it happen? (in short)	Manufacturing methods plus upscaling.
What is the benefit for society? (in short)	Sustainable H_2 production in scalable systems, for implementation in any desirable or necessary scale. Decentralisation of production of H_2 as fuel. Energy independence on local, regional and global level.

2. Existing R&I projects

Existing national/EU project	Final objective	TRL	Run-time	Funding Instrument

3. State-of-the-Art: where are we now?

Definitions: specific energy consumption (**SEC**) in GJ/t is the amount of energy that an average plant requires to produce a specific product. It includes net electricity and fuel consumption to provide heat, hence processes generating electricity or supplying excess steam are accounted for in the SEC. The **total energy demand** in addition to the SEC contributions also includes the energy required to produce the feedstock used in the process and the energy content of the feedstock which is built in the product.
Carbon footprint: Emissions during synthesis of the target product comprise energy related emissions (i.e. heat and electricity) and process related emissions (e.g. CO2 generated in ammonia synthesis), i.e. **cradle to gate** contributions (Production of methanol from hydrogen and CO2 includes the supply of electricity for electrolysis of water to produce hydrogen, the electrolysis process itself, capture and supply of CO2 and subsequent methanol synthesis).

Technological solution to be developed in SUNRISE	**PEC Buried Junction**
TRL	~3 (now), 7-8 in 2050
Cost	Projected
Energetic conversion yield	>10% (record @19% Cheng 2018 10.1021/acsenergylett.8b00920) Target > 20%.

Stability	10th of hours today, 80000h in 2050
Product separation yield	Near 100% as hydrogen and oxygen are produced in separated places.
Total energy demand [GJ/t]	Unknown
Electricity needs [GJ/t]	Unknown
Energy demand utilities [GJ/t]	Unknown
Steam balance [GJ/t]	None
CO2 emissions [tCO2 eq/t] (cradle-to-gate, including feedstock production)	Strongly depend on the manufacturing processes and recyclability.
Water consumption	Low
Air separation unit	None
Compressors	Yes
DOI References	

Conventional fossil-based process	**Steam-reforming of natural gas**
Global annual production volume	70 Mt (total production) < 0,1% from electrolysis of water (IEA 2019)
Total energy demand [GJ/t]	165 GJ/t
Energy feedstock [GJ/t]	Natural gas (methane): 205 billion m^3 Coal: 107 Mt
Fuel demand [GJ/t]	
Steam balance [GJ/t]	I don’t know what this means
Electricity [GJ/t]	?
Air separation unit	?
Compressors	?
CO2 emissions [tCO2 eq/t] (cradle-to-gate, including feedstock production)	12 t CO_2/t H_2 net emissions (<u>not</u> including feedstock production) Up to 9% higher emissions due to source leakage

Water consumption per t product	6,6 m^3/t
Current TRL	9
Current cost per t product	1000 USD (1 $/kg), with no CCUS Approx 2000 – 2500 USD (2-2,5$/kg) with CCUS
DOI References	“The future of hydrogen”, IEA 2019. https://www.iea.org/topics/hydrogen/

Biomass-based process (if any)	
Global annual production volume	
Energy demand [GJ/t]	
Feedstock demand [GJ/t]	
CO2 emissions [tCO2 eq/t] (cradle-to-gate, including feedstock production)	
Water consumption per t product	
Electricity needs [GJ/t]	
Current TRL	
Current cost per t product	
DOI References	

4. Available techno-economical analysis:

DOI Reference	James et al. (2009) “Technoeconomic Analysis of Photoelectrochemical (PEC) Hydrogen Production” https://www.energy.gov/sites/prod/files/2014/03/f12/pec_technoeconomic_analysis.pdf Architectures for scalable integrated photo driven catalytic devices-A concept study, R. van de Rol et al., (2016) International journal of hydrogen energy, 41, 20823 DOI:10.1016/j.ijhydene.2016.05.088

Summary	

5. Deliverables, milestones

Define a set of deliverables that provide a series of stepping stones from the current state to the future application/vision.

Define the associated time dimension.

Define time: **short-/medium-/long-term, x years**	Medium term (2 – 10 years)
Deliverable, milestone	Improving the stability of traditional PV materials, maintain high STH conversion efficiency at between ~15 to 20%, and producing demonstrators at a higher TRL level (meter square scale, TRL 5 to 6).
Solved Challenges / Lifted barrier (in bullet points)	Currently, traditional PV materials, such as Si and III/V semiconductors, show the highest STH efficiencies in PEC water splitting devices (up to ~16%). However, their poor water stability and high processing cost preclude commercial viability. The key challenges are: ● protection methods to improve the stability of traditional PV materials -. this will require the development of new and scalable coating methods to stabilize traditional PV materials such as c-Si in an aqueous environment (e.g. weeks to months without substantial corrosion and loss of performance). Such materials should be used to fabricate prototypes at TRL 4 to 6 (i.e. bench to large scale). ● TEA and LCA of promising prototypes - to guide materials choice and development.
What was necessary to solve the challenge? Did it depend on advances in other fields?	Possible advancements in coating science (e.g. atomic layer deposition, chemical vapour deposition etc) may better enable the development of scalable protection methods of such materials.
TRL	5 – 6 (i.e. pilot and large scale)
Stability	Several months with less than 20% loss in efficiency
Energetic conversion efficiency	Target between ~15 and 20% STH (higher than inherently stable materials, as traditional PV materials are likely to be more expensive to produce and

	protect)
Scale	Demonstrate >1 m2 scale prototypes
DOI Reference	10.1039/C6EE03036J 10.1021/cr1002326 10.1038/nenergy.2017.28

Define time: short-/medium-/long-term, x years	Medium-long-term, 5-10 years (depending on what you mean by long-term)
Deliverable, milestone	Demonstrate the integrated PEC concept in tandem PEC device (“artificial photosynthesis”) and/or buried-junction PV+electrolysis (“hybrid tandem” a.k.a. “artificial leaf”) made of abundant materials
Solved Challenges / Lifted barriers (in bullet points)	● Proof-of-concepts exist for both tandem PECs and buried-juncrion PV+electrolysis at varying STH efficiency, however catalyst materials still partially or completely based on noble-metals (metallic or oxides)
What was necessary to solve the challenge? Did it depend on advances in other fields?	…Research…?
TRL	3
Stability	Several days (?)
Scale	Tandem PECs : ~1% Buried-junction or hybrid PV/electrolysis: 10-20%
Energetic conversion efficiency	Small lab scale (in the order of cm^2)
DOI Reference	DOI: 10.1073/pnas.1414290111 DOI: 10.1021/acsenergylett.8b00920 DOI: 10.1021/acs.jpcc.7b00533

Define time: short-/medium-/long-term, x years	Long-term, 15+ years

Deliverable, milestone	Discover and develop OER catalysts from abundant, non-platinum group metals working at medium/low overpotential. Either metal oxides (for hybrid or buried junction devices), or molecular catalysts (for liquid phase dye-sensitized devices).
Solved Challenges / Lifted barriers (in bullet points)	● Several metal oxides with OER activity at relatively low overpotential are available and have been tested in proof-of concepts devices with PV and Pt-based HER electrodes (e.g. WO_3, $BiVO_4$, α-Fe_2O_3) ● Remaining challenge: Molecular OER catalysts that are stable and efficient are still lacking for nano-particle and/or dye-sensitized systems
What was necessary to solve the challenge? Did it depend on advances in other fields?	
TRL	3
Stability	Varying, from hours to a few days
Scale	
Energetic conversion efficiency	~1-6%
DOI Reference	DOI: 10.1126/science.1246913 DOI: 10.1126/sciadv.1501764 DOI: 10.1021/acs.jpcc.7b00533

Define time: short-/medium-/long-term, x years	Long-term, 15+ years
Deliverable, milestone	Discover and develop HER catalysts from abundant, non-platinum group metals working at medium/low overpotential. Either metal oxides (for hybrid or buried junction devices), or molecular catalysts (for liquid phase dye-sensitized devices).
Solved Challenges / Lifted barriers (in bullet points)	● Efficient molecular HER catalysts are available, mainly Ni- and Fe-based. ● Remaining challenge: Good metal oxide HER catalsysts based on non-platinum group metals are still lacking
What was necessary to solve the challenge? Did it depend on advances in other fields?	

TRL	3
Stability	Hours time scale. Stability and efficiency of molecular Fe complexes can be improved by incorporation in MOFs or other “inert” frameworks.
Scale	
Energetic conversion efficiency	
DOI Reference	DOI: 10.1021/ar900110c DOI: 10.1039/c7cc00022g DOI: 10.1021/jacs.6b03889 DOI: 10.1039/c4cs00448e

Define time: short-/medium-/long-term, x years	Long-term, 15+ years
Deliverable, milestone	Developing or adapting new PV materials (i.e. tandem perovskytes)
Solved Challenges / Lifted barriers (in bullet points)	● Stability issue of those emerging materials toward hydrogen production environment (liquid electrolytes). ● Lift the cost barrier linked with multiple junction PV materials.
What was necessary to solve the challenge? Did it depend on advances in other fields?	Strongly depends on the development of the PV fields.
TRL	3
Stability	Hours time scale. Stability and efficiency of the PV part of the device is key.
Scale	
Energetic conversion efficiency	
DOI Reference	10.1021/ja511739y 10.1039/C8CS00699G

Link to TRL level

At TRL 5-6:

Production volume	
Light harvesting area needed per t/product	
Political/societal barriers to be overcome	
Market barriers to be overcome	

At TRL 7-8:

Production volume	
Light harvesting area needed per t/product	
Political/societal barriers to be overcome	
Market barriers to be overcome	

At TRL 9:

Production volume	
Light harvesting area needed per t/product	
Political/societal barriers to be overcome for market introduction	
Market barriers to be overcome	

6. Opportunity criteria

What are the criteria that make this technology an opportunity when ready?
Score the potential opportunity from 0 (very low) to 12 (very high).
Each contributor provides an individual score (we average afterwards).

Opportunity criteria	Individual Score

7. Feasibility criteria

What factors determine the feasibility of the final application?
Score the potential feasibility from 0 (very low) to 12 (very high).
Each contributor provides an individual score (we average afterwards).

Feasibility criteria	Individual Score

8. Key learning points

From the exploration of the selected topic, what are the key learning points?
(Resources, enablers, barriers, decision points, knowledge gaps, risks)

Decision points	
Knowledge gaps	
Risks	

Resources

Suggestion	Please detail
Critical, rare elements	
Non-fluctuating energy	

sources	
Hydrogen storage	
CO2 storage	
Water purification	
CO2 from the atmosphere	
Concentrated, pure CO2	
Specific, new infrastructures	
Low-cost, low-carbon electricity	
Renewable energy	
Renewable heat	

Breakthroughs in key enabling disciplines

Scale-Up	
System integration	
Novel reactor designs	
Novel catalyst materials: earth-abundant, non-toxic, efficient, stable	
Novel absorber materials: earth-abundant, non-toxic, efficient, stable	
Standardized life-cycle assessment methodologies	
Further developments in quantitative sustainability	

analysis	
Strain robustness	
Genomic stability	
Preservation (culture collection)	

Political/societal/market barriers

EU-wide, homogeneous regulatory frameworks	
Adaptation/ novel regulations (e.g. genetics, use of waste CO2, ..)	
EU/national regulations for the deployment of the technology/product	
EU/national incentives for the deployment of the technology/product	
Fast idea protection (patenting, etc.)	
Large capital investment for market introduction	
Standardization of efficiencies, etc.	
Societal acceptance	
Political security	
EU supply chain	

Funding/research frameworks

International collaboration	
Funding schemes for demonstrators, pilots, etc.	
Large-scale EU research initiatives	

Hydrogen photoproduction by photosynthetic microorganisms

Technology	**Hydrogen photoproduction by photosynthetic microorganisms**

Targeted product

H_2	NH_3	CH_3OH	EtOH	CH_4	Jet fuel	CO_2	Other
x							

Nature of active material		Solid-state Inorganic		Molecular		Biomolecular	X	Biological (living cells)
Sunrise approach		PV-powered electrocatalysis		Photoelectrochemical direct conversion	X	Biological and biohybrid direct conversion		Key enabler*, Other
Device category		Electrolyzer		Photo(bio)electrolyzer	X	Photo(bio)reactor		fermentors, thermocatalytic reactors

Contribution to SUNRISE goals (what?)

	Sustainable low-carbon production of carbon-based fuels with high efficiency and competitive costs
	Sustainable low-carbon production of carbon-based commodity chemicals with high efficiency and competitive costs
	Sustainable low-carbon production of ammonia with high efficiency and competitive costs
X	Sustainable low-carbon production of hydrogen with high efficiency and competitive costs
	CO_2 as a valuable feedstock
	Sustainable building materials, mineralization, long-lasting C-based materials

Sustainability criteria

	Carbon capture from the atmosphere
	Carbon capture from point sources/ flue gas
x	Exclusive use of abundantly available, non-toxic and non-critical elements
x	Sunlight as the primary energy source
x	Low resource consumption
x	Solar to products yields tenfold to hundredfold higher than current biomass practice

Envisaged production system	x	Decentralized, local production at small scale (households, niche applications)				
		Large-scale production using existing centralized infrastructure				
		Large-scale production necessitating new centralized infrastructure				
Rough timeline (when?)	Short term (2020-25)		Medium term (2025–30)		Long term (2030–50)	
	TRL°3-5		TRL°5-6		TRL°7-8	
Who are the main actors? Who has to be involved?	Uppsala Univ., Sweden University of Turku, Finland CEA, France BRC, Szeged, Hungary Tel Aviv University, Israel University of Münster, Germany Aarhus, Denamark RUB, Bochum, Germany Bielefeld Univ., Germany Humboldt Univ NREL, USA Helmholtz. C. Leipzig					

* key enabler: fundamental for diverse technological approaches ° TRL: see Annex

Please indicate who gave concrete input; this is **optional**, but allows us to quantify the reach of the proposed technological solution.

Contributors	Yagut Allahverdiyeva-Rinne (Turku), Gustav Berggren (Uppsala), Joanna Kargul (Warsaw), Peter Lindblad (Uppsala)

1. Short description of the proposed technological solution

Main technological elements, working principle (max. 5 lines)	**Hydrogen photoproduction by photosynthetic microorganisms (algae & cyanobacteria)** Long-term efficient hydrogen photoproduction by photosynthetic microorganisms, using sunlight and water. Some photosynthetic green algae and cyanobacteria possess hydrogen producing enzyme (hydrogenase or nitrogenases). They naturally photoproduce H2 gas under specific environmental conditions. Due to regulatory, metabolic and also technical limitations, the light-to-product conversion efficiencies in photosynthetic cyanobacteria and algae are about 1-2% (under specific lab-scale cultivation conditions and/or with engineered microalgae it can be as

	high as 4%), this strongly limits their industrial application. Integration of whole cells with artificial semiconductors provides possible route towards systems circumventing the inherent limitations of the photosynthetic apparatus, enabling efficiencies beyond the 10-13% limit.
Why is this technology not commercially available right now? What are the major challenges?	The theoretical light energy to H2 energy conversion efficiency (LHCE) is around 10-13% in green algae, which is high enough for industrial applications. Despite this, there are many metabolic hindrances and technological barriers to the application of algae for H2 photoproduction at industrial levels. The major metabolic bottlenecks include: (i) the high sensitivity of the [Fe-Fe]-hydrogenase to O2; (ii) the non-dissipated proton gradient across the thylakoid membrane and (iii) alternative electron transport pathways competing for photosynthetic reducing power. High costs of algal/cyanobacteria cultivation (feedstock production) strongly affects cost effectiveness of the process.
What does it take to make it happen? (in short)	1. Mining novel, more efficient and O2 tolerant hydrogenases and nitrogenases (including metatranscriptomics, metagenomics, metasecretome) 2. Uncover electron-transport network in unicellular and heterocyst forming cyanobacteria in order to increase H2 production. Primary focus on heterocyst forming N2 fixing cyanobacteria. 3. Funneling more solar electrons to hydrogenase / nitrogenase by eliminating competing pathways 4. Developing novel production protocols which do not require nutrient starvation (resulting low cell fitness) but induce efficient and long-term H2. 5. Construction of special photobioreactors for cultivation (efficient biomass accumulation) and production phases (where biomass production should be limited and energy directed to products, e/g/ solid state production).
What is the benefit for society? (in short)	Production of sustainable “green” hydrogen. The main advantage of this technology is that the photosynthetic cells act as long-lived and self assembled biocatalysts enabling sustained production process. For the production platform only water and sunlight and some minerals are needed. For decreasing production costs even waste-water and sea water can be used.

2. Existing R&I projects

Existing national/EU project	Final objective	TRL	Run-time	Funding Instrument

3. State-of-the-Art: where are we now?

Technological solution to be developed in SUNRISE	**Hydrogen photoproduction by photosynthetic microorganisms**
TRL	3-4
Cost	
Energetic conversion yield	Up to 1%
Stability	months
Product separation yield	Gas mixture
Total energy demand [GJ/t]	
Electricity needs [GJ/t]	
Energy demand utilities [GJ/t]	
Steam balance [GJ/t]	
CO_2 emissions [tCO_2 eq/t] (cradle-to-gate, including feedstock production)	
Water consumption	
Air separation unit	
Compressors	
DOI References	

4. Available techno-economical analysis:

DOI Reference	W. A. Amos (2004) “Updated cost analysis of photobiological hydrogen production from *Chlamydomonas reinhardtii* green algae.” NREL, Department of Energy, US. Milestone report NREL/MP-560-35593.
Summary	Costs as low as 0.57 USD/kg are conceivable

5. Deliverables, milestones

Define a set of deliverables that provide a series of stepping stones from the current state to the future application/vision. Define the associated time dimension.

Define time: **short-/medium-/long-term, x years**	Mining biodiversity for hydrogen producing enzymes (hydrogenases and nitrogenases) with increased efficiency and O2 tolerance. Short, 2-4 years
Deliverable, milestone	Hydrogenases stable under atmospheric oxygen; FeFe hydrogenases that show a high degree of promiscuity towards electron donors (ferredoxins) in cyanobacteria and algae. More efficient nitrogenases.
Solved Challenges / Lifted barrier (in bullet points)	
What was necessary to solve the challenge? Did it depend on advances in other fields?	
TRL	4-5
Stability	
Energetic conversion efficiency	
Scale	
DOI Reference	

Define time: short-/medium-/long-term, x years	Mapping out and optimizing relevant electron transfer pathways in cyanobacteria (main focus on heterocysts) and algae Medium 4-6 years
Deliverable, milestone	Identification of key ferredoxins; optimization of electron transfer pathways funneling electrons to N2ase or H2ase.
Solved Challenges / Lifted barriers (in bullet points)	
What was necessary to solve the challenge? Did it depend on advances in other fields?	
TRL	4-5
Stability	
Scale	
Energetic conversion efficiency	
DOI Reference	

Define time: short-/medium-/long-term, x years	Engineered cyanobacterial and algal cells acting as a long term biocatalysts producing photoH2 at competitive price
Deliverable, milestone	
Solved Challenges / Lifted barriers (in bullet points)	● O2 tolerant and highly active enzymes ● Efficient and cheap synthetic biology tools for diverse organisms ● Highly efficient tools (switches) for funneling photosynthetic electron transfer to targeted enzymes
What was necessary to solve the challenge? Did it depend on advances in other fields?	
TRL	6-7
Stability	

Scale	
Energetic conversion efficiency	
DOI Reference	

Link to TRL level

At TRL 5-6:

Production volume	
Light harvesting area needed per t/product	
Political/societal barriers to be overcome	
Market barriers to be overcome	

At TRL 7-8:

Production volume	
Light harvesting area needed per t/product	
Political/societal barriers to be overcome	
Market barriers to be overcome	

At TRL 9:

Production volume	
Light harvesting area needed per t/product	
Political/societal barriers to be overcome for market introduction	

Market barriers to be overcome	

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Score the potential opportunity from 0 (very low) to 12 (very high).
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Opportunity criteria	**Individual Score**

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Decision points	
Knowledge gaps	

Risks	

Resources

Suggestion	**Please detail**
Critical, rare elements	
Non-fluctuating energy sources	
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CO2 storage	
Water purification	
CO2 from the atmosphere	
Concentrated, pure CO2	
Specific, new infrastructures	
Low-cost, low-carbon electricity	
Renewable energy	
Renewable heat	

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System integration	
Novel reactor designs	
Novel catalyst materials: earth-abundant, non-toxic, efficient, stable	

Novel absorber materials: earth-abundant, non-toxic, efficient, stable	
Standardized life-cycle assessment methodologies	
Further developments in quantitative sustainability analysis	
Strain robustness	
Genomic stability	
Preservation (culture collection)	

Political/societal/market barriers

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Adaptation/ novel regulations (e.g. genetics, use of waste CO2, ..)	
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EU/national incentives for the deployment of the technology/product	
Fast idea protection (patenting, etc.)	
Large capital investment for market introduction	
Standardization of efficiencies, etc.	

Societal acceptance	
Political security	
EU supply chain	

Funding/research frameworks

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Funding schemes for demonstrators, pilots, etc.	
Large-scale EU research initiatives	

Hydrogen photoproduction by biomolecular technologies

Technology	**Hydrogen photoproduction by biomolecular technologies**

Targeted product

H_2	NH_3	CH_3OH	EtOH	CH_4	Jet fuel	CO_2	Other
x							

Nature of active material		Solid-state Inorganic		Molecular	X	Biomolecular		Biological (living cells)
Sunrise approach		PV-powered electrocatalysis	x	Photoelectrochemical direct conversion		biological and biohybrid direct conversion		Key enabler*, Other
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Contribution to SUNRISE goals (what?)

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	Sustainable building materials, mineralization, long-lasting C-based materials

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<tr><td>TRL°4-7</td><td>☐</td><td>TRL°7-8</td><td>☐</td><td>TRL°8-9</td><td>☐</td></tr>
<tr><td>Who are the main actors? Who has to be involved?</td><td colspan="6">Very interdisciplinary group of scientists/engineers with expertise in natural photosynthesis (biochemistry, biophysics, molecular biology, genomics), photophysics, material science, electrochemistry and chemical catalysis due to the hybrid nature of the working biomolecular assemblies.
CeNT,UW, Poland
CEA, Grenoble, France
RUB, Germany
TH Wildau, Germany
Leiden Uni., the Netherlands
Amsterdam University, the Netherlands
Bristol Uni., UK
Cambridge Uni., UK
Leeds Uni., UK
DTU, Denmark
Harvard Uni., USA
Vanderbilt Uni, USA
Penn Uni, USA
Uni. of Tennessee, USA
Utah Uni., USA
ES-y Labs, Germany
Freiburg Uni., Germany
Arizona State Uni., USA
Berkeley, USA
VUA, Netherlands
Padova Uni., Italy
UC Louvain, Belgium
Photovoltaic Center for Energy (AIT), Austria
NUS, Singapore
IPCF, CNR, Bari, Italy
CNRS, Marseille, France
ENS, France
Osaka Uni., Japan
e-conversion consortium including LMU Munich, Germany

For upscaling:
Fraunhofer, Germany</td></tr>
</table>

	Leiden Uni., the Netherlands Wuerzburg Uni.,Germany

* key enabler: fundamental for diverse technological approaches ° TRL: see Annex

Please indicate who gave concrete input; this is **optional**, but allows us to quantify the reach of the proposed technological solution.

Contributors	Joanna Kargul (Warsaw), Yagut Allahverdiyeva-Rinne (Turku), Juliette Jouhet (Grenoble), Gustav Beggren (Uppsala)

1. Short description of the proposed technological solution

Main technological elements, working principle (max. 5 lines)	Development of green hydrogen producing technologies from water based on natural light harvesting catalyst that have been optimised for light capture and electron transfer. Biomolecular assemblies composed of electrode + large biomolecules with light harvesting and/or catalytic activities, e.g. robust extremophilic photosystem I, extracted from living microalgal cells that is used as the light harvester and charge separator and hydrogenases. This technology stems from the use of “living solar cells” because light harvesting components are capable of self-assembly and self-renewing through the processes that have been optimized for over 3.5 billion years of evolution for efficient solar energy conversion.
Why is this technology not commercially available right now? What are the major challenges?	Limitations due to stability of the components and wasteful back reactions. Stability, nanostructuring and interfacing of the working modules need to be optimised for efficient DET. No Life Cycle Assessment studies. For scaling up, business plan/cost evaluation need to be established.
What does it take to make it happen? (in short)	Need for upscaling studies (see key enabler: Upscaling artificial photosynthesis - Fraunhofer-led key enabler PRD) Engineering of efficient interfaces between electrode and photoelectrochemical compounds. Nanostructuring the biocomponents to increase light absorption and through the use of plasmonics and minimise back reaction and short-circuiting.
What is the benefit for society? (in short)	It is envisaged that biohybrid technologies, when optimised, will provide a viable technological alternative to costly synthetic solar-converting technologies based on the classical

	photovoltaics. The biocomponents used in these technologies are non-toxic originating from living photosynthetic microorganisms. Not much energy input needed to synthesize photoactive molecules inside the cells, since the main challenge is to optimise the biomass production for extraction of photoactive biomolecular components. 20% loss of photochemical activity observed during intermittent measurements of photochemical activity of immobilised photosystem I from extremophilic algae over 12 months under 3500 uE/m2/s illumination with white light.

2. Existing R&I projects

Existing national/EU project	Final objective	TRL	Run-time	Funding Instrument
e-conversion	Fundamental studies on solar conversion processes. Development solar-conversion devices for production of electricity, H2 and other chemicals.	2-3	2019-2026	DFG, Germany
OPUS14	Development of optimal organic interface for linking biophotocatalysts with various electrode materials	2-3	2018-2021	NCN, Poland

3. State-of-the-Art: where are we now?

Technological solution to be developed in SUNRISE	Integrated biomolecular systems for photocatalytic H2 production from water
TRL	2-3
Cost	
Energetic conversion yield	~ 1%
Stability	With 1 year of intermittent white light illumination of robust PSI

	catalyst integrated with semiconductor (hematite, p-Si) lab-scale device, 20% of photochemical activity observed.
Product separation yield	
Total energy demand [GJ/t]	
Electricity needs [GJ/t]	
Energy demand utilities [GJ/t]	
Steam balance [GJ/t]	
CO2 emissions [tCO2 eq/t] (cradle-to-gate, including feedstock production)	
Water consumption	
Air separation unit	
Compressors	
DOI References	10.1002/adfm.201401399 10.1039/C8PP00426A doi.org/10.1021/nn900748j 10.1038/s41560-018-0232-y 10.1016/j.jplph.2012.05.018 and references therein 10.1016/j.bbabio.2013.12.013 and references therein

4. Available techno-economical analysis:

DOI Reference	
Summary	

5. Deliverables, milestones

Define a set of deliverables that provide a series of stepping stones from the current state to the future application/vision. Define the associated time dimension.

Define time: short-/medium-/long-term, x years	***Short-term: 1 year***

Deliverable, milestone	- Genome mining for 1st generation novel robust enzymes, - Selection of biocompatible electrode materials, - Selection of redox-tuned conductive interfaces, - Selection of novel 1st generation robust proton reduction catalysts (PRCs), - Kinetic modelling of ET at the interfaces and hydrogenase enzyme catalytic centres.
Solved Challenges / Lifted barrier (in bullet points)	- Identification of ET competing pathways in the integrated biomolecular systems - Identification of biocompatible electrode materials - Identification of the 1st generation PRCs, hydrogenases and embedding matrices for increased O2 tolerance of the (bio)catalytic modules
What was necessary to solve the challenge? Did it depend on advances in other fields?	Thorough investigation of ET processes at the interface between electrode and enzymes or PRCs using STOA spectroelectrochemical approaches and kinetic modelling
TRL	3-4
Stability	
Energetic conversion efficiency	
Scale	
DOI Reference	10.1021/jacs.5b01194 10.1039/C8FD00168E 10.1021/acs.nanolett.8b04935 10.1038/s41560-018-0232-y and many other examples

Define time: **short-/medium-/long-term, x years**	***Medium-term: 3 – 5 years***

Deliverable, milestone	● Genome mining for 2nd generation novel robust hydrogenase enzymes, ● Selection of novel 2nd generation robust PRCs, ● Interfacing robust photosynthetic RCs with electrode and novel hydrogenase enzymes, ● Interfacing robust photosynthetic RCs with electrode and novel PRCs, ● Interfacing whole cell biocatalysts with artificial photosensitisers; proof-of-concept devices with solar to energy efficiencies >10% with regards to target products, ● Modelling of ET at the biohybrid nanoassemblies ● Nanostructuring of each module of the biohybrid nanodevices to ensure the optimisation of DET, ● LCA modelling of the laboratory prototypes of the biohybrid nanoassemblies. **Milestones in 3-5 years:** ● Libraries of novel O2-tolerant hydrogenase enzymes and PRCs, ● Kinetic models of ET at the interfaces and hydrogenase enzyme/PRC catalytic centres identifying ET competing pathways, ● Medium-scale demonstrators for bias-free biomolecular H2-production with LCA assessment, ● LCA evaluation of the device performance.
Solved Challenges / Lifted barriers (in bullet points)	● Use of (bio)catalytic components with significantly improved stability, activity and O2-tolerance ● Development of redox-compatible molecular interfaces for oriented deposition of catalytic modules ● Rational, ET modelling-driven design of the integrated biomolecular systems with amelioration of the competing pathways for significant improvement of STH efficiencies ● Improved light harvesting of the biocatalytic modules

	(photosynthetic reaction centres)
What was necessary to solve the challenge? Did it depend on advances in other fields?	- Identification of novel robusts enzymes, catalysts and compatible interfaces for improved DET - Taking advantage of plasmonic interactions to improve light harvesting of biocatalytic modules - Efficient molecular wiring of the light-harvesting biocatalysts, PRCs and electrode materials for improved DET
TRL	5-7
Stability	Essential to improve it for all the working modules of the biomolecular devices
Scale	Medium, ideally all-solid-state configuration
Energetic conversion efficiency	5%
DOI Reference	

Define time: short-/medium-/long-term, x years	***Long-term: 10 – 20 years***
Deliverable, milestone	- Construction of viable solar-to-hydrogen biomolecular devices, - Macroscaling of the viable laboratory prototypes based on the results of LCA modelling yielding the TRL8 of the solar hydrogen production installations based on the best performing biomolecular systems. **Milestones in 10-20 years:** - Libraries of 3rd generation novel O2-tolerant hydrogenase enzymes and PRCs, - Large-scale demonstrators for biomolecular H2-production with LCA assessment, - LCA evaluation of the large-scale device performance.

Solved Challenges / Lifted barriers (in bullet points)	● As for medium-term challenges but also with complete LCA studies and full assessment of stability and performance ● Fully integrated solid-state systems operational at a medium scale (1 m2) with STH efficiencies of 10%.
What was necessary to solve the challenge? Did it depend on advances in other fields?	No significant progress in biomolecular technologies can be made without a highly interdisciplinary approach (for rapid development of catalysts of increased stability and activity when interfaced with electrode materials, more robust enzymes, compatible electrode materials and interfaces).
TRL	7-8
Stability	Essential to improve the stability of (bio)catalytic components
Scale	
Energetic conversion efficiency	
DOI Reference	

Link to TRL level

At TRL 5-6:

Production volume	
Light harvesting area needed per t/product	
Political/societal barriers to be overcome	
Market barriers to be overcome	

At TRL 7-8:

Production volume	
Light harvesting area needed per t/product	
Political/societal barriers to be overcome	

Market barriers to be overcome	

At TRL 9:

Production volume	
Light harvesting area needed per t/product	
Political/societal barriers to be overcome for market introduction	
Market barriers to be overcome	

6. Opportunity criteria

What are the criteria that make this technology an opportunity when ready?
Score the potential opportunity from 0 (very low) to 12 (very high).
Each contributor provides an individual score (we average afterwards).

Opportunity criteria	**Individual Score**
Decentralised production of H2 for further reduction processes leading to chemical synthesis of complex molecules	12
Low-cost of biophotocatalytic and synthetic PRCs with the minimised use of rare or toxic elements	12
Use of light harvesting and redox active biocatalysts that are self assembling, self-renewing and optimised for primary solar conversion process (nearly 100% efficiency of primary charge separation)	12
Cost-effective purification of biocatalysts from large-scale cultures of extremophilic microorganisms taking advantage of laboratory evolution (for improved O2-stability, activity and oriented nanostructuring, e.g. by genetic introduction of affinity tags, DNA origami etc.)	12

7. Feasibility criteria

What factors determine the feasibility of the final application?
Score the potential feasibility from 0 (very low) to 12 (very high).
Each contributor provides an individual score (we average afterwards).

Feasibility criteria	Individual Score
Improved efficiency of the complete biomolecular H_2-producing systems by optimising the stability, nanostructuring, light-harvesting and ET properties of the working modules and interfaces	12

8. Key learning points

From the exploration of the selected topic, what are the key learning points?
(Resources, enablers, barriers, decision points, knowledge gaps, risks)

Decision points	Identification of ET competing pathways Synthesis of matrices for embedding (bio)catalytic working modules that improve their O_2 tolerance and stability Identification of nanostructured biocompatible plasmonic materials to boost the light harvesting and photochemical activity of the catalysts in medium-to-large scale devices
Knowledge gaps	
Risks	

Resources

Suggestion	Please detail
Critical, rare elements	
Non-fluctuating energy sources	

Hydrogen storage	
CO2 storage	
Water purification	
CO2 from the atmosphere	
Concentrated, pure CO2	
Specific, new infrastructures	
Low-cost, low-carbon electricity	
Renewable energy	
Renewable heat	

Breakthroughs in key enabling disciplines

Scale-Up	essential
System integration	Development of highly conductive interfaces that can improve DET and O2-tolerance of the catalytic modules. The biocatalysts have been used with novel matrices which show significantly improved O2 tolerance and stability.
Novel reactor designs	yes
Novel catalyst materials: earth-abundant, non-toxic, efficient, stable	yes for PRCs
Novel absorber materials: earth-abundant, non-toxic, efficient, stable	Use of natural light harvesting properties of biophotocatalysts that can be further improved by plasmonic resonance interactions
Standardized life-cycle assessment methodologies	Essential when developing medium-to-large scale devices

Further developments in quantitative sustainability analysis	yes
Strain robustness	Use of extremophiles for isolation of the most robust photosynthetic reaction centres and redox active enzymes
Genomic stability	
Preservation (culture collection)	

Political/societal/market barriers

EU-wide, homogeneous regulatory frameworks	
Adaptation/ novel regulations (e.g. genetics, use of waste CO2, ..)	
EU/national regulations for the deployment of the technology/product	
EU/national incentives for the deployment of the technology/product	
Fast idea protection (patenting, etc.)	
Large capital investment for market introduction	
Standardization of efficiencies, etc.	
Societal acceptance	
Political security	
EU supply chain	

Funding/research frameworks

International collaboration	X
Funding schemes for demonstrators, pilots, etc.	X
Large-scale EU research initiatives	X

Baggies with particulate systems

Technology								
Targeted product	H_2	NH_3	CH_3OH	EtOH	CH_4	Jet fuel	CO_2	Other
	X							

Nature of active material	X	Solid-state Inorganic		Molecular		Biomolecular		Biological (living cells)
Sunrise approach		PV-powered electrocatalysis	X	Photo(electro)chemical direct conversion		biological and biohybrid direct conversion		Key enabler*, Other
Device category		Electrolyzer		Photo(bio)electrolyzer	x	Photo(bio)reactor		fermentors, thermocatalytic reactors

Contribution to SUNRISE goals (what?)		Sustainable low-carbon production of carbon-based fuels with high efficiency and competitive costs
		Sustainable low-carbon production of carbon-based commodity chemicals with high efficiency and competitive costs
		Sustainable low-carbon production of ammonia with high efficiency and competitive costs
	X	Sustainable low-carbon production of hydrogen with high efficiency and competitive costs
		CO_2 as a valuable feedstock
		Sustainable building materials, mineralization, long-lasting C-based materials

Sustainability criteria		Carbon capture from the atmosphere
		Carbon capture from point sources/ flue gas
		Exclusive use of abundantly available, non-toxic and non-critical elements
	X	Sunlight as the primary energy source
	X	Low resource consumption
	X	Solar to products yields tenfold to hundredfold higher than current biomass practice

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<tr><td>Who are the main actors? Who has to be involved?</td><td colspan="7">Univ Tokyo
Tokyo Univ. Science
Dalian Institute of Chemical Physics
Jiangsu Key Laboratory for Carbon-based Functional Materials and Devices
Univ Houston
Kyoto Univ
Tokyo Tech
Mitsubishi
HyperSolar ? (UCSB)</td></tr>
</table>

* key enabler: fundamental for diverse technological approaches ° TRL: see Annex

Please indicate who gave concrete input; this is **optional**, but allows us to quantify the reach of the proposed technological solution.

Contributors	Leif Hammarström (Uppsala University)

1. Short description of the proposed technological solution

Main technological elements, working principle (max. 5 lines)	Simple and cheap baggie-type reactors where semiconductor particles in water solution harvest light and separate charge. “Co-catalyst” material is deposited to collect charges and catalyse HER and OER, respectively. The HER and OER reactions could occur on a single particle, or on separate particles. In the latter case, the HER and OER particles can be linked as tandem particles, or connected via a diffusional redox shuttle (e.g. iodate). HER and OER particles may be in separate bags (product separation).
Why is this technology not commercially available right	Present materials do not show good enough performance.

now? What are the major challenges?	
What does it take to make it happen? (in short)	Better materials. Better solutions for separating charge and connecting the HER and OER reactions. Product separation technologies
What is the benefit for society? (in short)	Sustainable H_2 production in scalable systems, for implementation in any desirable or necessary scale. Decentralisation of production of H_2 as fuel. Energy independence on local, regional and global level.

2. Existing R&I projects

Existing national/EU project	**Final objective**	**TRL**	**Run-time**	**Funding Instrument**
None in the EU?				
Good funding in Japan and Dalian				

3. State-of-the-Art: where are we now?

Technological solution to be developed in SUNRISE	**H2 from particulate systems**
TRL	3-5 (now), >10 (commercial) in 2050
Cost	Projected
Energetic conversion yield	2% record (*Nature Nanotech.* 2014, 9, 69–73). 1% realised on photocatalytic sheets (*Nature Materials* 2016, 15, 611–615)Typically <1% for solution systems
Stability	Several months today (best systems), > 5 years in 2050
Product separation yield	Depends on reactor design
Total energy demand [GJ/t]	Unknown

Electricity needs [GJ/t]	None
Energy demand utilities [GJ/t]	For separation and compression of product
Steam balance [GJ/t]	None
CO2 emissions [tCO2 eq/t] (cradle-to-gate, including feedstock production)	Probably comparatively low, depending on the manufacturing processes and recyclability.
Water consumption	Low
Air supply unit	no
Compressors	Yes
DOI References	

4. Available techno-economical analysis:

DOI Reference	James et al. (2009) “Technoeconomic Analysis of Photoelectrochemical (PEC) Hydrogen Production” https://www.energy.gov/sites/prod/files/2014/03/f12/pec_technoeconomic_analysis.pdf
Summary	H2 production at 1.63 USG/kg is possible

5. Deliverables, milestones

Define a set of deliverables that provide a series of stepping stones from the current state to the future application/vision. Define the associated time dimension.

Define time: short-/medium-/long-term, x years	Medium term (2 – 10 years)
Deliverable, milestone	• Improved charge transport and reduced charge recombination, allowing for much higher STH efficiencies than SOTA. • New methods for cheap product separation (single bag systems). Improved mass transport between HER and OER + good gas separating membranes (two-bag systems). • Good performance with only scalable catalyst elements.

Solved Challenges / Lifted barrier (in bullet points)	● A large range of functional materials discovered, many without precious elements. “Co-catalysts”, however, are based on precious/non-scalable elements (Pt, Ru, Rh, Ir) in all the best performing systems. ● Tandem systems with higher efficiency than a single bandgap system. ● Asymmetric single-particle systems with intrinsic electric fields, directing electrons and holes to the respective (HER and OER) catalyst.
What was necessary to solve the challenge? Did it depend on advances in other fields?	Research, mainly within this field. Improved methods for materials synthesis and characterization of nanoparticle structure and electronic properties.
TRL	5-7
Stability	Several months with less than 20% loss in efficiency
Energetic conversion efficiency	Target >5% STH
Scale	Demonstrate >1 m2 scale prototypes
DOI Reference	10.1039/c3cs60378d 10.1038/natrevmats.2017.50 10.1039/c5ee01434d 10.1021/ar300227e

Define time: **short-/medium-/long-term, x years**	
Deliverable, milestone	
Solved Challenges / Lifted barriers (in bullet points)	
What was necessary to solve the challenge? Did it depend on advances in other fields?	
TRL	
Stability	

Scale	
Energetic conversion efficiency	
DOI Reference	

Define time: short-/medium-/long-term, x years	
Deliverable, milestone	
Solved Challenges / Lifted barriers (in bullet points)	
What was necessary to solve the challenge? Did it depend on advances in other fields?	
TRL	
Stability	
Scale	
Energetic conversion efficiency	
DOI Reference	

Define time: short-/medium-/long-term, x years	
Deliverable, milestone	
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TRL	
Stability	

Scale	
Energetic conversion efficiency	
DOI Reference	

Link to TRL level

At TRL 5-6:

Production volume	
Light harvesting area needed per t/product	
Political/societal barriers to be overcome	
Market barriers to be overcome	

At TRL 7-8:

Production volume	
Light harvesting area needed per t/product	
Political/societal barriers to be overcome	
Market barriers to be overcome	

At TRL 9:

Production volume	
Light harvesting area needed per t/product	
Political/societal barriers to be overcome for market introduction	

Market barriers to be overcome	

6. Opportunity criteria

What are the criteria that make this technology an opportunity when ready?
Score the potential opportunity from 0 (very low) to 12 (very high).
Each contributor provides an individual score (we average afterwards).

Opportunity criteria	**Individual Score**

7. Feasibility criteria

What factors determine the feasibility of the final application?
Score the potential feasibility from 0 (very low) to 12 (very high).
Each contributor provides an individual score (we average afterwards).

Feasibility criteria	**Individual Score**

8. Key learning points

From the exploration of the selected topic, what are the key learning points?
(Resources, enablers, barriers, decision points, knowledge gaps, risks)

Decision points	
Knowledge gaps	

Risks	

Resources

Suggestion	**Please detail**
Critical, rare elements	
Non-fluctuating energy sources	
Hydrogen storage	
CO2 storage	
Water purification	
CO2 from the atmosphere	
Concentrated, pure CO2	
Specific, new infrastructures	
Low-cost, low-carbon electricity	
Renewable energy	
Renewable heat	

Breakthroughs in key enabling disciplines

Scale-Up	
System integration	
Novel reactor designs	
Novel catalyst materials: earth-abundant, non-toxic, efficient, stable	

Novel absorber materials: earth-abundant, non-toxic, efficient, stable	
Standardized life-cycle assessment methodologies	
Further developments in quantitative sustainability analysis	
Strain robustness	
Genomic stability	
Preservation (culture collection)	

Political/societal/market barriers

EU-wide, homogeneous regulatory frameworks	
Adaptation/ novel regulations (e.g. genetics, use of waste CO2, ..)	
EU/national regulations for the deployment of the technology/product	
EU/national incentives for the deployment of the technology/product	
Fast idea protection (patenting, etc.)	
Large capital investment for market introduction	
Standardization of efficiencies, etc.	

Societal acceptance	
Political security	
EU supply chain	

Funding/research frameworks

International collaboration	
Funding schemes for demonstrators, pilots, etc.	
Large-scale EU research initiatives	