NOVEMBER 2019

TECHNICAL APPENDIX

PART 4 - SUSTAINABLE CARBON CAPTURE AND SUNRISE KEY ENABLERS

Sunrise

SOLAR ENERGY FOR A CIRCULAR ECONOMY

SUNRISE

Solar Energy for a Circular Economy

Technological Roadmap

Technical Appendix

Part 4 - Sustainable Carbon Capture and SUNRISE Key Enablers

November 2019

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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 Carbon Capture

Carbon Capture by chemical absorption

Technology	**Capture of CO2 from industrial point sources by chemical absorption**							
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		Biological (living cells)
Sunrise approach		PV-powered electrocatalysis		Photoelectrochemical direct conversion		biological and biohybrid direct conversion	X	Key enabler*, Other

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
	Sustainable low-carbon production of hydrogen with high efficiency and competitive costs
X	CO_2 as a valuable feedstock
	Sustainable building materials, mineralization

Sustainability criteria

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

Envisaged production system	<table><tr><td></td><td>Decentralized distribution production</td></tr><tr><td></td><td>Large-scale production using existing centralized infrastructure</td></tr><tr><td></td><td>Large-scale production necessitating new infrastructure</td></tr></table>

Rough timeline (when?)	Short term (2020-25)		Medium term (2025–30)		Long term (2030–50)		
	TRL°8		TRL°9		TRL°		
Who are the main actors? Who has to be involved?	Main suppliers of amine technology: Fluor, Mitsubishi, Siemens (amino-acid), Aker solutions (Advanced Carbon Capture^{TM}), Shell (Cansolv) + Advanced systems: CO_2 solutions (enzymes), C_Capture						

* 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	Helene Lepaumier (ENGIE)

1. Short description of the proposed technological solution

Main technological elements, working principle (max. 5 lines, for scientists not expert in the field)	CO_2 emitted from industrial point sources is captured according to a cyclic absorption process using a solvent. Different types of solvents can be used (amine, amino-acid,carbonates), amine being the most commonly used. - In the absorber, the flue gas is injected at counter-current from the solvent: CO_2 reacts with the amine and the treated flue gas is released at the top. - The CO_2-rich solvent is then sent to the desorber where it is heated. . After heating of the solvent, the CO_2 is recovered and the solvent is regenerated and sent back to the absorber.
Why is this technology not commercially available right now? (major challenges)	This technology is already commercially available for CO_2 capture from Power Plant flue gases. The major challenges limiting the wide deployment of this technology for industrial CO_2 point sources are: - High energy requirements - Environmental aspects; solvent emissions, degradation, toxicity… - Costs (incl. Purification of the exhaust gas)

What does it take to make it happen? (in short)	R&D needs: - Scale-up at demonstration scale with industrial CO_2 sources - Development of advanced solvents with reduced energy requirements and increased stability
What is the benefit for society? (in short)	At the current stage, amine-based CO_2 capture is one of the most mature technology enabling to produce a CO_2 stream with a high purity and which could be applied for short-term commercial application.

2. Existing R&I projects

Existing national/EU project	Final objective	TRL	Run-time	Funding Instrument
Japan – COURSE50	Iron & Steel Industry: CO_2 Ultimate Reduction in Steelmaking process by innovative technology for cool Earth 50 – Pilot testing with proprietary solvent http://www.jisf.or.jp/course50/outline/index_en.html	7	Step 1: 2008-2012 Step 2: 2013-2017	
CEMCAP	Cement production: Evaluation and testing of CO_2 capture technologies for the cement industry in an industrially relevant environment	7	2015-2018	H2020
Norway	Cement production: Norcem's Brevik cement plant: testing of different carbon capture technologies included amine absorption	7	2013-2017	Climit-programme (Gassnova)
Norway	Waste-to-Energy and cement plants: Feasibility study for a large scale CO_2 capture plant (400 000 tpy CO_2) at Norcem Brevik (cement plant) and at Klemetsrud (Waste-to-energy plant) - 2019: Pilot testing with amine solvent at Klemetsrud (capacity : ~2000 tpy)	7	2018-2019	

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

Technological solution to be developed in SUNRISE	Amine-based CO_2 capture technology
TRL	7 (cement) – 7 (Iron & Steel) - 7 (Waste-to-Energy)
Cost	Cement plant (CEMCAP - 1 Mt clinker per year) + CAPEX: 76M€ (MEA) – 149 M€ (Chilled Ammonia Plant [CAP]) + OPEX: 76M€ (MEA) – 66 M€ (CAP) 80.2 € / t CO_2 avoided (MEA) // 66.2 € / t CO_2 avoided (CAP) // 83.5 € / t CO_2 avoided (membrane) Iron & Steel production: Average cost between 50-100 €/tCO_2
Energetic conversion yield	
Stability	Based on the levels of impurities present in the flue gas, risk of solvent degradation and emission
Product separation yield	> 90% CO_2 emissions captured
Total energy demand [GJ/t]	3.81 GJ/ton CO_2 (with Blast Furnace Gas) (announced to be able to reduce down to 2 GJ / t CO_2 with solvents improvements)
Electricity needs [GJ/t]	Specific power consumption: 0.52-0.55 GJ / t CO_2
Energy demand utilities [GJ/t]	Reboiler duty (CO_2 desorption): ~3.7-3.8 GJ/ t CO_2
Steam balance [GJ/t]	
CO2 emissions [tCO2 eq/t] (cradle-to-gate, including feedstock production)	Cement production: Equivalent CO_2 avoided: 64% (with MEA, reference solvent for amine technology) considering EU-28 electricity mix
CO2 quality	High (> 98-99%)
Water consumption	Yes
Air separation unit	No
Compressors	Yes (CO_2 compression unit)
DOI References	Cement production: 10.1021/acs.est.5b03508 – 10.3390/en12030559 - 10.3390/en12030542 Iron & Steel:

	Techno-economic study of integrated steel works with Oxygen Blast Furnace and CO_2 capture : 10.1016/j.egypro.2013.06.651 Iron and steel CCS study, Techno-economics integrated steel mill (IEA-GHG, 2013-04)

4. Available techno-economical analysis:

DOI Reference	Comparison of technologies for CO_2 capture for cement production: + 10.3390/en12030559 (2019) : Technical evaluation + 10.3390/en12030542 (2019) : Cost analysis Techno-economic study of integrated steel works with Oxygen Blast Furnace and CO_2 capture : 10.1016/j.egypro.2013.06.651 (2013)
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 (expected in 2023)
Deliverable, milestone	Large-scale demonstration of the CO_2 capture technology by absorption planned for waste-to-energy plant (Norway, 400 000 tpy) and cement plant (Norway, 400 000 tpy) by 2023.
Solved Challenges / Lifted barrier (in bullet points)	• Development of advanced solvent systems with a higher energy efficiency and an increased solvent stability. • Recovery of waste heat sources
What was necessary to solve the challenge? Did it depend on advances in other fields?	Technology already commercially available to capture CO_2 from Power Plants flue gas (e.g. Boundary Dam, 1 Million ton CO_2 per year) - TRL9
TRL	7 (Iron and Steel) – 7 (cement production) – 7 (Waste-to-Energy plants)
Stability	
Energetic conversion efficiency	
Scale	400 000 t CO_2 / year

DOI Reference	

Define time: **short-/medium-/long-term, x years**	Short-term
Deliverable, milestone	Evaluate the environmental risk associated with amine technology for industrial sources of CO_2
Solved Challenges / Lifted barriers (in bullet points)	
What was necessary to solve the challenge? Did it depend on advances in other fields?	Full characterization of the industrial flue gas composition (gaseous pollutants, dust, particles) Identification of mitigation measures (e.g. flue gas treatment)
TRL	
Stability	
Scale	
Energetic conversion efficiency	
DOI Reference	

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**
Technology maturity level for a short-term application	10
‘Production’ of a CO_2 stream with a high CO_2 purity	10

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**
Increase the energy efficiency	10
Development of advanced solvent systems with improved chemical stability and lower energy requirements	10 (e.g. enzymes promoted amines …)

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	- Level of CO_2 purity required for the further conversion steps - Techno-economic comparative assessment with other types of CO_2 capture technologies (membranes, calcium looping …)
Knowledge gaps	- Upscaling amine technology with industrial flue gases from cement production, Iron & Steel
Risks	

Polymeric membranes based carbon capture

<table>
<tr><th>Technology</th><th colspan="8">Capture of CO2 from industrial flue gases by Polymeric Membranes</th></tr>
<tr><td>Targeted product</td><td colspan="8"><table><tr><td>H_2</td><td>NH_3</td><td>CH_3OH</td><td>EtOH</td><td>CH_4</td><td>Jet fuel</td><td>CO_2</td><td>Other</td></tr><tr><td></td><td></td><td></td><td></td><td></td><td></td><td>X</td><td></td></tr></table></td></tr>
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</table>

system	X	Large-scale production using existing centralized infrastructure				
		Large-scale production necessitating new infrastructure				
Rough timeline (when?)	Short term (2020-25)		Medium term (2025–30)		Long term (2030–50)	
	TRL°7		TRL°8-9		TRL°9	
Who are the main actors? Who has to be involved?	HZG (Helmholtz-Centre Geesthacht) operated small container (≤ 25 m^2 membrane area) in real flue gas from a hard coal fired power plant Known activities also at NTNU and in particular and in much larger scale MTR (US company)					

* 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	Stefan Baumann (FZJ)

1. Short description of the proposed technological solution

Main technological elements, working principle (max. 5 lines, for scientists not expert in the field)	- Polymeric membranes separating CO2 from point sources such as flue gases. Typically two-stage process to achieve high purity (>95%) requiring turbomachinery, but very flexible due to its modular nature. Optimization to entire process chain (from CO2-source to conversion technology) possible/necessary. - Power consumption is key - Permeate vacuum – not feed compression. - A total separation needs a multi stage process. - Process needs very high permeance membranes (>1,500 gpu). - CO2/N2 mixed gas selectivity (25) is enough.
Why is this technology not commercially available right now? (major challenges)	- Tests in real flue gas revealed the necessity of flue gas pre-treatment increasing energy demand. This, of course, depends on the gas source. - Capture rate, purity, capture cost etc. highly depend on intended use of the CO2, which is often not well-defined.
What does it take to make it happen? (in short)	- Simulation and experimental verification of membrane modules at different point sources

	- LCA/TEA considering the entire process chain - Long term testing - Scale up
What is the benefit for society? (in short)	- Membrane technology is in contrast to many other technologies equally efficient at all scales and, thus, in particular useful for decentralized CCU. Today CO2 is not utilized efficiently from smaller point sources. - Moreover, membrane technology is flexible in capture rate and purity. In case of lower requirements with regard to CO2 purity and/or capture rate, the membrane process can be adapted requiring less turbomachinery and, thus, providing lower carbon footprint and less CAPEX/OPEX compared to high requirements - Low Capex , Low Opex[1] - Small footprint - Modular (containerized) construction - Uses (renewable) electricity , no steam - No emissions , no hazardous waste - Simple flow sheet , easy to operate - Cold start to steady state in 15 minutes

2. Existing R&I projects

Existing national/EU project	Final objective	TRL	Run-time	Funding Instrument
MemKoR	Test in real flue gas of coal fired power plnats both hard coal and lignite	6-7	2016-2019	COORETEC BMWi (German Ministry of Econominc Affairs and Energy)
NanoGloWa	?	?	?	EU
MTR	Pilot 20 TPD achieved, 200 TPD (~10 MW_{el}) planned	7-8? ?	2017 ?	DoE

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

Technological solution to be developed in SUNRISE	Polymeric membrane CO_2 Capture from point sources
TRL	6-7 (MTR maybe higher)
Cost	35-45 $/t_{CO2}$ (99.5%, 150 bar) at 40-80 % capture rate according to MTR[1]
Energetic conversion yield	N/A
Stability	Effect of relative humidity and impurities including particulates pre-treatment, e.g. drying, potentially required
Product separation yield	40-80% CO_2 separated depending on process design
Total energy demand [GJ/t]	Depending on process design
Electricity needs [GJ/t]	Depending on process design
Energy demand utilities [GJ/t]	Depending on process design
Steam balance [GJ/t]	No steam needed
CO_2 emissions [tCO2 eq/t] (cradle-to-gate, including feedstock production)	
Water consumption	Non
Air separation unit	No
Compressors	Yes
DOI References	https://doi.org/10.1016/j.ijggc.2016.07.033 https://doi.org/10.1016/j.ijggc.2015.03.010 https://dc.engconfintl.org/cgi/viewcontent.cgi?article=1015&context=co2_summit3

4. Available techno-economical analysis:

DOI Reference	
Summary	

5. Deliverables and milestones

[1] Baker et al. https://dc.engconfintl.org/cgi/viewcontent.cgi?article=1015&context=co2_summit3

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
Decentralized sources of CO_2	10

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	Scale-up Life Cycle Assessment
Risks	

Resources

Suggestion	Please detail
Critical, rare elements	Presumably no
Non-fluctuating energy sources	
Hydrogen storage	No
CO_2 storage	Yes
Water purification	No
CO_2 from the atmosphere	No
Concentrated, pure CO_2	Yes
Specific, new infrastructures	No
Low-cost, low-carbon electricity	
Renewable energy	
Renewable heat	

Breakthroughs in key enabling disciplines

Scale-Up	X
System integration	X
Novel reactor designs	X
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)	

Low Temperature Direct Air Capture

Technology	Low Temperature Direct Air Capture							
Targeted product	H_2:	NH_3:	CH_3OH:	EtOH:	CH_4:	Jet fuel:	CO_2: X	Other:
Nature of active material		Solid-state Inorganic		Molecular		Biomolecular		Biological (living cells)
Sunrise approach		PV-powered electrocatalysis		Photoelectrochemical direct conversion		biological and biohybrid direct conversion	X	Key enabler*, Other
Device category		Electrolyzer		Photo(bio)electrolyzer		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
		Sustainable low-carbon production of hydrogen with high efficiency and competitive costs
	X	CO_2 as a valuable feedstock
		Sustainable building materials, mineralization, long-lasting C-based materials

Sustainability criteria		
	X	Carbon capture from the atmosphere
		Carbon capture from point sources/ flue gas
		Exclusive use of abundantly available, non-toxic and non-critical elements
		Sunlight as the primary energy source
		Low resource consumption
		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
		Comment: Currently small scale for niche applications. Potential for decentralized but large scale production will probably be targeted to reduce cost

Rough timeline (when?)	Short term (2020-25)		Medium term (2025–30)		Long term (2030–50)	
	TRL 7		TRL 8		TRL 9	

Comment:	Comment: On the short term, Direct Air Capture will compete with capture from point source (DOI: 10.1021/acs.est.5b03474). DAC large deployment will probably not be observed before 2030, or even 2050, depending on emission reduction ambitions (Negative Emission to achieve targets in terms of climate change?)
Who are the main actors? Who has to be involved?	Climeworks, Antecy, Global Thermostat

* 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	Han Huynh (ENGIE)

1. Short description of the proposed technological solution

Main technological elements, working principle (max. 5 lines)	Direct air capture (DAC) is the physical or chemical **separation** and **concentration of CO_2** from **ambient air**. Actor such as Climeworks has developed Low Temperature Solid Sorbent DAC. Air is driven by fan and comes into contact with a filter material (solid sorbent) where CO_2 is absorbed. CO_2 is then released in the regeneration, an energy intensive step at 80-100°C. Absorption and desorption (regeneration) occurs in a cyclic process.
Why is this technology not commercially available right	This technology is not fully commercially available because of the following challenges:

now? What are the major challenges?	- Direct air capture technologies exist today, but are expensive: dilute stream magnifies costs - Low CO_2 concentration in the atmosphere (Around 400 ppmv vs 3-70% CO2 from point source) High energy demand to capture and regenerate solvent (4-5 times than capture from point source) - Need of low-carbon power and heat (Carbon footprint)
What does it take to make it happen? (in short)	R&D needs : - Solvent/sorbent: development of new solvents/sorbents with reduced regeneration energy requirements, improved kinetics and stability. - Contactors: designs with enhanced surface area, low pressure drop and reduced capital costs - Identification of renewable sources of electricity and especially heat – Better integration
What is the benefit for society? (in short)	Decentralized source of CO_2 In theory, DAC could be located anywhere DAC can capture the CO_2 emitted by sources that Point Source Carbon Capture cannot (e.g. planes) Modular systems that can be packed can lead to compact technology (0.4 - 1.5 km²/Mt CO_2 reported DOI: 10.1016/j.jclepro.2019.03.086)

2. Existing R&I projects

Existing national/EU project	Final objective	TRL	Run-time	Funding Instrument
	Demo plant in Hinwil. Capture rate: 2460 kg CO_2/day (900 ton/year), CO2 is sold to Gebrüder Meier for use in the greenhouse, waste heat supplied by the incinerator Kenzo	7	Commissioned on 31st May 2017	
CarbFix2	Demo Plant in Hellisheidi. Capture rate: 135 kg CO_2/day (50 ton/year), CO_2 is mineralized into carbonates underground and can be sold as a carbon compensation. Heat from geothermal.	7	Commissioned on 11th October 2017	H2020, R&I program. Grant agreement N° 764760

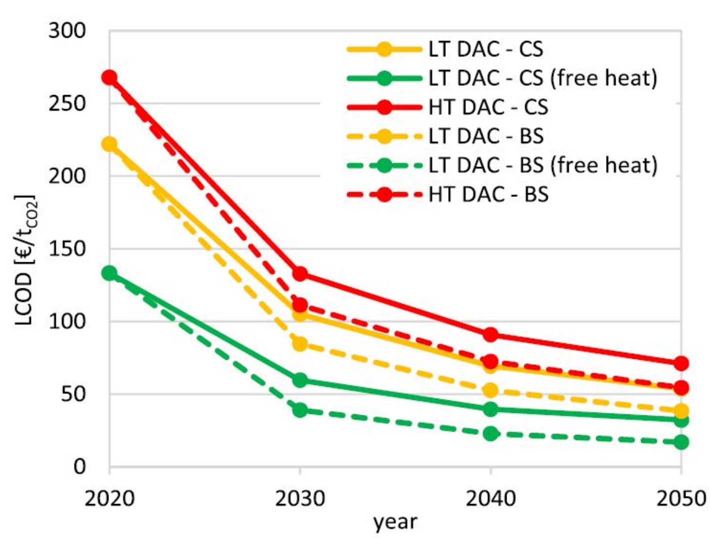
Kopernicus Power to liquid Fuel	Climeworks provides infrastructure to capture CO_2 from air. Liquid fuels production combining high temperature co-electrolysis (Sunfire) and Fischer-Tropsch-reactor (Ineratec).		Commissioned in 2019	Federal Ministry of Education and Research, Germany
Store & Go	Second-generation Direct Air Capture plants (DAC-3) in Troia, Apulia (Italy) – Lower energy consumption. Capture rate: 150 ton CO_2/year. The CO_2 will serve as a feedstock to methanation process Atmostat.		Commissioned in October 2018	H2020, R&I program. Grant agreement No 691797

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

Technological solution to be developed in SUNRISE	**Direct Atmospheric CO_2 Capture with a cyclic process using aqueous KOH sorbent**
TRL	7
Cost	Current cost: up to 600 €/ton CO_2 depending on assumptions. Cost reduction roadmap: Reduction to 300 €/ton CO_2 by 2022/2025 and to 100 €/ton CO_2 by 2025/2030
Energetic conversion yield	Not applicable
Stability	Effect of dust and atmospheric pollutants on sorbent filter material
Product separation yield	Not applicable
Total energy demand [GJ/t]	1.1 (electricity needs) + 7.2 (waste heat)
Electricity needs [GJ/t]	200-450 kWhe/ton CO_2 for fans and control systems
Energy demand utilities [GJ/t]	1500-2000 kWhth/ton CO_2
Steam balance [GJ/t]	
CO_2 emissions [tCO2 eq/t] (cradle-to-gate, including feedstock production)	Manufacturing: 0.069 kg CO_2 eq. per kg of captured CO_2 Use: Depending on the source of energy

Water consumption	+ 0.8-2 ton water / ton CO_2 (LT DAC captures water as a by-product)
Air separation unit	No
Compressors	Yes
DOI References	10.1016/j.jclepro.2019.03.086 Climeworks Company Presentation Glynn, ETSAP, 18th June 2018 Lozanovski, 17th ICCDU 2019

4. Available techno-economical analysis:

DOI Reference	10.1016/j.jclepro.2019.03.086
Summary	Current cost announced for DAC is high (some cases in the range of 400 – 600 €/ton CO_2). However, it is assumed that the maintenance costs will be reduced along with equipment capex due to mass production, along with lower energy consumption due to technical advances in the long term.  **Fig. 9.** LCOD for LT and HT DAC systems with 8000 FLh and 7% WACC for the conservative scenario (CS) and base case scenario (BS) assumptions.

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 (1-3 years)
Deliverable, milestone	Technology improvements, cost and energy reduction
Solved Challenges / Lifted barrier (in bullet points)	Improvement of sorbent and filter material : improved kinetics, better stability and lower regeneration energy Improved process design: optimization of air contactor, optimization of sorbent/solvent regeneration cycling concepts to maximize equipment usage intensity and minimize equipment degradation and material replacement requirements Identification of renewable sources of heat – Improved integration Alternative DAC technologies: Membrane...
What was necessary to solve the challenge? Did it depend on advances in other fields?	
TRL	7
Stability	
Energetic conversion efficiency	
Scale	
DOI Reference	**ICEF Roadmap 2018**

Define time: short-/medium-/long-term, x years	Medium-term (2-8 years)
Deliverable, milestone	Demonstration at 1000 t CO_2 /year
Solved Challenges / Lifted barriers (in bullet points)	
What was necessary to solve the challenge? Did it depend on advances in other fields?	
TRL	8

Stability	
Scale	
Energetic conversion efficiency	
DOI Reference	**ICEF Roadmap 2018**

Define time: **short-/medium-/long-term, x years**	Long-term
Deliverable, milestone	Demonstrate integrated system at 100 000 t CO_2/year
Solved Challenges / Lifted barriers (in bullet points)	
What was necessary to solve the challenge? Did it depend on advances in other fields?	
TRL	8-9
Stability	
Scale	
Energetic conversion efficiency	
DOI Reference	**ICEF Roadmap 2018**

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**
Decentralized sources of CO_2	10
Negative-emission technologies	10

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
Cost	10
Life Cycle Assessment	10
Development of sorbent with reduced regeneration energy and higher stability	10
Availability of abundant renewable energy	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	
Knowledge gaps	Scale-up Life Cycle Assessment (is it really sustainable in the end?)
Risks	

Resources

Suggestion	Please detail
Critical, rare elements	Presumably no
Non-fluctuating energy sources	
Hydrogen storage	No
CO2 storage	Yes

Water purification	No
CO_2 from the atmosphere	Yes
Concentrated, pure CO_2	No
Specific, new infrastructures	Yes
Low-cost, low-carbon electricity	
Renewable energy	
Renewable heat	

Breakthroughs in key enabling disciplines

Political/societal/market barriers

EU-wide, homogeneous regulatory frameworks	
Adaptation/ novel regulations (e.g. genetics, use of waste CO_2, ..)	
EU/national regulations for the deployment of the technology/product	
EU/national incentives for the deployment of the technology/product	Tax incentive: Legislation providing a tax incentive for DAC was enacted in the United States in early 2018. Known as the FUTURE Act or “45Q”. The law provides a tax credit of $28-50/t$CO_2$ captured from the air and stored in saline aquifers. The law also provides a tax credit of $17-35/t$CO_2$ captured from the air and used for enhanced oil recovery or converted into usable products.
Fast idea protection (patenting, etc.)	
Large capital investment for market introduction	X

Standardization of efficiencies, etc.	
Societal acceptance	X
Political security	
EU supply chain	

Funding/research frameworks

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

High Temperature Direct Air Capture

Technology	Low Temperature Direct Air Capture							
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		Biological (living cells)
Sunrise approach		PV-powered electrocatalysis		Photoelectrochemical direct conversion		biological and biohybrid direct conversion	X	Key enabler*, Other
Device category		Electrolyzer		Photo(bio)electrolyzer		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
		Sustainable low-carbon production of hydrogen with high efficiency and competitive costs
	X	CO_2 as a valuable feedstock
		Sustainable building materials, mineralization, long-lasting C-based materials

Sustainability criteria		
	X	Carbon capture from the atmosphere
		Carbon capture from point sources/ flue gas
		Exclusive use of abundantly available, non-toxic and non-critical elements
		Sunlight as the primary energy source
		Low resource consumption
		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 Comment: Currently small scale for niche applications. Potential for decentralized but large scale production will probably be targeted to reduce cost

Rough timeline (when?)	Short term (2020-25)		Medium term (2025–30)		Long term (2030–50)		
	TRL 7		TRL 8		TRL 9		
	Comment: On the short term, Direct Air Capture will compete with capture from point source (DOI: 10.1021/acs.est.5b03474). DAC large deployment will probably not be observed before 2030, or even 2050, depending on emission reduction ambitions (Negative Emission to achieve targets in terms of climate change?)						
Who are the main actors? Who has to be involved?	Carbon Engineering						

* 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	Han Huynh, Hélène Lepaumier (ENGIE)

1. Short description of the proposed technological solution

Main technological elements, working principle (max. 5 lines)	Direct air capture (DAC) is the physical or chemical **separation** and **concentration of CO_2** from **ambient air**. Carbon Engineering is the only actor using a solvent-based approach: - In the *air contactor*, CO_2 is captured by reacting with KOH to form K_2CO_3 The regeneration of the solvent uses a calcium caustic loop: - The solution is sent to a *pellet reactor*: K_2CO_3 reacts with $Ca(OH)_2$ which precipitates into $CaCO_3$ and regenerates the KOH solution - $CaCO_3$ is separated and sent to a *fluid-bed calciner* where it is decomposed to CO_2 and CaO at temperature around 900°C

	- In the *slaking process*, calcium hydroxide is regenerated via hydration of calcium oxide.
Why is this technology not commercially available right now? What are the major challenges?	This technology is not fully commercially available because of the following challenges: - Direct air capture technologies exist today, but are expensive: dilute stream magnifies costs - Low CO_2 concentration in the atmosphere (Around 400 ppmv vs 3-70% CO2 from point source) High energy demand to capture and regenerate solvent (4-5 times than capture from point source) - Need of low-carbon power and heat (Carbon footprint)
What does it take to make it happen? (in short)	R&D needs : - Solvent/sorbent: development of new solvents/sorbents with reduced regeneration energy requirements, improved kinetics and stability. - Contactors: designs with enhanced surface area, low pressure drop and reduced capital costs - Identification of renewable sources of electricity and especially heat – Better integration
What is the benefit for society? (in short)	Decentralized source of CO_2 In theory, DAC could be located anywhere DAC can capture the CO_2 emitted by sources that Point Source Carbon Capture cannot (e.g. planes) Modular systems that can be packed can lead to compact technology (0.4 - 1.5 km²/Mt CO_2 reported DOI: 10.1016/j.jclepro.2019.03.086)

2. Existing R&I projects

Existing national/EU project	Final objective	TRL	Run-time	Funding Instrument
	End-to-end DAC pilot plant operated in Squamish (Canada) including air contactor, pellet reactor, slacker, oxy-fired calciner, 1 ton CO_2 per day	7	Since 2015	
	Air-to-Fuel ™: pilot operated in Squamish (Canada) – 1 bbl/day of synthetic fuel with CO_2 captured from the atmosphere // Partnership with GreyRock	7	2017	
	Commercial validation for the engineering		2018-2021	

	and design of the world's largest DAC and sequestration plant (CE + Oxy Low Carbon Ventures) - Objective : 500 000 t CO_2 from the atmosphere per year - If approved, construction will start in 2021 with an operation in 2023.			

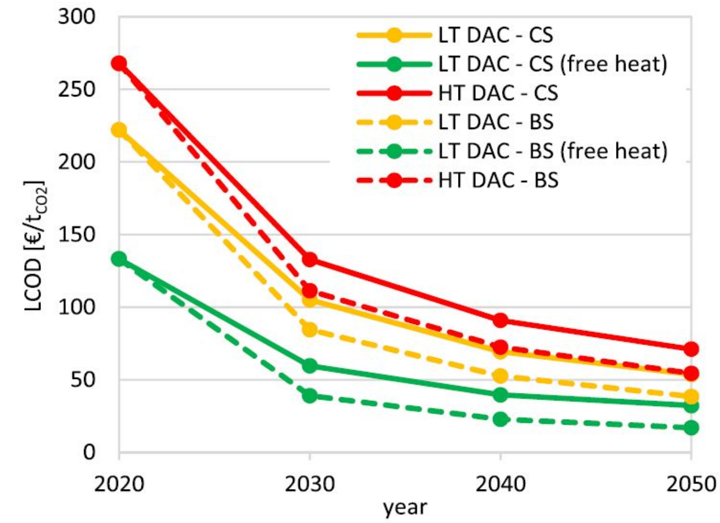
3. State-of-the-Art: where are we now?

Technological solution to be developed in SUNRISE	**Direct Atmospheric CO_2 Capture with a cyclic process using aqueous KOH sorbent**
TRL	6
Cost	Carbon Engineering: . 83-205 € / t CO_2 (announced by the supplier based on simulation data and pilot data of 1 ton CO_2/day) Socolow, 2011: 115-200 € / t CO_2 captured Fasihi, 2019: 186 € / t CO_2 captured
Energetic conversion yield	
Stability	Effect of dust and atmospheric pollutants on liquid sorbent solution
Product separation yield	~75 % CO_2 captured from the atmosphere
Total energy demand [GJ/t]	See document Joule: for CO_2 at 15 MPa. + 8.81 GJ (of CH_4) /t CO_2 extracted from the atmosphere for a process powered by natural gas only or 5.25 GJ of natural gas and 366 kWh of electricity /t CO_2 extracted = total 6.57 GJ/t CO_2 extracted Use of natural gas to supply high-grade heat demand + Air contactor: 82 kWh/t CO_2 (fan and fluid pumping energy) + Pellet reactor: 27 kWh/t CO_2 (fluid pumping energy) + Calciner: 4.05 GJ/t CO_2 + Slaker: 77 kWh / t CO_2 recovered (32 kWh/t CO_2 consumed) + ASU: 238 kWh/t CO_2 + CO_2 compressor: 132 kWh/t CO_2
Electricity needs [GJ/t]	366 kWh
Energy demand utilities [GJ/t]	5.25 GJ/t CO2 for high temperature heat (900°C)
Steam balance [GJ/t]	

CO_2 emissions [tCO2 eq/t] (cradle-to-gate, including feedstock production)	If the energy requirements are fully covered by using natural gas, then 0.5 ton of CO2 is 'released' per ton of atmospheric CO2 captured. LCA : doc 10.1016/j.ijggc.2018.11.011
Water consumption	Loss of water by evaporation Input estimated at 531 t / h H_2O (see fig 2 article Joule, to be confirmed?) / 4.7 tons of water per ton CO2 captured from the atmosphere at 20°C and 64 % Relative Humidity.
Air separation unit	Yes (use of pure O_2 during the calcination process)
Compressors	Yes (CO_2 compressor unit)
DOI References	Patent: US8119091 B2 10.1016/j.joule.2018.05.006 10.1016/j;jclepro.2019.03.086

4. Available techno-economical analysis:

DOI Reference	10.1016/j.jclepro.2019.03.086
Summary	Current cost announced for DAC is high (some cases in the range of 400 – 600 €/ton CO_2). However, it is assumed that the maintenance costs will be reduced along with equipment capex due to mass production, along with lower energy consumption due to technical advances in the long term.

	 **Fig. 9.** LCOD for LT and HT DAC systems with 8000 FLh and 7% WACC for the conservative scenario (CS) and base case scenario (BS) assumptions.

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 (1-3 years)
Deliverable, milestone	Technology improvements, cost reduction
Solved Challenges / Lifted barrier (in bullet points)	Improvement of sorbent and filter material : improved kinetics, better stability and lower regeneration energy Improved process design: optimization of air contactor, optimization of sorbent/solvent regeneration cycling concepts to maximize equipment usage intensity and minimize equipment degradation and material replacement requirements Identification of renewable sources of heat – Improved integration
What was necessary to solve the challenge? Did it depend on advances in other fields?	
TRL	7
Stability	
Energetic conversion efficiency	

Scale	
DOI Reference	**ICEF Roadmap 2018**

Define time: **short-/medium-/long-term, x years**	Medium-term (2-8 years)
Deliverable, milestone	Demonstration at 1000 t CO_2 /year
Solved Challenges / Lifted barriers (in bullet points)	
What was necessary to solve the challenge? Did it depend on advances in other fields?	
TRL	8
Stability	
Scale	
Energetic conversion efficiency	
DOI Reference	**ICEF Roadmap 2018**

Define time: **short-/medium-/long-term, x years**	Long-term
Deliverable, milestone	Demonstrate integrated system at 100 000 t CO_2/year
Solved Challenges / Lifted barriers (in bullet points)	
What was necessary to solve the challenge? Did it depend on advances in other fields?	
TRL	8-9
Stability	

Scale	
Energetic conversion efficiency	
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Knowledge gaps	Scale-up Life Cycle Assessment
Risks	

Resources

Suggestion	**Please detail**
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Non-fluctuating energy sources	
Hydrogen storage	No
CO2 storage	Yes
Water purification	No
CO2 from the atmosphere	Yes
Concentrated, pure CO2	No
Specific, new infrastructures	Yes
Low-cost, low-carbon electricity	
Renewable energy	
Renewable heat	

Breakthroughs in key enabling disciplines

Scale-Up	X
System integration	X

Novel reactor designs	X (improved design of air contactor)
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	X Tax incentive: Legislation providing a tax incentive for DAC was enacted in the United States in early 2018. Known as the FUTURE Act or “45Q”. The law provides a tax credit of $28-50/tCO2 captured from the air and stored in saline aquifers. The law also provides a tax credit of $17-35/tCO2 captured from the air and used for enhanced oil recovery or converted into usable products.

Fast idea protection (patenting, etc.)	
Large capital investment for market introduction	X
Standardization of efficiencies, etc.	
Societal acceptance	X
Political security	
EU supply chain	

Funding/research frameworks

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

SUNRISE key enablers

Computational materials modelling: from novel materials to solar fuel devices

Contributors: Carina Faber (UCLouvain), Henrik Koch (NTNU), Gian-Marco Rignanese (UClouvain), Thierry Deutsch (CEA), Julia Mortera (university roma tre), Marcus Lundberg (Uppsala University), Laura Lopez-Suarez (ICIQ), Irene Aguilera (FZ Jülich), Martin Roeb (DLR), Stefan Baumann (FZ Jülich)

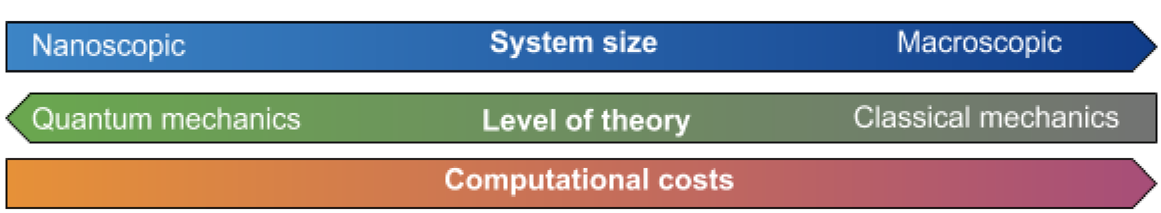
1. Priority research

1.1 Research Direction

The primary objective of *SUNRISE Computational Materials Modelling* is to employ advanced computer simulation techniques to guide experimental developments and to accelerate the large-scale deployment of SUNRISE technologies. An important challenge is the development and optimization of materials for artificial photosynthesis. Today's catalysts and photoabsorbers have to be significantly optimized in terms of efficiency and durability; novel materials are crucially needed that are earth-abundant and non-toxic in order to allow for a sustainable upscaling of the proposed technologies. Once efficient materials are found, these outcomes have to be tested in real device conditions and the nanoscopic scale has to be bridged to the macroscopic world.

The challenge is the intrinsic complexity of the considered thermo- and electrochemical, photoelectrocatalytic or bio-inspired systems, where one deals e.g. with complicated surface reactions, complex thermodynamic properties, the interplay between electrodes and electrolyte, photoabsorption and catalysis. Employed materials have to fulfill diverse requirements which are often competing and where a compromise has to be found. In order to allow for an efficient and targeted materials development, it is crucial to understand the underlying fundamental principles and reactions.

The ultimate goal is to describe a complete artificial photosynthesis system and its diverse reactions in a single simulation on the computer. However, this exceeds today's computational means and a compromise between accuracy and computational costs has to be made. The meaningful translation of results obtained on the nanoscopic onto the macroscopic level and vice versa is not straightforward.



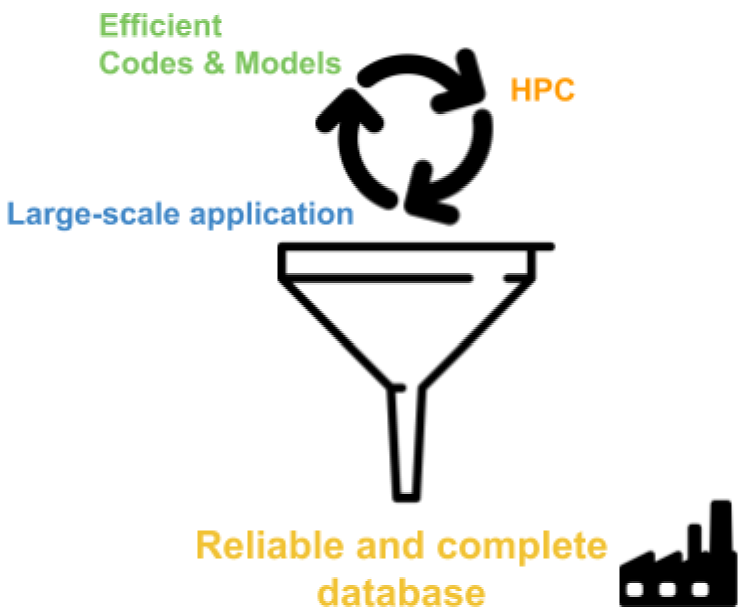
Reducing computational costs allows to treat systems comprising a large number of atoms or to screen millions of novel materials for their appropriateness.
Less demanding semi-classical or classical theories rely on empirical input parameters from experiment or take into account quantum properties only in an averaged way. They represent an important way of bridging the nanoscopic to the macroscopic world.
The purely quantum-mechanical level is inherently more demanding, but computational costs can be reduced by e.g. focusing on less demanding computational models. Another possibility of bridging nano to macro while limiting computational demands is to divide the system into different fragments; the most important part (e.g. the light absorption center in photocatalytic systems) is treated with high accuracy on the ab-initio level, whereas lower levels of theory are used to include the bigger part of the system. Another promising direction are machine-learning algorithms. These allow to predict properties of large systems based on the results of small constituents or to predict novel materials based on calculations of existing systems.

Treating materials for solar fuel systems by means of quantum-mechanical first-principles approaches seeks to predict material properties with high accuracy as compared to experimental measurements without depending on input parameters. For small systems or system parts (in the order of hundreds of atoms), underlying quantum-mechanical processes and fundamental principles are explored, which in the best case can be translated to a whole material class. Excited state properties, crucial in solar fuel devices for light absorption or charge transfer can be studied. For example, properties of excited electronic states and solid state diffusion, crucial in solar fuel devices for light absorption, charge transfer and ionic conduction, are accessible by this approach.

What is needed for efficiently predicting materials properties and translating these findings on the device level are four different dimensions (which inherently depend on each other and the advances made in one or the other field):

1) <u>Efficient and accurate codes and models</u>: methodological and code developments allow to calculate material properties both efficiently and accurately and to simulate real solar fuel device structures. Interfaces need special focus, since materials with an optimum property do not necessarily show the best performance in a device.
2) <u>High-performance supercomputers</u>: Innovation in HPC facilities and optimization of existing codes with respect to these infrastructures allows to go to more complex systems, higher reliability and billions of calculations of material properties.
3) <u>Large-scale application workflows</u>: simulations of artificial photosynthesis systems and calculation of material properties on a large-scale will prove the reliability of the developed methods and deliver key quantities for experimental studies;
   machine-learning algorithms allow for automated calculations and the study of millions of novel materials (combined with high-performance supercomputers). The lack of understanding of how to profit most effectively from artificial intelligence approaches for materials discovery and especially artificial photosynthesis has to be overcome. New big data analyses and high-throughput screening based on interoperable complex workflows will retrieve the most promising candidates instead of only predicting properties.

4) Efficient data sharing: reliable and complete databases are the prerequisite of all machine-learning approaches; the establishment of a SUNRISE database of most promising materials for artificial photosynthesis allows industry to pick out the most promising candidates and prevents a doubling of research efforts. The establishment of a common REST API allows to easily search in multiple existing databases and most promising candidates are selected using artificial intelligence.



1.2 Potential Impact

Materials design and discovery is a cross-cutting key enabler for the entire SUNRISE technologies. However, translating new materials from the laboratory to the market can take 10 to 20 years and is very expensive. According to the Energy Materials Industrial Research Initiative (EMIRI), advanced materials denote 50% of the manufacturing costs of clean energy technologies today and are expected to increase up to 80% in the near future. Significantly optimizing materials discovery crucially needs scientific breakthroughs to optimally design matter from the atomic up to the device scale.

Computational simulations can guide experiment, avoiding tedious sequences of trial and error in the lab; it significantly speeds up the innovation process and makes it much cheaper. Only the most promising materials are to be synthesized and tested in the lab and in solar fuel devices. Billions of hypothetical materials can be explored through high-throughput calculations and the most promising candidates are selected using artificial intelligence. Computational studies provide fundamental understanding enabling rational design. This accelerates the exploration, discovery and use of new high-performance, low-cost and non-toxic solar fuel materials.

2. Aims

2.1 Scientific Challenges

Challenge 1

Efficient and durable catalysts and photoabsorbers:

Challenge: catalyst durability is one of today's major issues for artificial photosynthesis technologies and new materials are urgently needed; in addition, catalysts reduce the energy needed for reactions; a small amelioration in catalyst efficiency has a large influence on energy reduction due to large-volume production of chemicals; also cheaper and earth-abundant materials have to be found, since today's low temperature catalysts rely on precious metals (e.g. platinum); the challenge is the large number of possible novel materials, too expensive and time-consuming to synthesize all in the lab. machine-learning approaches are most promising, but have to be transferred into the field of materials discovery; meaningful descriptors and structure-property relationships have to found for data-driven methods;

Modelling contribution: Ab initio high-throughput calculations allow for an efficient screening of thousands of candidate materials for novel catalysts and absorbers, which can drastically reduce the costs of the experimental materials search by direct synthesis. Whereas density functional theory can provide the ground state properties at a reasonable ratio of computational cost and accuracy, the treatment of excited state properties (like, e.g., the efficiency of photoabsorption) requires a higher level of theory. This can be achieved, for example, with many-body perturbation theory in the GW and the random-phase (RPA) approximations.

In spite of their computational cost, high-throughput calculations based on devoted workflows using a combination of DFT and many-body perturbation theory will reliably provide the candidates to be subsequently synthesised in the lab. As an example of such a workflow, one can start with density-functional theory to calculate structures and phonons, followed by many-body theory calculations for excited states properties.

Impact on: up-scaling of electrolysis (cheaper, earth-abundant, energy-efficient catalysts), photocatalysis (efficiency, sustainability, ..)

Challenge 2

Interfaces and hybrid structures:

Challenge: complex systems consisting of surface electrode, electrolyte, catalyst, absorber; all these different parts interact; state-of-the-art: model the whole system is too expensive for today's first-principles methods; therefore, most calculations done in vacuum; but crucial to understand the physical and chemical processes and to optimize the different parts taking into consideration the influence of the rest of the system; values of the calculated quantities significantly change!

Modelling contribution: since it is not possible to find in a reasonable time the configuration of the interfaces only by modelling, one needs to combine modelling and characterisation:

develop methodologies **combining nano-characterizations (cryo-TEM, FIB-SEM, HRTEM, 3D tomography)** and simulations (on the DFT and on higher level) able to simultaneously **characterize interfaces and** treat interacting parts of the device at reasonable computational cost; come as close as possible to experimental conditions;

Impact on: electrolysis, photoelectrocatalysis bio-approaches (understanding fundamental principles, ..), thermochemistry (gas-solid and solid-solid interfaces, surface absorption processes...)

Challenge 3
Charge accumulation and charge transfer:
Challenge: for solar fuel conversion, multi-electron multi-proton electrocatalytic processes; photogeneration of excited electrons and holes through light absorption on eventually already charged light absorbers; afterwards, dark, not light-driven, potential-driven electrocatalytic reactions; Molecular bonds are created through heterogeneous electrocatalysis at at a liquid electrolyte-solid interface.
Modelling contribution: go beyond ground state, calculate structure of excited state, photoabsorption of charged states; interfacial electron-transfer; advances in multi-electron multi-proton electrocatalysis (H2 evolution, CO2 reduction, water oxidation...); go beyond Marcus theory for charge-transfer;

Challenge 4
Dynamics of fuel forming reactions
Challenge: catalyst functioning, reaction kinetics, reaction barriers, multiple-electron/proton-coupled reactions;
Modelling contribution: time-dependent approaches, excited state, out-of-equilibrium processes;

Challenge 5
Ionic conduction
Challenge: The conduction of mobile species such as oxide ions in crystal systems is a crucial factor determining reaction kinetics and phase stability. It is necessary to develop methods for high throughput molecular dynamics calculations to model the ionic conduction in dependence of external parameters such as the temperature or electric fields.
Modelling contribution: high throughput molecular dynamics calculations with *ab-initio* calculation of force fields, potential overlap and combination with DFT calculations, automated data evaluation and calculation of properties such as the diffusion coefficient.

Challenge 5a
Thermodynamic properties
Challenge: Especially in the case of thermochemical reactions, the redox thermodynamics are a crucial factor governing the applicable temperature and atmosphere and the resulting redox energetics.
Modelling contribution: Evolution of thermodynamic models and further development of existing ones (such as in Vieten *et. al.*, DOI: 10.1039/C9EE00085B) including additional factors like vacancy concentration, ordered and disordered (solid solution) phases and high level accuracy with respect to temperature dependent effects.

Challenge 6
Direct conversion via bio-inspired systems
Challenge: especially for bio-approaches, systems contain non-negligible number of atoms; emerging concepts are e.g. organized assemblies of active (supra)molecular/biomolecular components or hybrid systems combining supra/biomolecular assemblies with nanostructured

materials (semiconductors, 2D-materials, possibly metal-organic frameworks); describe photoenzymes (assemblies of light-absorbing / electron-transport / catalytic units in proteins, *de novo* proteins)
Modelling contribution: treat systems with several thousands of atoms with unprecedented accuracy on ab initio level; multi-scale and embedding approaches, machine-learning on smaller units to predict whole system;

Challenge 7
Interoperable advanced workflows mixing simulation and characterisation
Challenge: it is becoming an established standard that one needs to use parallel computing and GPUs and many codes have already implemented this. To go one step further, it is now really important to have complex workflows mixing characterisation data and processing data, simulation associated to databases and machine learning. The challenge is to converge HPC, HPDA (High Performance Data Analytics), HTC (High Throughput Computing) and Characterisation data processing.
Current HPC structures allow to calculate material properties using thousands of processors at the same time (in parallel) using one method. Today, nano-characterisation methods need HPC to process large data in order to provide very accurate 3D information. This information can be used in simulation to refine models or calculate electronic properties. GPUs-based HPC , HTC (High Throughput Computing) and HPDA (High Performance Data Analytics) should be combined with the data processing from nano-characterisation. This necessitates the collaboration of different communities physicists/chemists/biologists who develop code and complex workflows with IT specialists.
Modelling contribution: Development of interoperable advanced workflows mixing simulation and characterisation.

Challenge 8
Bridging scales
Challenge: lengths scales: device modelling; millions of atoms,: bridging real devices to nanoscopic calculations (also related to Challenge 2, how to treat interfaces); time-scales: light absorption occurs in femtoseconds, vibrational relaxation in picoseconds, chemical bond formation in picoseconds; developed materials have to be stable for decades; different theories for each of these length and time scales, systematic methods connecting scales crucially needed. need reference calculations (very costly) to validate the different approximations
ex: large linear scaling DFT calculations (100,000 atoms) to validate QM/MM approaches and higher;
Modelling contribution: develop methods coupling different levels of theory, e.g. first principles - molecular dynamics - multiphysics - process simulation

Challenge 9
Efficient data sharing
Challenge: A European database containing reliable material properties of the most promising materials for artificial photosynthesis allows industry to quickly identify materials with the desired properties. Results are efficiently and reliably exchanged in between and between different communities, for the quantum-mechanical and the device community.
Modelling contribution: High-throughput screening studies allow to calculate material properties on the large-scale and to identify best-suited candidates. Nowadays, several large material

databases containing properties of millions of existing and hypothetical materials are already freely accessible:

- the AFLOW distributed materials property repository
- the Harvard Clean Energy Project Database
- the Materials Cloud
- the Materials Project (including the use of MPContribs)
- the NoMaD (Novel Materials Discovery) Repository
- the Open Quantum Materials Database
- the Computational Materials Repository
- the Data Catalyst Genome
- the ioChem-BD Platform
- …

Given this diversity and the relevance of certain databases for SUNRISE technologies, creating a completely new database is not necessarily required and risks to waste computational resources by repeating already existing calculations. However, formats, protocols and criteria (e.g. on the accuracy) differ strongly between the databases. One possible solution is to support efforts aiming at making materials databases interoperational by developing a common Representational State Transfer Application Programming Interface (REST API). This would clearly allow industrial stakeholders to interrogate all those databases as if there was one huge database. In a next step, the existing databases have to be complemented with new calculations targeting both specific materials and properties for artificial photosynthesis. Once key material properties for device design are identified, automated scripts searching the database for the most relevant results have to be developed and data scientists specialized in retrieving reliable data have to be trained. This database will facilitate the use of data mining and machine learning techniques in the future.

Challenge 10

Multivariate statistical analysis of complex systems

Challenge: The availability of large datasets, composed by a large number of variables (possibly with mixed measurement levels) and a very large number of observations, is a key feature of this project and a challenging multi-facet problem. It can be handled by modern statistics with the following approaches: probabilistic expert systems, causal inference and mixture models.

Modelling contribution:

Probabilistic expert systems

Probabilistic expert systems (PES), or Bayesian networks (BNs), are ideally suited to model complex multivariate interconnected systems characterized by having a large number of observations on many variables with complex structural interrelationships. The variables involved can be categorical, discrete, continuous, latent, unknown parameters and hypotheses. PES (and BNs) consists of two elements: the graphical representation (the network) and the inference engine. The statistical inference is simplified via a reduction of the global problem into local sub-problems, with no loss of information. Efficient algorithms exist that perform both the structural learning of the network and the inference. A key role is played by conditional independence relationships which yield the modularity of the graphical representation. The modularity makes PES an effective tool for dealing with complex problems by simplifying them both computationally and logically. Furthermore, PES can be augmented with decision and utility (cost) nodes yielding a decision support system under uncertainty. Another important feature of BNs is their importance in causal reasoning, since causal mechanisms can be easily represented by means of a network.

The advantages of using PES for this project are: they can exploit information about past events to predict the likelihood of future events; they can handle and interpret large, also incomplete data sets; they can help integrate information coming from different data sets with knowledge from experts; they can incorporate different types of variables (categorical, discrete, continuous, latent, unknown parameters, hypotheses) within the same model. Thanks to the inferential engine, they can quickly assess the impact of many different strategies and scenarios, performing so-called *what-if* analysis. All these features will help provide better, more flexible and robust strategies.

<u>Causal relationships</u>

Frequently, data come from observational studies, where several factors are outside statistical control, and play the role of confounders. In these circumstances, the comparison of results under different treatment levels becomes difficult, since parametric and non-parametric *standard* statistical methods (T-tests, Anova F-tests, Wilcoxon-Mann-Whitney test, etc.) cannot be used. The main problem is that *standard* methods are prone to a non-negligible source of bias: receiving a treatment is not a *purely random* event, and there could be relevant differences between observations corresponding to different treatment levels.

A promising approach consists in weighting observations on the basis of a preliminary estimate of the probability of receiving the treatment given the covariates. Using this approach, estimates of the distribution function (d.f.) of the variate of interest under treatments can be obtained. Such estimates essentially play a role similar to the empirical d.f. in nonparametric statistics, and paves the way to develop weighted versions of statistical methods to compare the effects of different treatments, and to discover possible causal relationships, mainly in a non-parametric perspective. Causal relationships could be also analyzed by using Bayesian Networks (BN), that have in addition an excellent potential role in estimating the probability of receiving treatments given the covariates. This could prelude to an integrated use of BNs and weighting methods.

<u>Environmental statistics using mixture models</u>

Environmental data take often the form of multivariate space-time series that include the observations on many variables at multiple points in time and space. These data are typically observed under heterogeneous conditions that vary across time and space. Such heterogeneity is often the source of complex correlation structures between the measurements, which complicate the identification of relevant patterns. Statistical mixture models address the heterogeneity issue by decomposing the joint distribution of the data according to a finite number of classes, which represent the conditional distributions of the data under specific environmental conditions. These conditional distributions have often simpler correlational structures than the joint distribution, and, therefore, they can be exploited to facilitate the identification of relevant patterns in environmental data. Two specific families of mixture models are of main interest in environmental studies: the hidden Markov models and the hidden Markov random fields (also known as hidden Gibbs fields), which respectively account for latent environmental conditions that vary over time and across space. These models were originally developed for Gaussian data, more recently, hidden Markov models have been extended to accommodate multivariate skew and heavy-tailed distributions and provide a standard strategy in the analysis of environmental data.

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

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1. Priority research

1.1 Research Direction

The rapid pace of technology development requires the development of new methods and software for the rapid assessment of the environmental, economic, and social impacts of emerging technologies. Existing methods also lack integration and new avenues of research should be explored.

Methods such as life cycle assessment (LCA), techno-economic assessment (TEA), and social impact assessment (SIA; e.g. including the study of societal acceptance of new technology) should be integrated and expanded. Current methods are able to assess existing, well-defined technological systems, but come short when emerging technologies need to be assessed and recommended, mainly because of two major gaps:

- Lack of data coverage for e.g. processes, environmental exchanges, market dynamics, social implications of technology diffusion, technology transition monitoring, etc.
- All models assess emerging technologies with existing methods, data, and software tools.

1.2 Potential Impact

Assessing the environmental, economic, and social impacts of emerging technologies early in innovation allows steering technology development towards more sustainable pathways. The development of a new set of methods and tools will allow a more effective support of technology and application design, and will allow early go/no-go decisions as well as frame the conditions for producing, distributing, storing and using renewable chemicals and fuels.

2. Aims

2.1 Scientific Challenges

<u>Challenge 1</u>

For all three sustainability dimensions:

- Combining qualitative and quantitative approaches
- Analysis (from the past, experimentation) → methodologies → tools
- Work with uncertainties of technology specification and of upscaling process (e.g. degree of efficiency, upstream products used, quality of output products achieved).
- Use new data sources, expand data collection to web, trade statistics, production data, material composition data, or use existing data sources in a novel way.
- Use qualitative techniques and consult technology experts to enlarge the pool of representative stakeholders.
- Use advanced techniques to harvest data from sparse data sources (e.g. using artificial intelligence to fill specific data gaps, e.g. inferring material and energy requirements from similar technologies, and from technological learning in the past). Additionally, use qualitative approaches, such as experimental economics, ergonomics, cognitive sciences.
- Use advanced techniques of data science (including knowledge management) to incorporate technology road-maps, policy interventions, and policy scenarios (e.g. 2°C scenario) in existing databases to ensure an adequate evaluation of impacts.
- Provide dynamic data sets and allocation methods in appropriate timely and special resolution considering fluctuating inputs, outputs and co-products and its application.
- Support decision-making including uncertainty information with results.
- Include decision theory techniques in the assessment of trade-offs and win-wins across the dimensions of sustainability.
- Consider the value-dimension of sustainability using an adequate system of indicators (related to the improvement of the measurement).
- Develop a SUNRISE indicator set and assessment methodology applying a multi-stakeholder approach along the value chain as well as the directly and indirectly impacted groups.
- Developing new methodological and software solutions to integrate the three dimensions of sustainability.

<u>Challenge 2</u>

Environmental (LCA):

- Develop new impact assessment methods for emerging materials (e.g. nanomaterials).
- Expand existing impact assessment methods to account for emerging materials and emerging technologies.
- Consideration of technology improvements for incumbent technologies (e.g. learning curves, upscaling scenarios and principles for the production of solar photovoltaics and batteries).
- Defining and adequately assessing multiple functional units and fluctuating process parameters and its dynamic impact representation and allocation.
- Focus on impacts from land and water-use (e.g. water footprint for hydrogen production)
- Impact of purification steps on energy demand
- Impact of Sunrise technologies on the change of impact of up-and downstream processes

- Assessment of co-products and by-products and their management
- Assessment of material scarcity
- Enhancement of standard methods with direct collaboration with experts, from e.g. climate science, scenario modelling

Challenge 3

Economic (TEA):

- Get an idea of the upscaling potential and cost at scale (e.g. learning curves, economies of scale)
- Policy effects
- rationalize H2 transport as a Trans-European Network (TEN)
- Market dynamics for renewables
- Market studies: supply, demand, governance, business models
- Investment potential and financial opportunities
- Actors: users, industries, authorities, financial funds, etc.
- Technological-risk analysis: financial, safety, landscape, etc.
- Integration of plants in municipal and landscape and water management

Challenge 4

Social (SIA):

- Social acceptance of technologies
- Social life cycle assessment
- Impact on climate-resilience as well as social inclusion and global equality
- Hydrogen transport and storage; welfare;
- Risk/safety
- Labor competences
- Communication
- Demonstrator/pathways of SUNRISE technologies, and comparison with historical trends for cognate technologies.

Challenge 5

Software development

- “Standardize” software in a way that it becomes useful to technology and application developers
- Speed up the sustainability screening process using state-of-the-art methodology, but in a way that it is quick and useful outside of academia
- Develop software that can support the assessment of SUNRISE technologies

- Integrate the environmental, economic and social dimensions practically in such a software, taking into account also decision theory techniques (e.g. multi-criteria decision analysis) to assess trade-offs across the dimensions of sustainability

- Develop a standard SUNRISE next-level tool for technology developers

2.2 Timescale:

What can be achieved in 1 year

- Reach out to existing initiatives (e.g. working group on LCA of CCU from Climate KIC, and DG Energy)
- Demonstrators feedback of selected technologies
- Define pathway to approach data-gaps
- Support demonstrator selection in SUNRISE through review of the relevant literature

What can be achieved in: 3 - 5 years

- Development of methods and software
- Creation of a platform for the assessment of the impacts of emerging technologies integrating all dimensions of sustainability
- Detailed sustainability assessment of SUNRISE technologies
- (New) Research questions, especially in relationship to the social aspects of new technologies

What can be achieved in 10-20 years

- SUNRISE methodologies and software recognized and adopted by the international community
- (New) questions to research

Redesigning photosynthesis for the biocatalytic production of chemicals and fuels

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1. Priority research

It is clear that the sustainability of bioeconomy cannot in a long-term be guaranteed only by exploiting and refining conventional plant biomass. Truly sustainable biofuel and chemicals production platforms relying on novel and advanced technologies are needed. This is possible by using the unique photosynthetic machinery of cyanobacteria and microalgae, either natural or re-designed. The main aim is to identify limiting factors of natural photosynthesis and to overcome these challenges for efficient photosynthetic bioproduction.

1.1 Research Direction

The photosynthetic machinery comprises a unique system where solar energy is utilized for the conversion of CO_2 into organic chemical bonds. Photosynthesis allows application of algae and cyanobacterial ***biomass*** in industrial production of different natural products. Large investments to develop R&D for new 'biorefinery' algae plants worldwide are currently being undertaken (*e.g*. USA DoE recently granted 17M$ to 7 projects to improve the efficiency of carbon utilization and productivity of algal systems and announced 79M$ for bioenergy R&D including intensification of algae cultivation, algae synthetic biology topics). Today around Europe about 150 SMEs (according to the EABA report) are involved in the algal business (*e.g*. Simris Alg, AstaReal AB, Algae Factory in Sweden, Algalif in Iceland, Ecoduna in Austria, MIAL, Cyano Biotech GmbH, BlueBioTech, Astaxa etc in Germany, Algaenergy in Spain, Fermentalg, Greensea in France and so on). There are ongoing projects which are based on algal CO_2 capture (as much as 40%) from cement plants before it enters the atmosphere. It is noteworthy that in most cases the algae companies using biomass for biorefineries have turned their focus from biofuel production to high-value products since it became clear that the biofuels derived from algae biomass would not be able to compete in price on the open market sector. However, the recently introduced and fast-progressing revolutionary ***synthetic biology*** toolboxes have opened enormous perspectives for the realization of algal-based production of renewable and sustainable biofuels and chemicals (see the child synthetic biology PRD). There are dozens of proof-of-concepts for ***direct production of a diversity of fuels and chemicals*** from sunlight using algae and cyanobacteria as real biocatalytic hosts secreting out the produced chemicals in continuous cultures. The second promising strategy includes the biohybrid systems, where photosynthetic microalgae or cyanobacteria function as biological solar cells (BPVs) harvesting solar energy and generating electrical current or acting as a component of a 'bionic leaf'. In this case, the advantage of the photosynthetic organisms over traditional catalysts is that they can repair damaged complexes and are able to survive under different environmental conditions, thus offering long lasting catalytic stability (see the child PRD Biohybrids). For these reasons, the DOE and USDA in the United States have recently made the decision to **consider microalgae as crops**.

Both biological approaches described above and in the generic (Emerging approaches 3) and two child PRDs ('Biohybrids' and 'Synthetic biology') integrate two cutting edge research fields: (i) fundamental photosynthesis in microbes; and (ii) man-made systems mimicking and/or fine-tuning natural photosynthesis. In all cases, a thorough understanding of photosynthesis is a starting point for developing robust industrial host organisms enabling the successful development of clean production technologies.

The theoretical light-to-product conversion efficiency of photosynthesis is about 10-13%. Even if the charge separation and the primary processes of photosynthesis occur at very high efficiency (nearly 99% for Photosystem -PS- I), the tight regulation mechanisms developed during the millions of years of evolution downscale the photosynthetic light reactions and instead favor cell fitness and survival under different environmental conditions. Thus, in the best case, 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%). A major challenge is to fine-tune photosynthesis for:

- o increasing biomass production (during feedstock production) and
- o the development of direct solar energy conversion technologies and cell factories.

1.2 Potential Impact

Scientific impact: User-inspired fundamental research will serve the molecular-level understanding of the efficiency and regulation of photosynthesis, the most unique and important process maintaining life on Earth.

Societal impact*:* Development of advanced biotechnological processes for direct solar energy conversion, CO_2 capture, nutrient recycling and their implementation through applied science. This will mitigate climate change and help in developing new strategies whose implementation would pave the way towards truly sustainable future economies and societies. Particular emphasis will be put on increasing both societal and political awareness of the feasibility of blue bioeconomy and novel emerging technologies including synthetic biology concepts.

2. Aims

2.1 Scientific Challenges

Challenge 1. Optimization of photosynthetic electron transport for improved solar-to-reducing power (bioproduct) conversion

- Photosynthetic light reactions. Increase the photosynthetic efficiency by enhancing light penetration (*e.g.* by truncating large light harvesting antenna and mitigating unwanted energy dissipation processes), by optimizing the stoichiometry of macromolecular complexes devoted to photochemical light energy conversion (and downstream electron flow); broaden the absorption spectrum range to improve solar light spectrum utilization.

- The mechanisms of photodamage to photosynthetic components, particularly the damage of PS II and PS I and their repair mechanisms. Increased knowledge of ROS production and action mechanisms in combination with interactive regulation networks that protect the photosynthetic machinery against photodamage upon solar energy conversion into chemical energy, will be used in redesigning the photosynthetic regulation for purposes of SUNRISE technology developments.
- Identification and elimination of waste points in photosynthetic light reactions.
- The role of *pmf*, ion channels and transporters, Cytochrome b_6f in regulation of photosynthetic electron transport chain.
- The redox and metabolic switches that regulate the distribution of photosynthetically excited high-energy electrons into various end products.
- Thylakoid membrane structure: analysis of proteins and lipids shaping thylakoid membranes
- Exploit biodiversity to obtain robust strains in terms of growth in industrial compatible conditions (temperature, CO_2 availability, flue gases). These strains will constitute the chassis of the next generation biofuel / chemicals production.

Achieved knowledge will enable efficient production of photosynthetically reduced ferredoxin (Fed) and NADPH for further utilization of the electrons in biological and biohybrid systems for bioproduction. Improvement of photosynthetic linear electron transport chain from water splitting to the reducing power will be evaluated as an efficient coupling of reductants (i) with redox enzymes for a direct synthesis of targeted chemicals *in situ* (also referred to as ‘oxyfunctionalization’ or ‘whole-cell biotransformation”, (ii) for biophotohydrogen production by green algae or cyanobacteria and (iii) for coupling with novel enzymes or engineered bacteria in electrochemical devices (see a child PRD Biohybrids).

Outcomes: (i) Efficient oxyfunctionalization or whole-cell biotransformation by photosynthetic organisms. A whole-cell photosynthetic biotransformation has remarkable potential in green chemistry due to the sustainable mode of producing a wide range of desired chemicals in a ‘substrate in - product out’ manner with small environmental impact. In this approach the redox enzymes, *e.g.* Baeyer-Villiger oxidases are directly coupled with the photosynthetic light reactions to catalyze a specific chemical reaction by utilizing photosynthetically produced reducing cofactors (NADPH, reduced ferredoxin) and O_2. This approach enables the conversion of a given substrate to a defined end-product and, in contrast to heterotrophic systems, can take advantage of photosynthetic production of O_2 and renewable reducing equivalents. Strategies to increase the reaction rate will include increasing availability of reducing equivalents, and mining diverse novel enzymes with different cofactor preferences.

(ii) Photobiohydrogen production. Many photosynthetic cyanobacteria and green algae are capable of catalyzing biological photohydrogen production via direct water biophotolysis or indirect photolysis. Despite great potential, there are many metabolic hindrances and technological barriers to the application of algae and cyanobacteria for H_2 photoproduction at industrial levels. The major metabolic bottlenecks include: (i) the high sensitivity of enzymes involved in H_2 metabolism (hydrogenases and nitrogenases) to O_2; and (ii) alternative electron transport pathways competing for photosynthetic reducing power. Recently, several protocols have been developed for induction of efficient H_2 photoproduction (light-to-hydrogen conversion efficiency, LHCE) in algal cultures (LHCE up to 1,7 - 4%) and will be further improved up to theoretical maximum 10-13% by applying the above mentioned strategies to photosynthetic light reactions and by:

- Managing competing pathways (using switchable devices) to boost H_2 production without reducing the cell fitness and introducing new components such as novel or more efficient and O_2 tolerant enzymes.
- Mining novel, more efficient and O_2 tolerant hydrogenases and nitrogenases (including metatranscriptomics, metagenomics)
- Uncover electron-transport network in heterocyst of N_2-fixing cyanobacteria in order to increase H_2 production
- Developing novel protocols and cultivation strategies for induction of efficient and long-term H_2 photoproduction in green algae and cyanobacteria.

Challenge 2. Coupling efficient photosynthetic light reactions with CO_2 fixation

Improving existing enzymes and pathways for CO_2 concentration, to replace wasteful photorespiration pathways with more cost-effective ones by introducing novel efficient biological and synthetic components. Managing competing pathways to increase the efficiency and rate of CO_2 fixation. Optimizing carbon fluxes towards production of targeted chemicals rather than sugar reserves.

- Maximizing carbon flux through existing and introduced pathways to achieve economically relevant titers. Improving existing pathways and introducing new components or pathways, including novel or more efficient enzymes. The improvement of carbon capture mechanisms and metabolic pathways as thermodynamically efficient sinks.
- Elucidation of the role of various signaling cascades that originate from the photosynthetic apparatus and orchestrate the metabolic pathways to optimize the performance of the cells
- Unlocking the potential for enhancing the final sinks of excited electrons, thus allowing the relaxation of the feedback inhibition of photosynthetic light energy and carbon capture reactions. (e.g. by secretion of products in microalgae)
- Computational models to be used for facilitating the redesign of photosynthesis for different SUNRISE technology purposes.
- Redesign of photosynthetic regulation considering protein post-translational modifications (PTM), novel regulatory proteins and regulatory switches.
- Ammonia production by N_2 fixing cyanobacteria, utilizing heterocysts as microoxic production factory for ammonia production.
- Excreting hydrocarbons from microalgae. Proof-of-principle heterologous production of various hydrocarbons, including terpenoids, has been demonstrated with both cyanobacteria and microalgae. Metabolic engineering and synthetic biology approaches benefit from robust basal fluxes towards hydrocarbon precursors (fatty acids, terpenoids) in these systems and inherent metabolic flexibility of microalgal strains. Synthetic biology approaches need to focus on enhancing heterologous over-expression of downstream

pathway enzymes coupled to maximize carbon channeling to these pathways from central carbon metabolism following CO_2 fixation and optimized redox balances. Both bulk platform chemicals (e.g. isoprene) as well as specialty compounds (diterpenoids, triterpenoids, carotenoids and their derivatives) are target molecules.

Outcomes: *e.g.* diverse hydrocarbon platforms for biofuel -lipids, alkanes, terpenes, ammonia …

Challenge 3. Uncover the regulation mechanisms of photosynthetic machinery

Photosynthetic light reactions not only provide the energy for all cell metabolism but also guide the signaling processes to change gene expression, eventually leading to changes in the primary and secondary cell metabolism. This emerging knowledge can be harnessed for targeted photosynthetic bioproduction.

- Unlocking the photosynthetic performance from environmentally-induced regulation systems that heavily limit the efficiency of photosynthetic productivity.
- Flux enforcement: creating *controllable uncoupling/coupling* mechanisms between the flux through the product-forming pathway and the growth of the photosynthetic cell factory, to enhance genetic stability of the system.

Outcomes: *e.g.* produce switchable devices to modulate metabolism without reducing performances. Create predictive tool to forecast the consequences of metabolism transgenesis on productivity.

Challenge 4. Development of efficient cultivation and production systems

- Development of novel, energetically sustainable, efficient and scalable photobioreactor components and systems comprising automatization and new control systems based on machine learning and providing efficient light harvesting, CO_2 fixation and solar fuels and chemicals production. Consider minimal water use, recycling of waste waters and the fixation of CO_2 and atmospheric N_2 via utilization of different energy sources (e.g. light and reduced carbon from industrial or urban waste).
- Development of novel protocols and cultivation strategies for induction of efficient and long-term photobioproduction in green algae and cyanobacteria.
- Development and demonstration of cost-efficient product secretion, enrichment and/or purification of selected solar fuels and chemicals ready for market introduction.
- Identification of cyanobacterial/microalgae strains that can outcompete invading bacteria or live under extreme conditions (pH, temperature, osmolarity) that inhibit bacterial growth.
- Engineering of robust strains towards higher transgene expression (remove silencing mechanisms), expression of multi-gene pathways (selection marker and reporter recycling) and increased performance in secreting products
- Identifying promoters, introns, terminators as powerful expression tools for microalgae.
- Design and engineer devices or production systems with day and night control applicable for a production of solar fuels and high value chemicals under natural outdoor conditions.

- Demonstration of functional production units producing solar fuels and chemicals at high light and carbon efficiencies (water-soluble, water-insoluble-, non-volatile products, volatile products)
- Develop efficient technology for harvesting volatile compounds such as hydrogen, short chain hydrocarbons, which allow recovery of drop-in fuel molecules by avoiding biomass harvesting and chemical processing.

Outcomes: reduce the cost of biomass production to make all the above-mentioned application economically viable.

2.2 Timescale:

What can be achieved in 1 year.

- Selection and characterization of robust strains with high photosynthetic efficiency
- Integration of new control systems based on predictable models (machine learning) for phototrophic cultivation using sunlight.

What can be achieved in: 3 - 5 years.

- Develop novel protocols and cultivation strategies for induction of efficient, long-term and continuous photobioproduction in green algae and cyanobacteria
- Exploit knowledge on the regulation of photosynthesis, electron flow and CO_2 assimilation to implement the yield of biological photohydrogen and chemicals production.
    - o Achieve light to hydrogen conversion efficiency 8-10 %
    - o Product titters of 10-20 g/L, production rates of 5 mM/h, cellular activities above higher than 50 U /g cell (via oxyfunctionalization)

What can be achieved in 15-20 years

- Large-scale demonstration plants (TRL 8-9) producing renewable fuels and chemicals.

Synthetic Biology

1.1 Research Direction

State of the Art

Photosynthetic organisms are capable of hosting novel synthetic production pathways and enzymes that allow exploitation of photosynthetic microorganisms to function as ***microbial cell factories***, which can catalyze the entire process for the production of solar fuels and chemicals. For heterotrophic (non-photosynthetic) microorganisms (bacteria and fungi) that are employed in our biohybrid approaches, the synthetic biology toolboxes are currently more advanced compared to photosynthetic microorganisms. Yet, a robust and efficient modelling, systems biology and automatization of the synthetic biology toolboxes (encompassing the design-build-test-learn cycle) are necessary for both photosynthetic and heterotrophic microorganisms towards commercially profitable cell factories.

While the theoretical light to product conversion efficiency of photosynthetic light reactions is about 10-13%, the actual efficiency is less than 1 %, in some specific cases reaching about 2-4 %. Redesigning photosynthetic light reactions in order to increase light conversion efficiency is described in Biocatalysts PRD. Concomitantly, the improvement of CO_2 fixation into target molecules ensures increase in production of fuels and chemicals via fermentative and completely new synthetic production pathways.

Currently there are two different directions in synthetic biology field: top-down and bottom-up approaches. The top-down approach aims to remove redundancies in a host cell such as native regulation, thus decrease the complexity of the existing cells to minimum, while the bottom-up approach aims at identification of the building-blocks vital for the cell to be used in the design of completely new cells (synthesis of entire cell genomes from scratch). Recent breakthroughs in plant science demonstrated that crops engineered with a synthetic photorespiratory shortcut are 40% more productive in real-world agronomic conditions.[2] Besides the conventional CO_2 fixation pathway (Calvin Benson cycle) of oxygenic photosynthetic organisms, there are several other CO_2 assimilating pathways already discovered in microbes (T. Erb 2011), and learning from previously unknown catalytic principles of CO_2 assimilation now allows even more efficient synthetic CO_2 fixation routes to be developed. This opens up new directions to be utilized in the development of synthetic metabolic pathways to convert CO_2 into complex organic molecules. Thus, synthetic biology not only stringing together known biotransformations into pathways, but also allowing new transformations that currently have no biological route (though this is an emerging technology).

The current challenge is to fuse the existing information and ongoing work to generate more efficient standardized synthetic biology practices for a wide array of organisms. In practice, this requires finding more robust ways for effectively altering cellular functions in a predetermined manner by the introduction of new activities (foreign or deregulated native genes) or downregulation of interfering endogenous functions (gene knock-outs or knock-downs). This

[2] P. South ... D. Ort 2019 Science 363, eaat9077

can now be accomplished by combining i) most optimal characterized regulatory elements and genetic parts with ii) suitable modular assembly strategies that enable the construction of versatile pathways in a flexible manner and iii) linking with adaptive evolution. In addition, the establishment of CRISPR-Cas and CRISPRi systems for a wide array of organisms now allows multiplexed gene inactivation or regulated repression, respectively. As part of this development, systems biology approaches including versatile bioinformatics and *in silico* modeling strategies are integrated into all phases of the synthetic biology workflow, and assist the design, data processing, interpretation and visualization.

1.2 Potential Impact

Fast-progressing and revolutionary synthetic biology tool boxes will open enormous perspectives for realization of algal/cyanobacterial-based production of renewable and sustainable chemicals. The choice of the starting chassis is of critical importance for industrial production. Out of the thousands of known species of algae/cyanobacteria, only a few strains are currently being utilized. Research must focus on selecting robust strains with favorable metabolic characteristics, and domesticating them, by reducing transposable elements, by increasing transformation efficiency, and by optimizing transgene expression efficiency. For heterotrophic organisms that in biohybrid approaches will be merged with photoelectrochemical devices to harvest and convert solar energy to chemical energy, the synthetic biology approaches are already providing automatic pathway design and implementation practices, but progress to real industrial breakthroughs still requires validation, synchronization and optimization.

Ultimately, synthetic biology sits at the interphase of molecular biology (genetic assemblies), the corresponding functional cascades (enzyme-catalyzed metabolic functions), and the resulting systemic entities (organism-level cellular processes) which together make up the production systems. The tools available for engineering different organisms are currently at different stages of development, but all share the same premises: Fusing the existing molecular information with optimized pathway construction will enable significantly higher flux towards the end products, and less adverse effects to the host from reactive intermediates, and thus more efficient conversion of the start materials into the final products. The main impact of the current development is that we can more effectively harness the biosynthetic capacity of the cells to industrial needs, incorporate the artificial pathways as part of the host metabolism, and minimize consequent imbalances in carbon distribution, cofactor availability, and the necessary housekeeping functions. At the level of scientific research, well-established approaches significantly save resources through more labor-effective strategies, and high-throughput preparative and analytical systems. This also advances the exchange of compatible materials and research protocols, resulting in more effective collaboration at the level of synthetic biology and strain engineering. Importantly, this also assists the transfer to alternative host strains, and increases the prospects for obtaining wider range of target chemicals produced at significantly higher efficiencies.

Performance benefits:

- A synthetic metabolic route for utilization of a specific nutrient could prevent contamination of cultures (*e.g.* only the constructed strain can metabolize phosphite).

- Implementation of heterologous pathways in new wild-type strains that have enhanced CO_2 fixation rate at high light relative to model strains. This “domestication” can provide new *base* strains with productivities > 300 mg/L-day. An excellent starting point for reaching > 1-2 g/L-day productivities.
- De-regulation of central carbon metabolic pathways using synthetic biology
  - Through elimination of allosteric regulation (provided we know allosteric sites from a systems-biology study). This could increase specific productivity 100%, an estimate based on small # examples from literature.
  - Through re-factored biosynthesis pathways (such example for N_2-fixation implemented in *Synechocystis*).
- An optimized controlled “metabolic switch” from growth to bioproduction.
- A platform for adaptive evolution for tolerance to environmental stresses, including product. Allow continuous production of titers up to >10 g/L
- New bioproduction pathways that use non-native reactions: can increase energy yield by 25-50%

2. Aims

2.1 Scientific Challenges

Challenge	Research opportunities
Finding the optimal genetic elements for strain-specific purposes required for rational synthetic biology engineering	Continued generation of libraries of standardized genetic elements, using strategies which allow the comparison of molecular-level research data from different sources to guide the design. Develop orthogonal expression systems that would work in all strains (like T7 RNA polymerase systems). Optimize elements for each given strain (GC content, codon usage, endogenous regulatory elements like introns).
Selecting the most appropriate pathway assembly strategies that would be sufficiently versatile and compatible with the systems used by the others (i.e. lack of consensus and synergy)	Establishment of easy-to-use assembly syntaxes that base on modular BioBrick-inspired systems or PCR-based designs (e.g. GoldenGate, Gibson Assembly) for new hosts. Development of plugins and extensions to currently existing systems such as the CyanoGate (DOI: https://doi.org/10.1104/pp.18.01401) recently published for cyanobacteria or Modular Cloning (MoClo) established for Chlamydomonas (Crozet et al, 2018).
Adequate controllability of the introduced pathways, operons and individual genes for maximal productivity and reduced metabolic stress to the host.	Characterization of strain-specific transcriptional and translational control elements and associated genetic factors, in context with the assembly, pathway optimization and screening strategies [i.e. considering the entire design pipeline]. Develop

	more logic-based control, with two or more inputs (*e.g.* AND gates).
Identify engineering targets	Quantum modelling of energy and electron transfer pathways to provide feedback loops for experimental engineering of enzymatic catalytic properties.
Improve catalytic efficiency, stability, substrate specificity or cofactor preference of enzymes	Careful selection of alternative enzyme homologs, in addition to structure-based engineering and enzyme evolution, to provide higher fluxes and system stability. Improving retrosynthesis ("pathway finding") software by including structural analysis of potential enzymes. (*Hadidi et al., PNAS 2019; Asplund-Sameulsson et al., Metabolic Engineering 2018)*
Selection of robust strains with favorable metabolic characteristics	
Understanding of the host metabolism, regulation, and molecular-level interactions for rational engineering (synthetic biology + systems biology)	Continued fundamental molecular-level research to fill in the critical knowledge-gaps and resolving the key bottlenecks that must be known for each specific host organism. Integrating metabolic flux data into kinetic models to propose regulatory networks.
Monitor effects caused by the introduced genetic changes for rational design of next round of engineering (synthetic biology + systems biology)	Continuous evaluation of the engineered production hosts at different levels (e.g. proteomics and metabolomics) to guide the engineering, as an integral part of the synthetic biology strategy. Testing strains in simulated large-scale in the laboratory (I.e. by simulated light limitation, temperature changes, incomplete mixing).
Finding ways to properly optimize complex multi-gene assemblies as part of the host metabolic network.	To maximize the target pathway flux, and to minimize adverse effects caused by the introduced new functions, high throughput assembly methods and screening methods must be systematically developed. Transformation of and expression from large DNA fragments has to be established. Alternatively, methods for reporter and selection marker recycling must be developed.
Finding the most appropriate, efficient and cost-effective cultivation strategy for different strains and purposes. Scalability, to ensure that the system can be transferred from lab-scale systems into up-scaled processes.	Photobioreactor system development, together with the integration of new functions to the existing systems with more user-friendly user interfaces. Filling in the gaps via stepwise advancement from simple batch systems to optimize small-scale continuous analytical photobioreactors systems, and towards real upscale.
Developing the production methods together with the	Evaluation of alternative product-specific batch culture and continuous cultivation methods, in

strategies for the extraction, enrichment and the purification of the product.	parallel to immobilization techniques and *in situ* extraction methods, for different volatile and soluble end-products. Introduction of product excretion systems as part of pathway design.
Need for acquiring reliable numerical data to evaluate the competence of the systems, in context with the complete value-chain (from the starting materials to the final commercial product)	Establishment of continuous cultivation systems and better analytical strategies, which increase reproducibility and provide reproducible data for direct comparison between the inputs and the outputs.
Complications in fusing biochemistry and *in silico* modeling in a synergistic and biologically relevant manner at a detailed level.	More critical evaluation of the possibilities and limitations. Tying in the communication gaps between the disciplines. More resources for integration of modeling as part of the synthetic biology design, data interpretation and visualization.
Environmental safety issues. Acquiring societal acceptance and involvement in science-based decision making.	Evaluation of potential environmental risks, in context with the local and international GM regulations. Continuous dedicated education of the public and decision makers at various levels and via different media.
Process optimization and piloting: Incorporation of new industrial solutions to the existing technology infrastructure.	

2.2 Timescale:

What can be achieved in 1 year.

- A platform for automated synthesis and assembly of genetic constructs
- Agreement on standards for synthetic biology to allow for interchangeability of parts (ideally MoClo syntax)
- A “domestication” roadmap for selected production strains, based on gene fitness across environmental conditions
- Implementation of new genetic parts in selected strains, including:
    - Logic gates that incorporate multiple inputs for increased robustness, such as an inducer molecule and O_2 level.
    - A conditional-dependent protein degradation system via a protease and target protein tagging

What can be achieved in: 3 - 5 years.

- Comprehensive libraries of genetic parts established for the host systems
- Parts for high-level transgene expression and secretion optimized
- Model systems optimized for high-level expression (silencing pathways removed etc.)
- Top down: Rapid removal of protein burden caused by non-essential genes using CRISPR/Cas. Large genome modifications possible in model strains.

- Bottom up: Synthesis of re-factored central carbon pathways (>50,000 kpb) that are designed to be de-regulated in host
- A metabolic "interaction map" for enzymes in selected strains to identify potential routes for deregulation. For example, which metabolites inhibit the MEP pathway enzymes? Identified via systems biology.
- Engineering efforts with several iterations completed
- Deregulated central carbon metabolism in selected strains, through targeted mutagenesis of allosteric sites
- Integration of retrobiosynthesis software with enzyme structure software
- Screening of novel, ATP and redox-efficient bioproduction pathways for product of interest
- Implementation of novel, energy-efficient CO_2-fixing pathways into model strains
- Integration of gene expression data from multiple host strains
- Stable production of compound without cell growth.
- Synthetic cells with on-demand growth and production properties

What can be achieved in 10 years

- Engineering principles established with model systems have been applied to optimal hosts from natural environments
- Libraries for genetic parts also established for new hosts
- Detailed mathematical models of fundamental processes established
- Feedback loop from first experience from industrial scale production back to engineering of hosts to improve performance at large scale

What can be achieved in 15-20 years

- Large scale production at industrial level achieved with model hosts
- Automated DNA synthesis and construction ("cell designer")
- Rapid design of enzymes to catalyze novel reactions, with native or characterized enzymes as a starting point

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

<table>
<tr><td>Enabling Technology</td><td colspan="8">Bottom-up chemical engineering of bioinspired artificial photosynthesis reactor materials that surpass the photon-to-product performance of natural photosynthesis</td></tr>
<tr><td>Nature of active material</td><td>X</td><td>Solid-state Inorganic</td><td>X</td><td>Molecular</td><td>X</td><td>Biomolecular</td><td>X</td><td>Biological (living cells)</td></tr>
<tr><td>Sunrise approach</td><td></td><td>PV-powered electrocatalysis</td><td>X</td><td>Photo(electro)chemical direct conversion</td><td>X</td><td>biological and biohybrid direct conversion</td><td></td><td>Other</td></tr>
<tr><td>Contribution to SUNRISE goals (what?)</td><td colspan="8"><table>
<tr><td>X</td><td>Sustainable low-carbon production of <u>carbon-based fuels</u> with high efficiency and competitive costs</td></tr>
<tr><td>X</td><td>Sustainable low-carbon production of carbon-based <u>commodity chemicals</u> with high efficiency and competitive costs</td></tr>
<tr><td>X</td><td>Sustainable low-carbon production of <u>ammonia</u> with high efficiency and competitive costs</td></tr>
<tr><td>X</td><td>Sustainable low-carbon production of <u>hydrogen</u> with high efficiency and competitive costs</td></tr>
<tr><td>X</td><td><u>CO_2</u> as a valuable feedstock</td></tr>
<tr><td></td><td>Sustainable <u>building materials</u>, mineralization</td></tr>
</table></td></tr>
<tr><td>Sustainability criteria</td><td colspan="8"><table>
<tr><td>X</td><td>Carbon capture from the atmosphere</td></tr>
<tr><td>X</td><td>Exclusive use of abundantly available, non-toxic and non-critical elements</td></tr>
<tr><td>X</td><td>Sunlight as the primary energy source</td></tr>
<tr><td>X</td><td>Low resource consumption</td></tr>
<tr><td>X</td><td>Solar to products yields tenfold to hundredfold higher than current biomass practice</td></tr>
</table></td></tr>
<tr><td rowspan="2">Rough timeline (when?)</td><td colspan="3">Short term (2020-25)</td><td colspan="2">Medium term (2025–30)</td><td colspan="2">Long term (2030–50)</td><td rowspan="2"></td></tr>
<tr><td colspan="2">TRL°3</td><td></td><td>TRL°4-5</td><td></td><td>TRL°7-9</td><td></td></tr>
<tr><td>Who are the main actors?</td><td colspan="8">LERU (represented by Leiden University and Imperial College London), University of Uppsala, Heyrovski Institute</td></tr>
</table>

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

Contributors	Huub de Groot (Leiden University), Vincent Artero (CEA), Leif Hammarstrom (Uppsala University), James Durrant (Imperial College), Tony Vlcek (Heyrovsky Institute)

1. Short description of the proposed technological solution

Main technological elements, working principle (max. 5 lines, for scientists not expert in the field)	Tailoring catalytic sites in chiral photoactive solid state and supramolecular nanostructures for nonadiabatic conversion of raw materials into products with high yield and using light or sometimes electricity as the energy source
Why is this technology not commercially available right now? (major challenges)	Reverse engineering of biological designs and processes such as photosynthetic proteins, membranes and organelles working in synergy for high forward yields with low back reaction and recombination losses is not yet possible
What does it take to make it happen? (in short)	Axiomatic design: A function based engineering theory for the design of robust molecular, inorganic particle PEC and hybrid smart matrix 3D modular architectures with vibronic coupling over avoided crossings of anticorrelated electronic states.
What is the benefit for other technologies? Why is it an enabler?	Advanced high performance reactor materials that go well beyond the current adiabatic practice are central to all Sunrise technologies
Why is it promising?	Route to high efficiency, high density, low cost

2. Existing R&I projects

Existing national/EU project	Final objective	TRL	Run-time	Funding Instrument
National	Biological underpinning of nonadiabatic conversion by adiabatic passage	0	2024	projects
National	Modeling of semiclassical coherent conversion	3	2021	projects

National	Second shell tuning of molecular catalysts	2-3	3-5 yrs	projects
National	Molecular design	2-3	3-5 yrs	projects
ERC, FET etc.	Molecular photochemistry, second shell tuning of catalysts, bottom-up design	1-3	3y	H2020 networks and research consortia

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

TRL	1-3
Current state of the art	Molecular photocatalysts have the potential for high absorption, catalytic rate and selectivity, and as all atoms are surface exposed, the required amount of material can be minimized. However, today such systems show only low efficiency, photochemical yield, and stability.
Limitations	Reverse engineering of biological designs and nonadiabatic processes such as photosynthetic proteins, membranes and organelles working in synergy for high forward photon to product yields with low back reaction and recombination losses is not yet possible and is the single principal bottleneck. An engineering theory is missing and is required for further development
DOI References	See e.g. 10.1021/acscatal.5b02950; 10.1142/9789813274440_0003; 10.1098/rsfs.2015.0014; 10.1021/acs.jpcc.6b08244

4. 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	1 year
Deliverable, milestone	Specification of technology concepts and applications formulated
Solved Challenges / Lifted barrier (in bullet points)	• Based on earth abundant elements • Catalytic sites with very few metal ions • High selectivity and efficiency for energy conversion

	● Operate under ambient temperature and pressure in aqueous media
What was necessary to solve the challenge? Did it depend on advances in other fields?	Data mining, to continuously adhere to the advances in other fields
TRL	1
Stability	Variable
Energetic conversion efficiency	70% photon to product yield
Scale	Scalable to the TW level
DOI Reference	DOI: 10.1142/9789813274440_0003

Define time: **short-/medium-/long-term, x years**	3-5
Deliverable, milestone	Characteristic proof of concept catalysts
Solved Challenges / Lifted barriers (in bullet points)	● Hydrogenases ● Nitrogenases ● Dehydrogenases ● Laccases ● others...
What was necessary to solve the challenge? Did it depend on advances in other fields?	Biomimicry for multi-electron multi-proton reactions such as CO2, O2, water and N2 activation in a laboratory environment
TRL	3
Stability	variable
Energetic conversion efficiency	Variable, depending on the product, target is 80% chemical yield
Scale	Scalable to the TW level
DOI Reference	10.1039/c4sc03720k

Define time: **short-/medium-/long-term, x years**	10-20

Deliverable, milestone	Artificial membranes
Solved Challenges / Lifted barriers (in bullet points)	• Efficient coupling of light harvesting and catalysis • Rapid separation of products
What was necessary to solve the challenge? Did it depend on advances in other fields?	Validate modules, explore self-assembly, compartmentalization, self-repair, regulation of functional arrays of modules; validation of modules and self-assemblies under relevant field conditions
TRL	4-5
Stability	variable
Energetic conversion efficiency	70% proton to product yield
Scale	Scalable to the TW level
DOI Reference	10.1039/C7EE00294G

Link to TRL level

At TRL 5-6:

Technological barriers to overcome	**Prototyping, long term stability**
Political/societal barriers to be overcome	**Those will be taken into account in the axiomatic design from the very start**
Market barriers to be overcome	**Cost, derisking (by government)**

At TRL 7-8:

Technological barriers to overcome	**Device integration in the existing technological infrastructure**
Political/societal barriers to be overcome	**Agency**
Market barriers to be overcome	**Cost, derisking**

At TRL 9:

Technological barriers to overcome	**Concentration of product (downstream) and possible raw material upstream (CO_2, H_2O)**
Political/societal barriers to be overcome for market introduction	**The moral and practical agency of citizens towards AP technology is essential. If within Sunrise we cannot empower the citizen with this kind of agency then we have failed to take the societal factor into account. What we do not want is that we prescribe how citizens should behave vis-à-vis the AP technology, in our integrated approach we want to create room for the fulfillment of what we have called societal and citizen needs, which implies that we need their moral and practical agency, and that we is aim at empowering this.**
Market barriers to be overcome	**Cost, derisking**

5. 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
Fuel	12
chemicals	10
CO_2 scrubbing	8

6. 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
Sustainability	12
Scalability	12
Concentration	10

Cost	10

7. 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	Bottom-up chemical engineering of bioinspired artificial photosynthesis reactor materials that surpass the photon to product performance of natural photosynthesis
Risks	Light harvesting not at 70% Recombination losses limit efficiency Leaching of photoabsorbers and catalysts during operation Limited stability of photoelectrode materials due to side reactions Instability of semiconductors and molecules in aqueous electrolyte Photocatalytic back reactions destroying the generated products

Breakthroughs in other key enabling disciplines

Modeling	Axiomatic design of smart matrices; nonadiabatic conversions
Industrial research	Device engineering and integration
Chemistry	Catalysts, photoabsorbers, semisynthetic components

Resources

Suggestion	**Please detail**
Critical, rare elements	Can be avoided
Non-fluctuating energy sources	Are taken care of by non-adiabatic methods
Hydrogen storage	Product will be release into grid or compressed for off-grid use
CO2 storage	In the ground, distributed
Water purification	Water will be collected from the air and is pure
CO2 from the atmosphere	Yes
Concentrated, pure CO2	When it is available

Specific, new infrastructures	Grids, possibly dynamic (drones)
Low-cost, low-carbon electricity	Can be handled but is not critical
Renewable energy	Will be “produced”
Renewable heat	Will be “produced”

<u>Political/societal/market barriers</u>

EU-wide, homogeneous regulatory frameworks	Yes, would help
Adaptation/ novel regulations (e.g. genetics, use of waste CO2, ..)	Will depend on country, important is a level playing field on the medium term with targeted support for a limited time (5 yrs)
EU/national regulations for the deployment of the technology/product	Possibly
EU/national incentives for the deployment of the technology/product	Yes, to stimulate agency
Fast idea protection (patenting, etc.)	Fast idea protection will be both possible and essential
Large capital investment for market introduction	Derisking with green bonds
Standardization of efficiencies, etc.	Common standards for yield and efficiency will be needed
Societal acceptance	We need agency with the population
Political security	Decentralized manufacturing of energy carriers and commodities will contribute to political security
EU supply chain	Is needed for concentration of products to achieve the TW scale

<u>Funding/research frameworks</u>

International collaboration	Europe has an edge with respect to the international competition, mainly from the US and China. Further collaboration in e.g. mission

	innovation will be beneficial.
Funding schemes for demonstrators, pilots, etc.	A distributed innovation network with hubs (a la SUNRISE valleys) and public-private funding will be necessary for demonstrators and pilots
Large-scale EU research initiatives	cPPP is the preferred instrument to move forward, as no single member state can do the development on its own.

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

Enabling 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	X	Molecular	X	Biomolecular		Biological (living cells)
Sunrise approach		PV-powered electrocatalysis		Photoelectrochemical direct conversion		biological and biohybrid direct conversion	X	Key enabler*, Other

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 product
		Sustainable building materials, mineralization

Sustainability criteria		
		Carbon capture from the atmosphere
	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

Rough timeline (when?)	Short term (2020-25)		Medium term (2025–30)		Long term (2030–50)		
	TRL°	4	TRL°	5	TRL°	9	
Who are the main actors? Who has to be involved?	Fraunhofer IME (light absorption, water splitting in biotic systems & HER biocatalysts) Fraunhofer ISC (abiotic material development & integration) Fraunhofer IMM (simulation & microfluidic integration) Leiden University (light absorption & water splitting in biotic systems; simulation) University of Würzburg (light absorption & water splitting in abiotic systems) University of Warsaw (plasmonics-driven improvement of light absorption of natural catalysts, developing optimal bio-organic interfaces and catalysts) University of Padova (water splitting in abiotic systems; HER catalyst) UC Louvain (abiotic material development & integration) Photovoltaic Center for Energy, AIT (abiotic material development & integration)						

* 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	
Affiliation	

1. Short description of the proposed technological solution

Main technological elements, working principle (max. 5 lines, for scientists not expert in the field)	Explore combinations of different biotic and abiotic components to develop a modular and fully cyclic tandem system capable of photocatalytic water splitting under solar light-conditions and simultaneous H_2 and O_2 evolution and find the best technological solutions to advance the current TRL from 1 to 9.
Why is this technology not commercially available right now? (major challenges)	Current biotic-abiotic artificial photosynthesis approaches for fuel production show still low conversion efficiency and are at TRL1: ● There are no long term-stable light harvesting systems available including an efficient charge separation and transportation to a highly active reaction centre. ● Inefficient catalysis - particularly due to slow O_2 evolution and to the formation of partially oxidized side products ● Short half-life of critical components e.g. photosystems ● Most of the existing molecular synthetic catalysts for water oxidation are based on costly, rare and toxic materials

	● Lack of technological solutions for implementation of bio-hybrid artificial photosynthetic systems for a larger-scale production amenable to industrial application.
What does it take to make it happen? (in short)	This technology needs optimization of each of the biotic and abiotic components used for light harvesting, charge transfer, water splitting and H_2 gas production The minimum requirements for achieving a functional system are: ● broad spectral absorption of solar light ● directional concentration of excitation energy at a stable and ideally self-renewable reaction centre for water splitting and ● efficient protons convey to optimized enzymatic catalysts for hydrogen production. ● component integration in a flexible, exchangeable and scalable environment
What is the benefit for society? (in short)	Solar-driven biotic/abiotic hybrid systems for hydrogen and fuel production contribute to: ● lowering the global warming by a significant reduction of CO_2 emissions and a drastically decreased usage of fossil fuels ● secure the demand for global energy supply ● provide energy at an affordable price ● securing a new market for high value manufacturing jobs ● decentralized production of hydrogen gas as clean and meanwhile accepted energy carrier to be converted into electricity or mechanical energy

2. Existing R&I projects

Existing national/EU project	Final objective	TRL	Run-time	Funding Instrument
CarbonCat (IMM)	Application of dye-modified diamond for light-driven CO_2 conversion to C_1 chemicals in a flow reactor	2-3	2016-2021	BMBF CO_2PLUS
SupraWOC (Uni Wü)	Supramolecular Architectures for Ruthenium Water Oxidation Catalysis	3	2018-2023	ERC Adv. Grant
Co-Pilot (Fraunhofer ISC)	Flexible Pilot Scale Manufacturing of Cost-Effective Nanocomposites through	6	2015-2017	H2020-EU.2. 1.2.4.

	Tailored Precision Nanoparticles in Dispersion			

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

Technological solution to be developed in SUNRISE	**Biotic-abiotic solar light-driven water splitting and hydrogen generation on large scale**
TRL	1-3 depending on single component of complete system
Cost	High, due to low efficiency and expensive materials (noble metals)
Energetic conversion yield	
Stability	Rather low; hours to days
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	A supramolecular ruthenium macrocycle with high catalytic activity for water oxidation that mechanistically mimics photosystem II (10.1038/NCHEM.2503) Cooperative water oxidation catalysis in a series of trinuclear metallosupramolecular ruthenium macrocycles (10.1039/c7ee01557g)

	Bias-Free photoelectrochemical water splitting with photosystem II on a dye-sensitized photoanode wired to hydrogenase. Nat. Energy 3, 944-951

4. Available techno-economical analysis:

DOI Reference	Technologien für Nachhaltigkeit und Klimaschutz – Chemische Prozesse und stoffliche Nutzung von CO_2 ISBN 978-3-89746-190-1
Summary	https://dechema.de/dechema_media/Bilder/Publikationen/CO2_Buch_Online-p-20003330.pdf

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 term, 3-5 years**
Deliverable, milestone	• High performance, cost-effective and stable components by Big Data Analysis and in-silico prediction for: light absorption water splitting hydrogen production, separation and storage • material interfaces for assembly of photocatalytic cell • Fast-track screening method for biotic catalyst components for enhanced stability and activity • Identify bottlenecks for scale-up for each topic in i-iv. • Holistic engineering concept for large-scale application of the most suitable technology components to overcome identified bottlenecks; simulation of reactor/half-cell components and rapid prototyping by additive manufacturing • Proof-of principle laboratory scale demonstrator • Method development / adaptation for life cycle analysis and cost analysis focusing on classes of biotic/abiotic components
Solved Challenges / Lifted barrier (in bullet points)	• Achieve panchromatic light absorption to improve light absorption up to 90% quantum efficiency

	● Increase the lifetime and stability of biotic components ● Improve the catalytic properties of supramolecular catalysts ● Develop semiconducting materials with efficient directional energy and electron transfer to achieve a long distance spatial charge separation ● Enhance rates of H_2 production up to 70% by molecular evolution of engineered hydrogenases using ● Economical and ecological footprints available for catalyst material classes
What was necessary to solve the challenge? Did it depend on advances in other fields?	Technology for Big Data Analysis and Dial-a-Molecule approaches for fast track screening of abiotic systems; Solid state chemistry for semiconductor development; Participation of engineering sector for additive manufacturing & rapid prototyping;
TRL	Achieve at least TRL4
Stability	Months
Energetic conversion efficiency	
Scale	Lab scale
DOI Reference	

Define time:	**Medium term, 5-7 years**
Deliverable, milestone	● Tailoring self-assembling complexes of biotic and abiotic light harvesting molecular components to extend the absorption spectrum of natural water oxidation catalysts ● Large-scale production of biotic material components with enhanced pH, temperature, and O_2 stability ● Large scale production of abiotic light harvesting systems and (supramolecular) catalyst assemblies by continuous flow plants ● Adaptation of available (immobilization/grafting/printing) technology for device manufacturing with novel abiotic and biotic components on plane surfaces ● Construction of a 1 m^2 bio-hybrid demonstrator for H_2 production beyond state of the art using optimized biotic and abiotic elements and its validation under laboratory conditions.

	• Fostering compatibility of novel technology to existing H_2 gas infrastructure and end user (check evolution of novel fuel cell designs or combustion motors for H_2) • Studies on societal acceptance of installation of solar light receiver and H_2 gas production in urban areas.
Solved Challenges / Lifted barriers (in bullet points)	• Technological solution for cost-efficient production of biotic/abiotic components/materials at larger scale (e.g. for a 20 m^2 pilot demonstrator) • Engineering concepts based on multiphysics simulation of microfluidic environments based on general simulation of reactor/half-cell concepts • Engineering concepts for integration of existing or novel technological solutions for H_2 separation / drying / storage • Technological solutions for light concentrators at larger scale for harvesting diffuse solar light • Technological solutions for recycling / regeneration of selected catalyst systems and technological components • Awareness raising on compatibility of SunRise technology with daily life in urban areas
What was necessary to solve the challenge? Did it depend on advances in other fields?	Participation of construction and engineering sectors for potential evaluation of SunRise technology to be used in urban areas and within an existing infrastructure; Participation of end user sector (mobility, electricity, …)
TRL	Achieve TRL 5
Stability	Months to years
Energetic conversion efficiency	
DOI Reference	

Define time: **short-/medium-/long-term, x years**	Long-term, 10 years
Deliverable, milestone	• Construction and validation of the most successful artificial photosynthesis demonstrator up to 20 m^2 based on the optimized biotic material components and non-toxic, abundant abiotic elements in relevant environment

	● Showcase for Installation of SunRise technology and usage of produced H_2 gas in daily life for e.g. automotive personal transportation or electricity generation with fuel cell
Solved Challenges / Lifted barriers (in bullet points)	● Life cycle analysis of business and technological aspects for a safe and sustainable large scale production ● Life cycle analysis of each of the selected biotic/abiotic components ● Use of materials/components derived from abundant resources to ensure production in large scale quantities ● Ensuring a long life of the entire system, e.g. by avoiding corrosion damage or "poisoning" of catalysts ● Consideration for price competitiveness in the design of the entire system
What was necessary to solve the challenge? Did it depend on advances in other fields?	Continuation of participation of all necessary industrial sectors for installing and running energy producing technology.
TRL	Achieve TRL 6
Stability	Years
Energetic conversion efficiency	
DOI Reference	

Link to TRL level

At TRL 5-6:

Production volume	X m^3 per 20 m^2 since we focus on the area, not on the amount of produced H_2 gas
Light harvesting area needed per t/product	
Political/societal barriers to be overcome	Regulatory issues related with H_2 production Safety assessment of hydrogen production facility
Market barriers to be overcome	Complexity of overall catalyst system; Societal acceptance on energy carrier production in urban areas; Development / advancement of technology for daily life H_2 gas usage;

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**
Solar light as earth-abundant, but fluctuating energy source	9
World-wide applicable	8
Infrastructure and technology for H_2 consumption/conversion already available	11
High societal acceptance in view of mimicking nature	10

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
Long term stability of biotic materials	7
Compatibility of biotic and abiotic components upon integration in reactor/half-cell	9
Alternative to expensive noble metals in abiotic catalyst system	7
Oxygen management in water splitting compartment necessary due to photocorrosion/singlet oxygen exposition of light harvesting system	8
Integration of artificial light sources for 24/7-production of H_2 with “renewable” electricity from around the world (grid integration of H_2 production)	9

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	Molecular and biomolecular development is superior to technological device development.
Knowledge gaps	How to increase quantum yield in light harvesting & charge separation? What is the perfect match between abiotic and biotic systems for high efficiency and long term stability?
Risks	Efficiency and stability of all catalyst systems

Resources

Suggestion	Please detail
Critical, rare elements	Substitution of ruthenium

Non-fluctuating energy sources	Integration of artificial light sources with “renewable” electricity from around the world
Hydrogen storage	Material development for high and low pressure H_2 storage
CO2 storage	/
Water purification	Depends on catalyst stability; biotic system runs in buffered solutions different to ionic solution of abiotic system
CO2 from the atmosphere	/
Concentrated, pure CO2	/
Specific, new infrastructures	Explosion protected system for HER and OER compartments
Low-cost, low-carbon electricity	For artificial light sources
Renewable energy	For artificial light sources
Renewable heat	/

Breakthroughs in key enabling disciplines

Scale-Up	Numbering-up of easily adaptable single modules
System integration	For device: integrated and exchangeable by component; Global: end user must be defined: automotive, electricity, …
Novel reactor designs	Manageable fabrication of reactor designs for efficient contacting of gas-liquid-solid-photonic phases; Reproducible immobilization of catalyst systems; Preparation of photoanodes based on novel light absorber materials (see below)
Novel catalyst materials: earth-abundant, non-toxic, efficient, stable	See below
Novel absorber materials: earth-abundant, non-toxic, efficient, stable	Development of multinuclear Macrocycles based on earth-abundant metal for water oxidation catalysis Development of MOFs and SURMOFs based on the most successful Ru-based WOCS and to be developed related earth abundant metallosupramolecular WOCs
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	Installations in urban areas must be made possible H_2 gas infrastructure must be standardized
EU/national incentives for the deployment of the technology/product	
Fast idea protection (patenting, etc.)	
Large capital investment for market introduction	From private collective over industry to investment by the state; Participation of private households can foster societal acceptance.
Standardization of efficiencies, etc.	e.g. for both light intensity and area; fully defined DIN for comparability of developed systems
Societal acceptance	Integration of energy carrier production needs to be implemented in daily life -> installation in urban areas Awareness of energy consumption must be trained!
Political security	

EU supply chain	

Funding/research frameworks

International collaboration	Expertise of each country must be funded within a global support measure → synergy must be generated between geographical areas (light, water, resources, …) and societal regions (science, work force, …)
Funding schemes for demonstrators, pilots, etc.	See above
Large-scale EU research initiatives	See above

Oxygen evolution (Water oxidation)

Enabling Technology								
Enabling Field								
Nature of active material	x	Solid-state Inorganic	x	Molecular		Biomolecular		Biological (living cells)
Sunrise approach	x	PV-powered electrocatalysis	x	Photo(electro)chemical direct conversion		biological and biohybrid direct conversion		Other
Contribution to SUNRISE goals (what?)	x	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						
	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						
Sustainability criteria		Carbon capture from the atmosphere						
	x	Exclusive use of abundantly available, non-toxic and non-critical elements						
	x	Sunlight as the primary energy source						
		Low resource consumption						
		Solar to products yields tenfold to hundredfold higher than current biomass practice						
Rough timeline (when?)	Short term (2020-25)			Medium term (2025–30)		Long term (2030–50)		
	TRL°			TRL°		TRL°		
Who are the main actors? Who has to be	Intensive research going on worldwide.							

involved?	

* 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	A. Vlcek
Affiliation	JHIPC

1. Short description of the proposed technological solution

Main technological elements, working principle (max. 5 lines, for scientists not expert in the field)	Requires robust and efficient catalysts: (photo)electrode materials, nanoparticle or (supra)molecular catalysts that could be homogeneous or immobilized in membranes, films, polymers. Natural photosynthesis uses a molecular catalyst in a protein environment.
Why is this technology not commercially available right now? (major challenges)	Low efficiency and instability of catalysts. Few stable and efficient catalysts exist but are prohibitively expensive and based on precious metals (Ir, Ru).
What does it take to make it happen? (in short)	Materials and catalytic research. Development of new oxide-based (nano)materials, stable molecular catalytic systems (e.g. based on polyoxometalates), their organisation in functional systems (membranes, quantasomes, electrode surface-immobilization), embedding of molecular catalysts in protein environment,… HPC materials modelling, QM/MM/MD of (supra)molecular systems
What is the benefit for other technologies? Why is it an enabler?	This is a necessary counter-reaction in all electrochemical and photo(electro)chemical processes where water is used to produce H2 and/or reduce CO2 or N2. It's a necessary prerequisite for approaches 1 and 2. Possibly also in approach 3, if bio-systems are used only on the reduction side.
Why is it promising?	Natural photosynthesis and existence of precious-metal catalysts demonstrate the feasibility of the process. Developing abundant-element based catalyst will underlie other SUNRISE technological solutions.

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?

TRL	
Current state of the art	
Limitations	
DOI References	

4. 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	Research on water oxidation needs to proceed in parallel with that on H_2 production, CO_2 and N_2 reduction
Deliverable, milestone	
Solved Challenges / Lifted barrier (in bullet points)	• Use of abundant elements • Stability • Integration with (photo)electrodes or light-absorbing/charge separating systems • Charge accumulation and coupling of O_2 production from water with proton transfer • Catalyst selectivity against chloride oxidation if seawater is used

What was necessary to solve the challenge? Did it depend on advances in other fields?	Depends on fundamental research in materials/catalyst development, mechanistic research, applications of advanced exp. techniques, and SUNRISE modelling platform
TRL	Has to keep pace with TLR of H_2 production, CO_2 and N_2 reduction
Stability	Challenge !
Energetic conversion efficiency	Has to keep pace with of H_2 production, CO_2 and N_2 reduction
Scale	As that of H_2 production, CO_2 and N_2 reduction
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	
Energetic conversion efficiency	
Scale	
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	
Energetic conversion efficiency	
Scale	
DOI Reference	

5. 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

6. 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

7. 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	

Breakthroughs in other key enabling disciplines

Resources

Suggestion	Please detail
Critical, rare elements	
Non-fluctuating energy sources	
Hydrogen storage	
CO_2 storage	
Water purification	Probably not, if the Cl^- selectivity problem is solved and the catalyst is not poisoned.
CO_2 from the atmosphere	
Concentrated, pure CO_2	

Specific, new infrastructures	
Low-cost, low-carbon electricity	x (when used in approach 1)
Renewable energy	x (Sunlight, when used in approach 2)
Renewable heat	

Political/societal/market barriers

EU-wide, homogeneous regulatory frameworks	
Adaptation/ novel regulations (e.g. genetics, use of waste CO_2, ..)	
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	needed
Funding schemes for	

demonstrators, pilots, etc.	
Large-scale EU research initiatives	Preferred

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