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TECHNICAL APPENDIX

PART 3 - SUSTAINABLE CARBON-BASED CHEMICALS
AND (JET)FUELS



SOLAR ENERGY FOR A CIRCULAR ECONOMY



SUNRISE

Solar Energy for a Circular Economy

Technological Roadmap

Technical Appendix

Part 3 - Sustainable carbon-based chemicals and (jet)fuels

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Definitions

4

Sustainable hydrogen production

Conventional process data

SUNRISE technologies

Large-Scale hydrogen production using PEM electrolysis

Hydrogen production using photoelectrochemical cell devices

Hydrogen via buried-junction photoelectrochemical cells

Hydrogen production by photosynthetic microorganisms

Hydrogen photoproduction by biomolecular technologies

Baggies with particulate systems

Sustainable ammonia production

Conventional process data

Biomass-based process

SUNRISE technologies

Renewable Haber-Bosch process

Electrochemical ammonia synthesis

Direct photoelectrochemical ammonia synthesis

Ammonium production by photosynthetic microorganisms

Plasma-assisted ammonia synthesis

Sustainable carbon-based chemicals and (jet)fuels

5

SUNRISE technologies

5

Dark electrochemical reduction of CO₂ to C₁/C₂/C₃ products

5

Electrochemical production of hydrocarbon fuels

17

Thermochemical production of hydrocarbons and jet fuels

28

Biocatalytic production of chemicals by microorganisms

45

Carbon-based fuel production by biomolecular approaches

57

Sustainable Carbon Capture

Amine-based Carbon Capture

Polymeric membranes based carbon capture

Low Temperature Direct Air Capture

High Temperature Direct Air Capture

SUNRISE key enablers

Computational materials modelling: from novel materials to solar fuel devices

Development of new methods and software tools for early quantitative sustainability

assessment of emerging SUNRISE technologies: bridging environmental, economic and social impacts

Redesigning photosynthesis for the biocatalytic production of chemicals and fuels

Synthetic Biology

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

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

Oxygen evolution (Water oxidation)

Definitions

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

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

Technology Readiness Level (TRL):

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

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

Sustainable carbon-based chemicals and (jet)fuels

SUNRISE technologies

Dark electrochemical reduction of CO₂ to C₁/C₂/C₃ products

Technology	Dark electrochemical reduction of CO ₂ to C ₁ /C ₂ /C ₃ products							
Targeted product	H ₂	NH ₃	CH ₃ OH	EtOH	CH ₄	Jet fuel	CO ₂	Other
				x	x	x		
Nature of active material	Solid-state Inorganic		X	Molecular		Biomolecular		Biological (living cells)
Sunrise approach	PV-powered electrocatalysis		X	Photoelectrochemical direct conversion		biological and biohybrid direct conversion		Key enabler*, Other
Device category	X	Electrolyzer		Photo(bio)electrolyzer		Photo(bio)reactor		fermentors, thermocatalytic reactors
Contribution to SUNRISE goals (what?)	X	Sustainable low-carbon production of <u>carbon-based fuels</u> with high efficiency and competitive costs						
	X	Sustainable low-carbon production of carbon-based <u>commodity chemicals</u> with high efficiency and competitive costs						
		Sustainable low-carbon production of <u>ammonia</u> with high efficiency and competitive costs						
		Sustainable low-carbon production of <u>hydrogen</u> with high efficiency and competitive costs						
		<u>CO₂</u> as a valuable product						
		Sustainable <u>building materials</u> , mineralization						
Sustainability criteria	Carbon capture from the atmosphere							
	X	Exclusive use of abundantly available, non-toxic and non-critical elements						

	Sunlight as the primary energy source					
	X	Low resource consumption				
	X	Solar to products yields tenfold to hundredfold higher than current biomass practice				
Envisaged production system		Decentralized, local production at small scale (households, niche applications)				
	✓	Large-scale production using existing centralized infrastructure				
	X	Large-scale production necessitating new infrastructure				
Rough timeline (when?)	Short term (2020-25)		Medium term (2025–30)		Long term (2030–50)	
	TRL°	4	TRL° 7	7	TRL°9	9
Who are the main actors? Who has to be involved?	<p>Universities to develop/synthesize the catalyst, do quantum chemical modelling and in-operando spectroscopy to see what is going on Industrial design players who develop suitable electrolyzer architectures and build demos. DFG Cluster of Excellence: e-conversion (LMU in Munich, Munich Univ., MPI Muelheim, TUM)</p> <p>Brooklyn, NYC (Staff Sheehan, Catalytic Innovations) Toronto University (Catalysts) JCAP (Catalysts) Berlin - Peter Strasser / Beatrice Roldan (Catalysts) Paris - Marc Fontecave (Catalysts) Szeged - Janaky (Engineering) OPUS 12 (Engineering) Dioxide Materials (Engineering/Materials) Univ. Leiden Danish Technical University EPFL</p>					

* 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	Various
Affiliation	

1. Short description of the proposed technological solution

<p>Main technological elements, working principle (max. 5 lines, for scientists not expert in the field)</p>	<p>The low-temperature electrolyser will need to avoid water reduction to hydrogen and in the same way allow selective reduction of CO₂. Ideally the electrolyser will work in gas phase, reducing pure CO₂ flow.</p> <p>Electrocatalysts will need to have a high overpotential requirement for proton reduction to suppress H₂ production and a low overpotential requirement for direct CO₂ reduction. They need to be good conductors, be selective and promote C-C bond formation. Most promising is a first step to reduce CO₂ to CO and a second step for further reduction of the CO to C₂/C₃ components. Here also a selectivity to one special species would be nice but hard to achieve.</p>
<p>Why is this technology not commercially available right now? (major challenges)</p>	<p>The main bottleneck is the stability of the current catalysts, mainly copper based. On the engineering/upscaling aspect, electrolyser manufacturer are only starting to envision this type of system.</p> <p>Academic work is directed to get nice papers and high H₂ factors. Not usable in practical life since all (except maybe U Toronto) catalysts degrade within few hours and cannot carry industrial relevant current densities. Only focus on catalyst itself and lack of work to embed it into a working system.</p>
<p>What does it take to make it happen? (in short)</p>	<p>In order to reach the objectives, one will require to master the C-C coupling and selectivity toward specific products. On the engineering side, material development will be required to achieve efficient systems working in gas-phase at room temperature. Ideally, those system will tolerate low-concentration CO₂ stream in order to reduce CO₂ out of air.</p> <p>Orchestrated collaboration of simulation, spectroscopic (live characterization) and chemical synthesis people with industrial people who know electrolyzer architectures.</p>
<p>What is the benefit for society? (in short)</p>	<p>Recycle the CO₂ to useful products. Generate a seasonal storage of PV energy as chemicals and empower mobility where batteries don't work.</p>

2. Existing R&I projects

Existing national/EU project	Final objective	TRL	Run-time	Funding Instrument
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Various. FHG and Siemens work on one called CO2EXIDE	Electrochemical synthesis of ethylene and hydrogen peroxide to produce ethylene oxide.	1-2	2019-2021	SPIRE
Strong and focused work at JCAP				
And probably in China/Korea				
TOTAL / Collège de France	Develop electrochemical CO2 valorization (To be completed)	3-4	2019-2024	TOTAL R&D funding
German National Funding	Conversion of CO2 to hydrocarbon (20 Mio)	1-2	2020-2022	CO2+ funding program
ITN eSCALED	PV+ electrolysis device for CO2 reduction	3	2018-2022	H2020-MSCA

e-conversion Cluster of Excellence in Germany (DFG-funded for 2019-2026)

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

Technological solution to be developed in SUNRISE	
TRL	Dependent on time, see above 4 □7□9
Cost (for projects)	R&D 20-30 Mio, Demonstrators 30 Mio for 10-50 MW scale Or product cost? 1 l fossil fuel is about 40 cents, 1 l synthetic fuel at good renewable conditions about triple of value and needs to come down by about 50%
Energetic conversion yield	Target: electrical energy □ molecules 60+%
Stability	At least 10.000h
Product separation yield	Tbd. input is CO2 pure, realistic output has 30% CO2, 3%H2, 50% (best) products and the balance is (perhaps also usable) by-products
Total energy demand [GJ/t]	Energy Content 30-50 GJ/T divided by overall efficiency, mainly electricity
Electricity needs [GJ/t]	See above
Energy demand utilities [GJ/t]	See above

Steam balance [GJ/t]	
CO2 emissions [tCO2 eq/t] (cradle-to-gate, including feedstock production)	
Water consumption	Each CO2 molecule will need 1-1.5 H2O molecules
Air separation unit	At first step CO2 will be taken from concentrated sources (exhaust from power plant cement, steel works)
Compressors	Minor share in energy balance
DOI References	

Conventional fossil-based process	
Global annual production volume	One power plant is about 10 MT/ a CO2, world wide 10-15 Gt/a
Total energy demand [GJ/t]	For values GJ/t see above. A refinery is about 30 GW power that would be needed (would need about 100x100km PV)
Energy feedstock [GJ/t]	
Fuel demand [GJ/t]	
Steam balance [GJ/t]	
Electricity [GJ/t]	
Air separation unit	
Compressors	
CO2 emissions [tCO2 eq/t] (cradle-to-gate, including feedstock production)	
Water consumption per t product	
Current TRL	
Current cost per t product	
DOI References	

Biomass-based process (if any)	Many in R&D, we might try to get data from the E10 production
Global annual production volume	
Energy demand [GJ/t]	
Feedstock demand [GJ/t]	
CO2 emissions [tCO2 eq/t] (cradle-to-gate, including feedstock production)	
Water consumption per t product	
Electricity needs [GJ/t]	
Current TRL	
Current cost per t product	
DOI References	

4. Available techno-economical analysis:

DOI Reference	
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, 4-5 years
Deliverable, milestone	Stable electrocatalyst formulation on small (10cm ²) lab scale
Solved Challenges / Lifted barrier (in bullet points)	<ul style="list-style-type: none"> Stable and able to carry realistic current needs (500mA/Cm²)

	<ul style="list-style-type: none"> • So the instability of surface morphology on atomic scale needs to be overcome (self repair, short regeneration pulses)
What was necessary to solve the challenge? Did it depend on advances in other fields?	See above co2work of simulation, spectroscopy, synthesis people with industrial people
TRL	4
Stability	10000h
Energetic conversion efficiency	40%
Scale	10 cm ² electrode surface
DOI Reference	To be published in some years

Define time: short-/medium-/long-term, x years	Medium, 8-10 years
Deliverable, milestone	Demonstrator unit at the several MW level
Solved Challenges / Lifted barriers (in bullet points)	<ul style="list-style-type: none"> • Include stable catalyst formulation in electrolyzer architectures • Develop new electrolyzer architectures to improve energetic efficiency, first safety aspects to be solved • Overall system / media flow control
What was necessary to solve the challenge? Did it depend on advances in other fields?	Catalyst people need to closely collaborate with engineers that design the layout of electrolyzers
TRL	7
Stability	10000h
Energetic conversion efficiency	60%
DOI Reference	

Define time: short-/medium-/long-term, x years	Long: 12-15 years
Deliverable, milestone	First industrial installation of technology on the 100MW scale

Solved Challenges / Lifted barriers (in bullet points)	<ul style="list-style-type: none"> • Scale up • Cheap manufacturing and quality control including safety aspects • Sensing, monitoring system control
What was necessary to solve the challenge? Did it depend on advances in other fields?	Convince society and investors Industrialization activities Public//governmental support to bring technology into the market
TRL	9
Stability	At least 10000h
Energetic conversion efficiency	60+%
DOI Reference	

[Link to TRL level](#)

At TRL 5-6:

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

At TRL 7-8:

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

At TRL 9:

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

6. Opportunity criteria

What are the criteria that make this technology an opportunity when ready?

Score the potential opportunity from 0 (very low) to 12 (very high).

Each contributor provides an individual score (we average afterwards).

Opportunity criteria	Individual Score

7. Feasibility criteria

What factors determine the feasibility of the final application?

Score the potential feasibility from 0 (very low) to 12 (very high).

Each contributor provides an individual score (we average afterwards).

Feasibility criteria	Individual Score

8. Key learning points

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

Decision points	
Knowledge gaps	Understanding/experience with electrocatalyst
Risks	H2 electrolyzers get widely industrialized and CO2 transformation is done with improved thermo-catalysis Too much liquid byproduct, which may be hard to separate

Resources

Suggestion	Please detail
Critical, rare elements	Currently Iridium is used in neutral/acidic electrolytes as counter electrode to generate O2 at the cathode. Availability is limited to several GW. So on the medium term need for replacements.
Non-fluctuating energy sources	Electrolyzer needs to be able to adapt its operation to the availability of renewable energy in the grid.
Hydrogen storage	
CO2 storage	Yes needed, but feasible (buffer storage)
Water purification	Yes at least purified (desalinated with existing technology)
CO2 from the atmosphere	For >10 a from concentrated source, later capture from air at current cost 1000€/t that needs to be reduced to 100€/t
Concentrated, pure CO2	
Specific, new infrastructures	Transportation of electricity to the place where CO2 is available & transport of products
Low-cost, low-carbon electricity	Needed for 1-2 Ct/kWh
Renewable energy	Yes, see above
Renewable heat	No

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Breakthroughs in key enabling disciplines

Scale-Up	From W to 100MW range
System integration	Catalyst + membranes + electrolyte + product separation
Novel reactor designs	Feed of CO ₂ which is badly soluble in water, avoid all ohmic conductance losses in the electrolyte
Novel catalyst materials: earth-abundant, non-toxic, efficient, stable	Yes, catalysts based on Cu needs to be developed as well as Ir replacements
Novel absorber materials: earth-abundant, non-toxic, efficient, stable	Here: new membrane materials, anion conducting polymeric membranes (AEMs) needed for improved electrolyzer architectures.
Standardized life-cycle assessment methodologies	10000h is hard to test, accelerated live time testing needs to be developed
Further developments in quantitative sustainability analysis	LCA techniques available, need to be applied
Strain robustness	
Genomic stability	
Preservation (culture collection)	

Political/societal/market barriers

EU-wide, homogeneous regulatory frameworks	Lack of supporting frameworks
Adaptation/ novel regulations (e.g. genetics, use of waste CO ₂ , ..)	No ethically critically topics involved
EU/national regulations for the deployment of the	Production safety regulations a in each chemical plant/refinery

technology/product	
EU/national incentives for the deployment of the technology/product	Needed for market introduction, e.g. CO2 taxes, tax benefits for green chemicals
Fast idea protection (patenting, etc.)	Ongoing on a worldwide scale
Large capital investment for market introduction	Yes, a refinery is about 10 Billion, a renewable refinery would need about twice the investment and about the fivefold for PV Cost payback in <10 years since a renewable refinery do not need to pay for crude
Standardization of efficiencies, etc.	
Societal acceptance	
Political security	Make the European Union independent on crude oil important
EU supply chain	Two options: deployment in Europe would need to cope with our amount of available sunshine and invest. Europa may manufacture the technologies which are deployed worldwide.

Funding/research frameworks

International collaboration	<u>X</u>
Funding schemes for demonstrators, pilots, etc.	<u>X</u>
Large-scale EU research initiatives	<u>XXX</u>

Electrochemical production of hydrocarbon fuels

Technology	Electrochemical production of hydrocarbon fuels (focus on jet fuel) – Power-to-Liquids (PtL)																									
Targeted product	<table border="1" style="width: 100%; border-collapse: collapse;"> <tr> <td style="text-align: center;">H₂</td> <td style="text-align: center;">NH₃</td> <td style="text-align: center;">CH₃OH</td> <td style="text-align: center;">EtOH</td> <td style="text-align: center;">CH₄</td> <td style="text-align: center;">Jet fuel</td> <td style="text-align: center;">CO₂</td> <td colspan="2" style="text-align: center;">Other</td> </tr> <tr> <td style="text-align: center;">(x)</td> <td></td> <td style="text-align: center;">(x)</td> <td></td> <td style="text-align: center;">(x)</td> <td style="text-align: center;">x</td> <td></td> <td colspan="2" style="text-align: center;">LPG, Naphtha, Diesel</td> </tr> </table>								H ₂	NH ₃	CH ₃ OH	EtOH	CH ₄	Jet fuel	CO ₂	Other		(x)		(x)		(x)	x		LPG, Naphtha, Diesel	
H ₂	NH ₃	CH ₃ OH	EtOH	CH ₄	Jet fuel	CO ₂	Other																			
(x)		(x)		(x)	x		LPG, Naphtha, Diesel																			
Nature of active material	x	Solid-state Inorganic		Molecular			Biomolecular		Biological (living cells)																	
Sunrise approach	x	PV-powered electrocatalysis		Photoelectrochemical direct conversion			biological and biohybrid direct conversion		Key enabler*																	
Contribution to SUNRISE goals (what?)	x	Sustainable low-carbon production of <u>carbon-based fuels</u> with high efficiency and competitive costs																								
	(x)	Sustainable low-carbon production of carbon-based <u>commodity chemicals</u> with high efficiency and competitive costs																								
		Sustainable low-carbon production of <u>ammonia</u> with high efficiency and competitive costs																								
	(x)	Sustainable low-carbon production of <u>hydrogen</u> with high efficiency and competitive costs																								
		<u>CO₂</u> as a valuable feedstock																								
		Sustainable <u>building materials</u> , mineralization																								
Sustainability criteria	x	Carbon capture from the atmosphere																								
	x	Carbon capture from point sources/ flue gas																								
	(x)	Exclusive use of abundantly available, non-toxic and non-critical elements																								
		Sunlight as the primary energy source																								
	x	Low resource consumption																								
	x	Solar to products yields tenfold to hundredfold higher than current biomass practice																								
Envisaged																										

production system	Decentralized, local production at small scale (households, niche applications)		
	x	Large-scale production using existing centralized infrastructure	
	x	Large-scale production necessitating new infrastructure	
Rough timeline (when?)	Short term (2020-25)	Medium term (2025–30)	Long term (2030–50)
	TRL° 1-6	TRL° 3-8	TRL° 6-9
Who are the main actors? Who has to be involved?	<p>German actors: Global alliance power fuels, PtX Allianz, BMWi, BMU, UBA, aireg</p> <p>C. Breyer (Lappeenranta University of Technology)</p> <p>Supporters: A. Sizmann, V. Batteiger (Bauhaus Luftfahrt) R.-U. Dietrich (DLR Stuttgart), T. Hirth, R. Dittmeyer (KIT) I. Hannula, J. Maninnen (VTT Technical Research Centre of Finland)</p> <p>Companies: Sunfire, Ineratec, Velocys</p>		

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

1. Short description of the proposed technological solution

Main technological elements, working principle (max. 5 lines, for scientists not expert in the field)	<p>Water electrolysis (electrochemical splitting of water into hydrogen and oxygen); part of the generated hydrogen is used to reduce CO₂ to carbon monoxide (CO) in a reverse water gas shift (RWGS) reaction; liquefaction of a mixture of the remaining hydrogen and CO (also called synthesis gas) to hydrocarbons via Fischer-Tropsch synthesis or to methanol (in case of methanol, H₂ and CO₂ can be directly reacted, avoiding the RWGS step). Hydrocarbon raw products need refining through hydroprocessing.</p> <p>Alternative: Co-electrolysis of water and CO₂ to directly yield synthesis gas (without RWGS).</p>
Why is this technology not commercially available right now? (major challenges)	<p>Main process steps (renewable electricity generation, water electrolysis, Fischer-Tropsch synthesis and hydroprocessing) are industrially mature. Major challenges lie in the integration of the individual process steps and in the adaption of the system to renewable energy supply (with, e.g., its intermittency); other challenges relate to the provision of CO₂ from renewable sources and the scale of the process: While conventional Fischer-Tropsch</p>

	<p>synthesis is conducted at very large scale and under stable process conditions, coupling with electrolysis and (potentially) intermittent renewable electricity supply requires smaller scales and load-flexible operation.</p> <p>Advanced electrolysis technologies (PEM, solid oxide electrolysis cell (SOEC)) could enable higher process efficiencies and need further development.</p> <p>A central challenge is economic and political in nature: Production of electrofuels is not cost-competitive with conventional fuel production. Regulatory/political measures are required to create a market and to provide a stable and reliable environment for the required large investments.</p>
<p>What does it take to make it happen? (in short)</p>	<p>Development of individual components</p> <ul style="list-style-type: none"> - Continued cost reduction of solar and wind electricity generation. - Electrolysis (PEM, SOEC, etc.) - CO₂ capture from air - Small-scale and load-flexible Fischer-Tropsch reactors and other liquefaction reactors, e.g. methanol synthesis) <p>Process integration</p> <ul style="list-style-type: none"> - Integrated production plants needed (pilot, demonstration, (pre-)industrial scale) <p>Electrochemical production of jet fuel (and other C-based liquid fuels) requires strong involvement of industrial players, as most involved process technologies are mature and the integrated processes now need demonstration in industrially relevant environments. Next to public funding of R&D activities, it is therefore important to implement policy/regulatory measures rendering commitment and investments attractive for the industry. Stable and reliable market conditions are crucial for industrial engagement. Policy/regulatory measures could aim for leveling the price gap between electrofuels and conventional fuels, e.g. through CO₂ taxes or effective emissions trading schemes. Other conceivable measures are quota for specific types of renewable fuels. A fair scheme for GHG accounting for electrofuels (using CO₂ and electricity as “feedstock”) in the context of (advanced) biofuels and electric (battery, fuel cell) vehicles is also vital to incentivize production and use of electrofuels.</p>

What is the benefit for society? (in short)	<p>The option to decarbonize aviation as a strongly growing transport sector that will continue to depend on liquid C-based fuels.</p> <p>To a lesser extent, this is also true for the maritime and heavy duty road transport. Additionally, electrofuels could help to reduce emissions in the personal automotive transport in the medium-term future, i.e. through fueling the existing fleet during the ramp-up of electromobility to replace ICE vehicles.</p>
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2. Existing R&I projects

Existing national/EU project	Final objective	TRL	Run-time	Funding Instrument
PowerFuel	Demonstration of an entire Power-to-Liquids production chain under load-flexible operational conditions.	6	3 years (2018 – 2021)	German Federal Ministry of Economic Affairs and Energy
KEROSyN100	Demonstration of PtL process	6		German Federal Ministry of Economic Affairs and Energy
Kopernikus Power-to-X		6		German Federal Ministry of Education and Research
Reallabore der Energiewende	several projects	>6		German Federal Ministry of Economic Affairs and Energy
Soletair	https://soletair.fi/			
Nordic Bluecrude Sunfire	commercialization	>6		commercial

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

Technological solution to be developed in SUNRISE	
TRL	5-6 (FT-SPK); 8 (Power-to-Methanol)
Cost	1.841 (1.086 – 1.926) EUR t ⁻¹ (assuming 2050 technologies) 1.348 – 4.165 EUR t ⁻¹ (assuming 2030 technologies)
Energetic conversion yield	40 – 55 % (electricity to final fuel product) 6 – 8.3 % (solar energy to final fuel product, assuming a 15% PV efficiency)
Stability	
Product separation yield	
Total energy demand [GJ/t]	80 – 110 GJ _{el} /t _{fuel} (at the PtL plant/refinery; energy for construction (also of PV or wind turbines etc) not included)
Electricity needs [GJ/t]	80 – 110 GJ _{el} /t _{fuel}
Energy demand utilities [GJ/t]	
Steam balance [GJ/t]	
CO2 emissions [tCO2 eq/t] (cradle-to-grave, including feedstock production)	1 – 28 gCO2eq /MJ or 0.044 – 1.23 tCO _{2eq} /t
Water consumption	about 0.038 to 0.040 m ³ of water per GJ of jet fuel or 1.3 to 1.4 liters of water per liter of jet fuel (process-related demand; water consumed in construction process not included)
Air separation unit	
Compressors	
DOI References	

4. Available techno-economical analysis:

DOI Reference	https://doi.org/10.1016/j.rser.2017.05.288 DOI: 10.1002/cite.201700129
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	3 years
Deliverable, milestone	Integrated (complete) PtL production chain demonstrated under relevant operational conditions (load-flexible; based on 100% renewable electricity) at pre-commercial scale
Solved Challenges / Lifted barrier (in bullet points)	•
What was necessary to solve the challenge? Did it depend on advances in other fields?	PtL producing jet fuel depends on progress especially in progress in CO ₂ capture, renewable electricity generation (low-cost!), and electrolysis. Aviation is not driving these developments, but benefitting from them.
TRL	>6
Stability	
Energetic conversion efficiency	
Scale	
DOI Reference	

Define time: short-/medium-/long-term, x years	5-10 years
Deliverable, milestone	Commissioning of first industrial (commercial) PtL plant, producing aviation-compatible fuel, based on fully renewable electricity and CO ₂ .

Solved Challenges / Lifted barriers (in bullet points)	•
What was necessary to solve the challenge? Did it depend on advances in other fields?	mainly investment and suitable political boundary conditions
TRL	8-9
Stability	
Scale	10 kt/yr or more.
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
GHG emissions	12
economic competitiveness	8 (depends very much price for CO ₂ , incentives etc.)
Scalability (substitution potential)	12

7. Feasibility criteria

What factors determine the feasibility of the final application?

Score the potential feasibility from 0 (very low) to 12 (very high).

Each contributor provides an individual score (we average afterwards).

Feasibility criteria	Individual Score

8. Key learning points

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

Decision points	
Knowledge gaps	
Risks	

Resources

Suggestion	Please detail
Critical, rare elements	Pt metals (as electrode materials in PEM fuel cells); rare earth elements for permanent magnets needed for wind power.
Non-fluctuating energy sources	Renewable electricity from hydropower and geothermal power can be applied instead of or in addition to intermittent wind, solar-thermal or PV electricity.
Hydrogen storage	Probably needed, depending on process design (scale of electrolyzer in relation to scale of liquefaction unit; load-flexibility of liquefaction unit)
CO2 storage	Depending on process design and CO ₂ sources, only small-scale storage (CO ₂ buffer) needed.
Water purification	Needed
CO2 from the atmosphere	Sustainable and most scalable option; key technology!
Concentrated, pure CO2	Can be used but must come from sustainable sources.
Specific, new infrastructures	Needed for future large-scale applications in remote areas with good conditions for renewable electricity generation (e.g. deserts). First industrial plants can benefit from existing infrastructure. Large-scale ramp-up of renewable electricity generation will be necessary in any case.

Low-cost, low-carbon electricity	Crucial (prerequisite!)
Renewable energy	Crucial (prerequisite!)
Renewable heat	Needed, but can probably be provided from on-site waste heat (e.g. from exothermic Fischer-Tropsch synthesis)

Breakthroughs in key enabling disciplines

Scale-Up	Needed (especially under relevant operations conditions, e.g. with fluctuating electricity supply)
System integration	Very important; most individual process steps are already mature, but integration is far less advanced
Novel reactor designs	Small-scale liquefaction reactors (Fischer-Tropsch) matching scale of electricity supply and scale of electrolyzer and enabling load-flexible operation
Novel catalyst materials: earth-abundant, non-toxic, efficient, stable	Catalysts enabling direct liquefaction of CO ₂ ; this would help to avoid the preceding RWGS step (reduction of CO ₂ to CO).
Novel absorber materials: earth-abundant, non-toxic, efficient, stable	
Standardized life-cycle assessment methodologies	Needed to enable consistent comparison with biofuels and other production pathways; problem of proper accounting of the CO ₂ fed into the system is still subject of debate; for example: can a fuel produced from CO ₂ from a fossil source (e.g. coal-fired power plant) be sustainable? How is this CO ₂ feedstock accounted for in the overall life cycle balance?
Further developments in quantitative sustainability analysis	
Strain robustness	
Genomic stability	

Preservation (culture collection)	

Political/societal/market barriers

EU-wide, homogeneous regulatory frameworks	Required, e.g. in order to enable economic competitiveness; consistent sustainability assessment
Adaptation/ novel regulations (e.g. genetics, use of waste CO ₂ , ..)	Required, e.g. consistent accounting of CO ₂ feedstock
EU/national regulations for the deployment of the technology/product	Required; e.g. quota, sustainability safeguards/rules
EU/national incentives for the deployment of the technology/product	Required, e.g. effective emissions trading, CO ₂ tax, proper accounting with respect to renewable energy quota (e.g. multipliers in EU-RED II), etc.
Fast idea protection (patenting, etc.)	
Large capital investment for market introduction	Urgently needed
Standardization of efficiencies, etc.	
Societal acceptance	Needed, as ramp-up would require large-scale installation of additional renewable power plants (PV, wind etc.)
Political security	Mandatory, as huge investments are only conceivable in reliable policy/regulatory frameworks
EU supply chain	
Technical approval of fuel for use in commercial aviation	Crucial; fuel specifications (e.g. ASTM D7566) very strict, as safety is prerequisite. FT-based jet fuel is already approved (with syngas from whatever sources: coal, natural gas, biomass, PTL, etc.)

Funding/research frameworks

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

Thermochemical production of hydrocarbons and jet fuel

Technology	Thermochemical production of hydrocarbons and jet fuel									
Targeted product	H ₂	NH ₃	CH ₃ OH	EtOH	CH ₄	Jet fuel	CO ₂	Other		
			x	x	x	x				
Nature of active material	x	Solid-state Inorganic		Molecular			Biomolecular		Biological (living cells)	
Sunrise approach	x	PV-powered electrocatalysis		x	Photoelectrochemical direct conversion		biological and biohybrid direct conversion		x	Other
Contribution to SUNRISE goals (what?)	x	Sustainable low-carbon production of <u>carbon-based fuels</u> with high efficiency and competitive costs								
		Sustainable low-carbon production of carbon-based <u>commodity chemicals</u> with high efficiency and competitive costs								
		Sustainable low-carbon production of <u>ammonia</u> with high efficiency and competitive costs								
		Sustainable low-carbon production of <u>hydrogen</u> with high efficiency and competitive costs								
		<u>CO₂</u> as a valuable product								
Sustainability criteria	x	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								
		Solar to products yields tenfold to hundredfold higher than current biomass practice								
Envisaged production system		Decentralized distribution production								
	x	Large-scale production using existing centralized infrastructure								
	x	Large-scale production necessitating new infrastructure								

Rough timeline (when?)	Short term (2020-25)	Medium term (2025–30)	Long term (2030–50)	
	TRL° 4-6	TRL° 5-7	TRL° 9	
Who are the main actors? Who has to be involved?	<p>In bold: Sunrise supporters</p> <p><u>Research Institutes in Europe:</u> DLR, Germany TU Dresden, Germany KIT, Germany Bauhaus Luftfahrt, Germany Solar-Institut Jülich, Germany ETH Zurich, Switzerland GDR Solar Fuels, France University of Zurich, Switzerland EPFL, Switzerland CNRS, France ENEA, Italy PSA Ciemat, Spain IMDEA Energy, Spain APTL, Greece</p> <p><u>Research Institutes around the World (non-exhaustive list):</u> Sandia National Laboratories, USA Arizona State University, USA University of Colorado, Boulder, USA University of Florida, USA Colorado School of Mines, USA Lawrence Berkeley National Laboratory, USA Caltech, USA Pacific Northwest National Laboratory, USA Georgia Tech, USA State Key Laboratory of Multiphase Flow in Power Engineering, China University of Adelaide, Australia Victoria University of Wellington, New Zealand Korea Institute of Energy Research, South Korea Niigata University, Japan</p> <p><u>Industrial companies which could play a key role for market implementation:</u> BASF, Germany Casale, Switzerland Total, France Synhelion, Switzerland Toyota, Japan/Belgium Abengoa, Spain Brightsource, Israel Helpe, Greece</p>			

* 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	Josua Vieten (DLR), Martin Roeb (DLR)
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1. Short description of the proposed technological solution

<p>Main technological elements, working principle (max. 5 lines, for scientists not expert in the field)</p>	<p>Hydrocarbons are currently used as fuel and as a feedstock for the chemical industry. The overwhelming majority of these hydrocarbons are currently of fossil origin. Upon combustion of these fuels, large amounts of CO₂ are generated, contributing to global warming.</p> <p>For many application scenarios, alternatives are currently developed. For instance, battery-electric and fuel cell vehicles are developed for road-based transportation. However, in some cases, a very high energy density is required, which currently is only feasible using hydrocarbon-based fuels. This is especially important in aviation, where the energy density of hydrocarbon fuels is crucial to achieve intercontinental travel without refueling.</p> <p>It is possible to produce and use carbon-based fuels without net CO₂ emissions. This requires CO₂ capture from the air (or the use of a biological carbon source), synthetic production of hydrocarbon fuels and subsequent combustion using conventional technology. The synthetic fuel production process is usually based on the production of syngas (hydrogen, H₂ and carbon monoxide, CO), which is then converted to hydrocarbons in the so-called Fischer-Tropsch process. Syngas can be produced from renewable sources using CO₂ and water (H₂O).</p> <p>Besides electrochemical options, an appealing pathway for CO₂ and H₂O splitting are thermochemical routes, which require an input of heat instead of electricity. The heat input can be delivered renewably by concentrating solar technology, which is already used in desert areas to produce electricity. Since heat is directly converted to chemical energy without an intermediate electricity production step, the theoretical efficiency of such processes is higher than in electrolysis.</p> <p>The thermochemical redox cycle typically consists of two steps at different temperatures, with an oxygen-carrying redox material as key</p>
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	<p>element. The two steps are:</p> <ol style="list-style-type: none"> 1. Oxygen release from the redox material (reduction): At high temperature (1350-1700 °C), the material releases some of its chemically-bound oxygen. This step is called reduction. It may be assisted by continuously removing the produced oxygen to shift the chemical equilibrium. 2. H₂O/CO₂ splitting (oxidation): At lower temperatures (600-1200 °C), the material is re-oxidized, which means that it takes up the oxygen which it lost in step (1). Since H₂O and CO₂ molecules contain oxygen, the redox material will split these molecules and absorb the oxygen from them. By this means, H₂O is converted to H₂ (hydrogen), and CO₂ is converted to CO (carbon monoxide). A combination of hydrogen and carbon monoxide is called syngas and can be used to produce hydrocarbons such as jet fuel. This process is entirely reversible, meaning that the metal oxide is not consumed overall. <p>It is also possible to use hydrocarbons for other applications besides the use as a jet fuel. For instance, the chemical industry requires large amounts of hydrocarbon resources, which could be produced by renewable means. Additionally, sea and road-based transportation could use synthetic fuels as well. This is especially beneficial in cases where battery-electric propulsion may not be efficient, such as in long distance or heavy duty transportation.</p> <p>Due to the predicted price of solar hydrocarbon fuels at commercial level (~ 2 €/L kerosene, reference: Bauhaus Luftfahrt, study presented at Solarpaces 2019) and the higher TRL of battery-electric and hydrogen-based propulsion, the use of solar fuels in transportation other than intercontinental aviation will most likely remain a niche application.</p>
<p>Why is this technology not commercially available right now? (major challenges)</p>	<p>The main factors to consider are efficiency and cost.</p> <p>Despite the fact that this process is very efficient in theory, large heat losses decrease its efficiency drastically. A large amount of redox material has to be heated to very high temperatures in the reduction step, and currently only a fraction of this heat can be recovered during cool-down and oxidation. An optimization of redox materials can decrease the temperature gap and increase the hydrogen or carbon monoxide productivity.</p>

	<p>Moreover, the steam needs to be heated to the oxidation temperature. Additionally, auxiliary systems are required, for instance vacuum pumps or purge gases to lower the oxygen partial pressure in the reduction step.</p> <p>Associated with that, the low efficiency would lead to a high price per kg of produced H₂ or CO₂, if these processes were commercialized today. Another source of high costs is the fact that the reactors for this process are expensive, as they require advanced refractory materials to withstand the high temperatures in such redox processes. All in all, this technology is still far from being economically competitive, given the still rather inexpensive option of sourcing fuels from crude oil. Even in large scale demonstration plants and research projects, only very small amounts of fuel are produced with current technology. Therefore, further research and development is required.</p>
<p>What does it take to make it happen? (in short)</p>	<p>More efficient solar fuels production processes require the following optimization steps:</p> <ul style="list-style-type: none"> • Reduction of cost of concentrating solar components by production at larger scale and technological innovation • Improvement of thermochemical redox materials (chemistry, physics) • Improvement of heat recovery between oxidation and reduction step (engineering) • More efficient removal of oxygen at high temperature through oxygen pumps (redox materials or membranes) • More efficient separation of products from reactants • Reduction of operational temperature • Process and design innovation for cost reduction of solar reactors
<p>What is the benefit for society? (in short)</p>	<p>There is currently no other technologically feasible option for intercontinental commercial aviation than to use carbon-based fuels for propulsion. These significantly contribute to global warming, if they are of fossil origin. CO₂ emissions account for about 1/3 of the total adverse effect of aviation on the climate (with the other 2/3 being caused by water vapor, NO_x-induced ozone production, and induced cloud formation, Lee et al., Atmos. Environ. 43, 2009, 3520-3537). By using renewable solar fuels, the effect of aviation on global warming could therefore be significantly reduced.</p>

	<p>The positive effects of solar fuels only exist if the CO₂ used for their production is removed from the atmosphere, rendering combustion of such fuels carbon-neutral.</p> <p>Society will benefit from the reduced CO₂ emissions, as the adverse effects of global warming such as extreme weather, draughts, and an increase of the sea level are mitigated. Moreover, reducing the effect of aviation on global warming can potentially increase worldwide travel by air, as individuals who would have decided against long distance travel due to the negative effects on the climate may take a different decision when renewable fuels are used. This would create economic benefits to the airline industry and to society, especially in areas which benefit strongly from globalization.</p>
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2. Existing R&I projects

Existing national/EU project	Final objective	TRL	Run-time	Funding Instrument
Sun-to-Liquid	Demonstration of solar fuels production	5	2016-2019	EU H-2020
Solare Kraftstoffe	Technology assessment, test of combustion behavior of fuels	4	2019-2021	BMW, Germany
DRESDEN	Preparation of a H2020 project between EU and US partners on materials development for solar fuels production	2	2019-2020	BMBF, Germany
Energiesysteme 2050	Systems analysis for a vision of the energy systems in 2050	4	2015-2020	Helmholtz Association, Germany
Future Fuels 2	Systems analysis for fuels of the future	4	2018-2021	DLR cross-cutting project, Helmholtz Association, Germany
HYDROSOL BEYOND	Reactor development for solar fuels production	4	2019-2022	EU H-2020
MENAFuels	Systems analysis for future fuels in the Mediterranean and North African region	4	2018-2022	BMW, Germany

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

Technological solution to be developed in SUNRISE	Thermochemical production of hydrocarbons and jet fuel
<i>The following data is for solar hydrogen and carbon monoxide production. The production of fuels from these feedstocks is state of the art (Fischer-Tropsch).</i>	
TRL	4-5
Cost	Estimate: 2 €/L kerosene (Bauhaus Luftfahrt, under positive assumptions for future technology development)
Energetic conversion yield	~1-6 % (solar to hydrogen efficiency), commercialization target: 15-30 %
Stability	Long term
Product separation yield	> 99 % for H ₂ (H ₂ separation from steam is effective), lower for CO
Total energy demand [GJ/t]	2000-14000 GJ/ton H ₂ (commercialization target: 400-800 GJ/ton)
Electricity needs [GJ/t]	depending on the extent of pumping for reduction: 5-30 % of the total energy demand
Energy demand utilities [GJ/t]	pumping, compression, separation (depends on plant size, larger plants will use less auxiliary energy)
Steam balance [GJ/t]	depends on the redox material, 2-60 % of the total energy demand
CO ₂ emissions [tCO ₂ eq/t] (cradle-to-gate, including feedstock production)	0, if the used CO ₂ and all energy sources are renewable and the plant is built using carbon-neutral energy sources
Water consumption	approx 8 t/t of H ₂ (excluding water used for construction and for production and supply of redox materials and auxiliaries)
Air separation unit	none, if no sweep gas is used
Compressors	required for storage and transportation of hydrogen, need of compressors is significantly reduced if fuels are produced directly
DOI References	10.1039/C9EE00085B

4. Available techno-economical analysis:

DOI Reference	https://www.eesi.org/files/netl_emissions_060001.pdf
Summary	Life-Cycle Greenhouse-Gas Emissions Inventory For Fischer-Tropsch Fuels
DOI Reference	C. Falter, V. Batteiger, A. Sizmann, Climate Impact and Economic Feasibility of Solar Thermochemical Jet Fuel Production, Environmental Science & Technology 2016, 50 (1), 470–477, DOI 10.1021/acs.est.5b03515 To be published soon, Christoph Falter et. al, Bauhaus Luftfahrt
Summary	Jet fuel prices around 2 €/L achievable with solar fuels under the assumption of further technology development
DOI Reference	http://www.lbst.de/news/2016_docs/161005_uba_hintergrund_ptl_barrierrefrei.pdf
Summary	Power-to-Liquids Potentials and Perspectives for the Future Supply of Renewable Aviation Fuel
DOI Reference	10.1039/C5EE02573G
Summary	A comparative technoeconomic analysis of renewable hydrogen production using solar energy
DOI Reference	10.1039/C8EE00111A
Summary	The future of solar fuels: when could they become competitive?
DOI Reference	10.1039/C1EE01311D
Summary	Methanol production from CO ₂ using solar-thermal energy: process development and techno-economic analysis “The solar concentrator/reactor sub-system accounts for more than 90% of the capital expenditure.”

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	By 2025-2030; Medium; 10 years
Deliverable, milestone	Increase in solar-to-fuel efficiency for solar-thermochemical hydrogen production to 15 %, demonstrated in pilot scale (250 kW thermal)
Solved Challenges / Lifted barrier (in bullet points)	Removal of largest efficiency bottlenecks <ul style="list-style-type: none"> • Material thermodynamics • Low heat recovery efficiency increased • Oxygen removal energy demand
What was necessary to solve the challenge? Did it depend on advances in other fields?	<ul style="list-style-type: none"> • Targeted design of optimized solar-thermochemical redox materials (well-defined redox enthalpy, entropy change maximized) • Solid-solid heat recovery rate > 60 % • Steam heat recovery rate > 95 % • Oxygen removal more efficient (combination of mechanical pumps and thermochemical pumps or oxygen-conducting membranes) • Limitation of re-radiation losses and spillage of radiation at the solar receiver • Scale-up to improve efficiency • Improved separation of products and reactants
TRL	5-6
Stability	20 years
Energetic conversion efficiency	15% minimum
Scale	250 kW thermal
DOI Reference	-

Define time: short-/medium-/long-term, x years	Medium to long term (2035-2040)
Deliverable, milestone	Substantial decrease in cost per kg of jet fuel produced (< 4 \$/kg jet fuel)

Solved Challenges / Lifted barriers (in bullet points)	<ul style="list-style-type: none"> • High cost of reactors and solar fuel production technology
What was necessary to solve the challenge? Did it depend on advances in other fields?	<ul style="list-style-type: none"> • Less expensive materials used for reactor design through reduced temperature and lower differences in total pressure, better heat distribution • Decrease in cost of solar-thermal technology (heliostats, towers) due to implementation of concentrated solar power plants on a larger scale • Optimization and integration of Fischer-Tropsch plants and solar fuel production plants
TRL	6-7
Stability	20 years
Energetic conversion efficiency	15-20%
Scale	> 10 MW thermal
DOI Reference	

Define time: short-/medium-/long-term, x years	2050, long-term
Deliverable, milestone	Commercialization and further efficiency increase, lower cost (max. 2 \$/kg jet fuel)
Solved Challenges / Lifted barriers (in bullet points)	<ul style="list-style-type: none"> • Efficiency increased • Cost decreased (scale-up)
What was necessary to solve the challenge? Did it depend on advances in other fields?	<ul style="list-style-type: none"> • Further optimization of solid-solid heat recovery (target: 80 %) • Decreased temperature difference between reduction and oxidation through further materials optimization • Scale-up and therefore decreased component cost • Decrease in the amount of steam to be produced per mol of hydrogen • Process optimization using experience from existing pilot plants
TRL	8-9
Stability	20 years
Energetic conversion efficiency	20-30%

Scale	Industrial scale, solar-plant similar to Ivanpah plant, USA
DOI Reference	10.1115/POWER2011-55248

Link to TRL level

At TRL 5-6:

Production volume	1 kg H ₂ / h at 250 kW thermal energy input (15 % solar-to-hydrogen efficiency) or approx. 30 kg CO (similar molar amount and efficiency) $2n \text{ H}_2 + n \text{ CO} \rightarrow \text{C}_n\text{H}_{2n} + \text{H}_2\text{O}$ ⇒ approx. 4 kg fuel per h
Light harvesting area needed per t/product	For hydrogen production at about 20% solar-to-hydrogen efficiency one needs 2km ² for the production of 50 tons of H ₂ (11 hours from the sun and 13 hours from an electricity grid). Idriss et al. SABIC- TechnoEconomy Report, Dec. 2018 (Classified). At 15 % efficiency one needs 2.66 km ² for 50 tons => 0.05 km ² /t of product
Political/societal barriers to be overcome	
Market barriers to be overcome	High price of solar fuel

At TRL 7-8:

Production volume	~200-250 kg fuel per h at 10 MW thermal heat input and 20 % solar-to-fuel efficiency
Light harvesting area needed per t/product	For hydrogen production at about 20% solar-to-hydrogen efficiency one needs 2km ² for the production of 50 tons of H ₂ (11 hours from the sun and 13 hours from an electricity grid). Idriss et al. SABIC- TechnoEconomy Report, Dec. 2018 (Classified).
Political/societal barriers to be overcome	Construction of large solar arrays for testing and technology development at pilot scale
Market barriers to be overcome	Solar fuel still not competitive at this TRL

At TRL 9:

Production volume	~30 t fuel per h at 1 GW thermal energy input and 25 % solar-to-fuel efficiency (~ 1h needed to produce enough fuel for a flight from New York to London on an A350-900 aircraft)
Light harvesting area needed per t/product	For hydrogen production at about 20% solar-to-hydrogen efficiency one needs 2km ² for the production of 50 tons of H ₂ (11 hours from the sun and 13 hours from an electricity grid). Idriss et al. SABIC- TechnoEconomy Report, Dec. 2018 (Classified).
Political/societal barriers to be overcome for market introduction	The cost of hydrogen and fuels is still higher than from fossil sources, needs government engagement to define the needed phases (incentives to use carbon-neutral processes, carbon tax or effective emissions trade)
Market barriers to be overcome	High price of solar jet fuel compared to fossil jet fuel. One recent study estimates 2 USD/kg under optimistic assumptions, compared to around 0.50 USD/kg for fossil fuel. Combustion of 1 kg of jet fuel produces 3.15 kg of CO ₂ emissions. A carbon emissions price of ~ 480 USD/t would be required to lead to equal cost. However, the commitment of airlines and customers to a decrease of CO ₂ emissions may lead to a higher acceptance of price increases in aviation – especially when considering that fuel costs account for less than half of the total cost of airline operations. Moreover, fossil fuel is not available in unlimited amounts, which may increase the price of conventional jet fuel.

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
Environmental regulations	12
Excess or high deployment of renewable electricity	6
Need for energy storage	8
Widespread implementation of concentrating solar power (synergy effects due to decreasing cost of heliostats and towers)	11

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
Efficiency of solar hydrogen and CO production	11
Sub-criteria:	
Thermochemical materials optimization	8
Heat-recovery efficiency	12
Product gas separation	6 (hydrogen), 11 (carbon dioxide)
Improved reactor design	9
Improved oxygen pumping	9
Improvement of operational parameters	10
Cost of concentrating solar equipment (mainly heliostats)	10
Integration with Fischer-Tropsch technology	9
Improvement of reactor design	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	Need for carbon-neutral jet fuels as consensus in politics, society, and industry Carbon emission pricing as an incentive to search for alternative fuels
Knowledge gaps	Efficiency improvement: need for improved redox materials, process innovation (heat recovery, lower differences in oxidation and reduction temperatures, better product gas separation), pathways to lower cost
Risks	Long-haul aviation may most likely be one of the last fields to become carbon-neutral due to high technological challenges in producing

	<p>carbon-neutral fuels. At the time when carbon-neutral fuels reach a sufficient TRL, the crude oil price may be very low due to the drastically reduced demand from other sectors in the decades before. It may be economically unfavorable to move to carbon-neutral fuels, especially since the impact of CO₂ emissions from long haul flights is small in comparison. Without political incentives, reducing the CO₂ emissions of long haul flights may never be economically favorable.</p> <p>Producing solar fuels at competitive prices is challenging. It is crucial that significant technological advancements are made quickly, especially in terms of solar-to-fuel efficiency.</p> <p>Carbon dioxide capture from the air is still expensive. Companies may be incentivized to use other CO₂ sources to “greenwash” their fuel production process without actually producing carbon-neutral fuels.</p> <p>Public funding bodies must ensure that CO₂ is removed from the air to the same extent at which it is produced upon fuel production.</p> <p>Synthetic fuel production requires high amounts of water, but concentrating solar plants are usually located in the desert. Access to water must be available without competing with the water supply of the local population.</p>
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Resources

Suggestion	Please detail
Critical, rare elements	Some of the redox materials for solar fuel production require rare earth elements such as cerium, lanthanum and samarium. Many novel perovskite materials, however, require only little or no rare earth metals and are entirely made from abundant resources.
Non-fluctuating energy sources	The Fischer-Tropsch process is net exergonic. This means that auxiliary electricity can at least partially be produced from waste heat of this process. 24 h operation requires thermal energy storage or external electricity sources.
Hydrogen storage	Only small amounts of hydrogen storage are required, as hydrogen is used on-site for fuel production.
CO ₂ storage	Only small amounts of CO ₂ storage are required, as CO ₂ is used on-site for fuel production.
Water purification	Required in desert areas (desalination of sea water)
CO ₂ from the atmosphere	Required
Concentrated, pure CO ₂	Will be produced from the atmosphere

Specific, new infrastructures	Concentrating solar plants coupled with fuel production infrastructure
Low-cost, low-carbon electricity	24 h operation requires thermal energy storage or external electricity sources.
Renewable energy	From concentrating solar power
Renewable heat	See above

Breakthroughs in key enabling disciplines

Scale-Up	1 ton of hydrogen/day from fully renewable source would be a breakthrough.
System integration	Integration of Fischer-Tropsch plant and solar fuels production
Novel reactor designs	Better temperature distribution and lower heat losses
Novel catalyst materials: earth-abundant, non-toxic, efficient, stable	New perovskite redox materials
Novel absorber materials: earth-abundant, non-toxic, efficient, stable	
Standardized life-cycle assessment methodologies	Standardization of materials performance metrics, currently done in a project coordinated by Arizona State University
Further developments in quantitative sustainability analysis	
Strain robustness	
Genomic stability	
Preservation (culture collection)	

Political/societal/market barriers

EU-wide, homogeneous	Carbon emission pricing as a strong incentive must be applicable
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regulatory frameworks	worldwide (airlines can otherwise choose a different country to base their operations in)
Adaptation/ novel regulations (e.g. genetics, use of waste CO2, ..)	
EU/national regulations for the deployment of the technology/product	Decarbonization of long-haul aviation
EU/national incentives for the deployment of the technology/product	Carbon tax and incentives for energy storage (in chemicals)
Fast idea protection (patenting, etc.)	Worldwide IP protection required
Large capital investment for market introduction	Concentrating solar plants have very high CAPEX
Standardization of efficiencies, etc.	
Societal acceptance	Good acceptance by airlines and passengers expected, as long as prices do not increase too much Local acceptance of concentrating solar fuels production plants challenging (especially in developing countries, many people could not afford long-haul airline tickets, so they would not benefit from the plants)
Political security	Willingness for decarbonization must be a premise of environmental politics worldwide for the next decades
EU supply chain	Rare earth elements may be required in small amounts Net import of fuels from countries with good solar irradiance is required (new potential political/economical dependencies)

Funding/research frameworks

International collaboration	H2020 and activities between Germany and the United States, EERA, IEA tasks
Funding schemes for demonstrators, pilots, etc.	Horizon Europe, H2020, national and regional research funding, at a later stage: oil companies and airline industry
Large-scale EU research initiatives	Secure, Clean and Efficient Energy https://ec.europa.eu/programmes/horizon2020/en/h2020-section/sec

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Biocatalytic production of chemicals by microorganisms

Technology	Biocatalytic production by engineered microorganisms (microalgae, cyanobacteria and photosensitised heterotrophic bacteria)																						
Targeted product	<table border="1" style="width:100%; text-align:center;"> <tr> <td>H₂</td> <td>NH₃</td> <td>CH₃OH</td> <td>EtOH</td> <td>CH₄</td> <td>Jet fuel</td> <td>CO₂</td> <td>Other</td> </tr> <tr> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td>X diverse number of carbon-based chemicals (terpenes, monomers, polymers...)</td> </tr> </table>							H ₂	NH ₃	CH ₃ OH	EtOH	CH ₄	Jet fuel	CO ₂	Other								X diverse number of carbon-based chemicals (terpenes, monomers, polymers...)
H ₂	NH ₃	CH ₃ OH	EtOH	CH ₄	Jet fuel	CO ₂	Other																
							X diverse number of carbon-based chemicals (terpenes, monomers, polymers...)																
Nature of active material	Solid-state Inorganic		Molecular			Biomolecular		X Biological (living cells)															
Sunrise approach	PV-powered electrocatalysis		Photoelectrochemical direct conversion			X Biological and biohybrid direct conversion		Key enabler*, Other															
Device category	Electrolyzer		Photo(bio)electrolyzer			X Photo(bio)reactor		fermentors, thermocatalytic reactors															
Contribution to SUNRISE goals (what?)	<table border="1" style="width:100%;"> <tr> <td style="width:5%;"></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></td> <td>Sustainable low-carbon production of <u>ammonia</u> with high efficiency and competitive costs</td> </tr> <tr> <td></td> <td>Sustainable low-carbon production of <u>hydrogen</u> with high efficiency and competitive costs</td> </tr> <tr> <td></td> <td><u>CO₂</u> as a valuable feedstock</td> </tr> <tr> <td></td> <td>Sustainable <u>building materials</u>, mineralization, long-lasting C-based materials</td> </tr> </table>									Sustainable low-carbon production of <u>carbon-based fuels</u> with high efficiency and competitive costs	X	Sustainable low-carbon production of carbon-based <u>commodity chemicals</u> with high efficiency and competitive costs		Sustainable low-carbon production of <u>ammonia</u> with high efficiency and competitive costs		Sustainable low-carbon production of <u>hydrogen</u> with high efficiency and competitive costs		<u>CO₂</u> as a valuable feedstock		Sustainable <u>building materials</u> , mineralization, long-lasting C-based materials			
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Rough timeline (when?)	Short term (2020-25)	Medium term (2025–30)	Long term (2030–50)							
	TRL ^o 1 (new chemicals) - 6 (e.g. lactic acid)	TRL ^o 7-8	TRL ^o 9							
Who are the main actors? Who has to be involved?	University of Turku, Uppsala University, CEA, Stockholm University, Bielefeld, Cambridge, Wageningen, University of Amsterdam, Graz University, TU Kaiserslautern, University of Copenhagen, VTT Oy, NREL, Berkeley, Harvard Industry: Photanol, Ecoduna, Synthetic Genomics, Euglena Oy									

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

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

Contributors	Yagut Allahverdiyeva-Rinne (Turku), Juliette Jouhet (CEA, Grenoble), Joanna Kargul (Warsaw), K. Hellingwerf and many other Sunrise community
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1. Short description of the proposed technological solution

Main technological elements, working principle (max. 5 lines)	Production of various carbon-based chemicals of industrial interest by engineered photosynthetic microorganisms, using sunlight, water and CO ₂ . Main advantage of this technology is a sustainable production of complex chemicals by the newly designed cell factories acting as self-assembled, long-term efficient biocatalysts.
Why is this technology not commercially available right now? What are the major challenges?	Low solar-to-chemicals conversion efficiency (below 1%) due to competing routes and also technical limitations (cultivation, cell harvesting and product separation, purification, suboptimal interfacing of photosensitisers with CO ₂ -fixing heterotrophic bacteria etc). High costs for microorganisms cultivation (feedstock production). A major

	<p>challenge is to fine-tune photosynthesis to increase photosynthetic performance and engineer stable and efficient strains producing desired end-product. Challenges: strain instability, product toxicity, not all production pathways (chemicals) are naturally available, short production phase (few days) compared to the biomass accumulation phase (weeks). Some chemicals production are available at high TRL (e.g. lactic acid by Photanol), however further improvement of strains and production process is necessary for cost-efficient production.</p>
<p>What does it take to make it happen? (in short)</p>	<p>A need for screening robust strains with naturally high production capacities. More efficient engineering tools and synthetic biology approach, combined with system biology level strain characterization and optimization. Engineered new strains with enhanced metabolic pathway for various chemicals production and secretion. Construction of special photobioreactors for cultivation and production phases (see enabler). Improvement of photosynthetic performance and carbon metabolism. A reliable, low cost water supply is critical to the success of bioproduction. Utilisation of CO₂ from point sources can boost biomass accumulation during the algae cultivation stage. Positive impacts could occur when algae production is integrated into the treatment of water bodies already suffering from excess nutrient supply.</p>
<p>What is the benefit for society? (in short)</p>	<p>This technology offers (i) sustainable production platform for various carbon-based chemicals and fuels; (ii) minimum competition with food production since marginal land is used (also e.g. utilisation of marine strains) (iii) contribution to CO₂ mitigation. The system will also contribute to wastewater remediation and recycling of nutrients (reduce N, P loss).</p>

2. Existing R&I projects

Existing national/EU project	Final objective	TRL	Run-time	Funding Instrument
Photofuel	Biocatalytic production of alternative liquid transportation fuels, using only sunlight, CO ₂ , and water.	3-5	2015-2020	EU Horizon2020
Synbio Powerhouse	Synbio Powerhouse is an ecosystem and service operator accelerating synthetic			National - SITRA,

	biology based business growth in Finland in cooperation with a growing international network			Academy of Finland

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

Technological solution to be developed in SUNRISE	
TRL	Up to 7
Cost	
Energetic conversion yield	
Stability	
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	

Conventional fossil-based process	
Global annual production volume	

Total energy demand [GJ/t]	
Energy feedstock [GJ/t]	
Fuel demand [GJ/t]	
Steam balance [GJ/t]	
Electricity [GJ/t]	
Air separation unit	
Compressors	
CO2 emissions [tCO2 eq/t] (cradle-to-gate, including feedstock production)	
Water consumption per t product	At least 50 fold less
Current TRL	
Current cost per t product	
DOI References	

Biomass-based process (if any)	
Global annual production volume	
Energy demand [GJ/t]	
Feedstock demand [GJ/t]	
CO2 emissions [tCO2 eq/t] (cradle-to-gate, including feedstock production)	
Water consumption per t product	In some cases 80% water recycling; per t dry algae 10 t is lost during the drying process, and around 15t during processing (total approx 25t)
Electricity needs [GJ/t]	
Current TRL	6-8
Current cost per t product	5-30 €/kg
DOI References	

4. Available techno-economical analysis:

DOI Reference	https://doi.org/10.1016/j.biombioe.2012.12.019
Summary	R. Slade and A. Bauen 2013 Micro-algae cultivation for biofuels: Cost, energy balance, environmental impacts and future prospects

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, 2-5 years	
Deliverable, milestone	<ul style="list-style-type: none"> ● Selection characterization of robust photosynthetic strains with high photosynthetic efficiency ● Application of synthetic biology to introduce desired pathways ● Construct efficient methylotrophic or formatotrophic etc microorganisms, introduce novel metabolic routes of carbon assimilation. ● Adapt the engineered microorganisms to industrial conditions of production ● Deliver engineered strains with productivities > 500 mg/L-day. An excellent starting point for reaching > 2-5 g/L-day productivities. ● A platform for automated synthesis and assembly of genetic constructs ● A proof of concept for different product formation and quantification ● A platform for adaptive evolution for tolerance to environmental stresses, including product. Allow continuous production of titers up to >10 g/L ● Integration of new control systems based on predictable models (machine learning) for phototrophic cultivation using sunlight ● Controlled uncoupling stable production of chemicals and cell growth
Solved Challenges / Lifted barrier (in bullet points)	<ul style="list-style-type: none"> ● Toxicification of host by the product

	<ul style="list-style-type: none"> • Instability of strains, low light to product conversion efficiency
What was necessary to solve the challenge? Did it depend on advances in other fields?	
TRL	1-3 (for newly engineered strains)
Stability	
Energetic conversion efficiency	
Scale	Lab scale for novel products / strains
DOI Reference	

Define time: medium-term, 5-10 years	<ul style="list-style-type: none"> • Develop novel protocols and cultivation strategies for induction of efficient, long-term and continuous bioproduction in green algae, cyanobacteria and photosensitized heterotrophic microorganisms • New bioproduction pathways that use non-native reactions: can increase energy yield by 25-50% • Exploit knowledge on the regulation of photosynthesis, electron flow and CO₂ assimilation to implement the yield of biological photohydrogen and chemicals production. • Achieve light to product conversion efficiency 4-6 % • Product titters of 10-20 g/L, production rates of 5 mM/h, cellular activities above higher than 50 U /g cell (via oxyfunctionalization).
Deliverable, milestone	
Solved Challenges / Lifted barriers (in bullet points)	<ul style="list-style-type: none"> • Low light -to - product conversion • Diluted cultures and diluted product
What was necessary to solve the challenge? Did it depend on advances in other fields?	
TRL	3-6
Stability	

Scale	
Energetic conversion efficiency	
DOI Reference	

Define time: long-term, 15-20 years	
Deliverable, milestone	Large-scale demonstration plants (ton scale, TRL 7-9) producing renewable fuels and diversity of chemicals Automated DNA synthesis and construction (“cell designer”) Rapid design of enzymes to catalyze novel reactions, with native or characterized enzymes as a starting point
Solved Challenges / Lifted barriers (in bullet points)	•
What was necessary to solve the challenge? Did it depend on advances in other fields?	
TRL	7-9
Stability	Months
Scale	Ton scale
Energetic conversion efficiency	
DOI Reference	

[Link to TRL level](#)

At TRL 5-6:

Production volume	10 t/ year
Light harvesting area needed per t/product	
Political/societal barriers to be overcome	No, except a general GMO issue
Market barriers to be overcome	

At TRL 7-8:

Production volume	100 kton/year
Light harvesting area needed per t/product	
Political/societal barriers to be overcome	
Market barriers to be overcome	

At TRL 9:

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

6. Opportunity criteria

What are the criteria that make this technology an opportunity when ready?

Score the potential opportunity from 0 (very low) to 12 (very high).

Each contributor provides an individual score (we average afterwards).

Opportunity criteria	Individual Score

7. Feasibility criteria

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

Feasibility criteria	Individual Score

8. Key learning points

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

Decision points	
Knowledge gaps	
Risks	

Resources

Suggestion	Please detail
Critical, rare elements	
Non-fluctuating energy sources	
Hydrogen storage	
CO2 storage	
Water purification	
CO2 from the atmosphere	
Concentrated, pure CO2	
Specific, new infrastructures	

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

Breakthroughs in key enabling disciplines

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

Political/societal/market barriers

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

Funding/research frameworks

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

Carbon-based fuel production by biomolecular approaches

Technology	Carbon-based fuel photoproduction by biomolecular technologies																			
Targeted product	H ₂	NH ₃	CH ₃ OH	EtOH	CH ₄	Jet fuel	CO ₂	Other												
			X	X				X (formic acid)												
Nature of active material	Solid-state Inorganic		Molecular			X	Biomolecular	Biological (living cells)												
Sunrise approach	PV-powered electrocatalysis		X	Photoelectrochemical direct conversion			biological and biohybrid direct conversion	Key enabler*, Other												
Device category	Electrolyzer		X	Photo(bio)electrolyzer			Photo(bio)reactor	fermentors, thermocatalytic reactors												
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Large-scale production using existing centralized infrastructure																
Large-scale production necessitating new centralized infrastructure																
Rough timeline (when?)	Short term (2020-25)	Medium term (2025–30)	Long term (2030–50)													
	TRL°4	TRL°5	TRL°8-9													
Who are the main actors? Who has to be involved?	<p>Very interdisciplinary group of scientists/engineers with expertise in natural photosynthesis (biochemistry, biophysics, molecular biology, genomics), photophysics, material science, electrochemistry and chemical catalysis due to the hybrid nature of the working biomolecular assemblies.</p> <p>CeNT, UW, Poland RUB, Germany TH Wildau, Germany Leiden Uni., the Netherlands CEA, Grenoble, France Amsterdam University, the Netherlands Bristol Uni., UK Cambridge Uni., UK DTU, Denmark Harvard Uni., USA ES-y Labs, Germany Freiburg Uni., Germany Arizona State Uni., USA Berkeley, USA Photovoltaic Center for Energy (AIT), Austria NUS, Singapore e-conversion consortium including LMU Munich, Germany</p>															

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

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

Contributors	Joanna Kargul (Warsaw), Yagut Allahverdiyeva-Rinne (Turku), Juliette Jouhet (Grenoble), Gustav Beggren (Uppsala)
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1. Short description of the proposed technological solution

Main technological elements, working principle (max. 5 lines)	Development and nanoscale engineering of biophotoelectrodes with efficient charge transfer, which capture solar light and convert CO ₂
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	and water to carbon-based fuels (e.g., methanol and formic acid). This technology stems from the use of natural light harvesting components are capable of self-assembly and self-renewing through the processes that have been optimized for over 3.5 billion years of evolution for efficient solar energy conversion.
Why is this technology not commercially available right now? What are the major challenges?	Limitations due to stability of the components and back reactions, mainly at the interfaces. No LCA studies, limited (only intermittent) studies on the solar-to-power and solar-to-fuel efficiencies. For scaling up - business/cost analysis essential prior to selection of the target commodity chemical to be biosynthesised. LCA should be made as early on as possible following prototype manufacturing.
What does it take to make it happen? (in short)	Engineering interfaces for efficient electron transfer between electrode and natural photocatalysts as well as synthetic CO ₂ -reducing catalysts. Improving stability of hybrid biomolecular assemblies. Nanostructuring the biocomponents to: (1) increase absorption cross-section (newly discovered photosystem I forms, plasmonics effects, oriented nanostructuring), (2) minimise back reactions and short-circuiting.
What is the benefit for society? (in short)	It is envisaged that biomolecular technologies, when optimised, will provide a viable technological alternative to costly synthetic solar-converting technologies based on the classical photovoltaics. The biocomponents used in these technologies are non-toxic and don't employ any toxic elements. High TRL of the individual biocomponents already in place to conduct efficient light harvesting, charge separation and biocatalysis of complex molecules.

2. Existing R&I projects

Existing national/EU project	Final objective	TRL	Run-time	Funding Instrument
"Solar-driven chemistry" call coordinated by DFG	Fundamental studies into solar energy conversion into chemicals (biohybrid included as long as they work with molecular catalysts).	4	2020-2023	DFG, and national funding agencies in Poland, Finland, Switzerland and France

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

Technological solution to be developed in SUNRISE	Integrated biomolecular systems for photocatalytic CO₂ reduction into chemicals using reducing equivalents from water
TRL	2-3
Cost	n.d.
Energetic conversion yield	< 1%
Stability	<p>Up to 6 hours stable formate production observed in the biomolecular system of photosensitised TiO₂ nanoparticles physisorbed with formate dehydrogenase enzyme.</p> <p>A bias-free biocatalytic tandem PEC cell that converted CO₂ to formate at an average rate of 0.78 μmol h⁻¹ and an FE of 77.3% only using solar energy and water is successfully assembled.</p>
Product separation yield	
Total energy demand [GJ/t]	
Electricity needs [GJ/t]	
Energy demand utilities [GJ/t]	
Steam balance [GJ/t]	
CO ₂ emissions [tCO ₂ eq/t] (cradle-to-gate, including feedstock production)	
Water consumption	
Air separation unit	
Compressors	
DOI References	10.1002/anie.201814419 10.1002/aenm.201900029

10.1002/ente.201600610 and references therein

4. Available techno-economical analysis:

DOI Reference	10.1016/j.joule.2017.09.003 10.1016/j.chempr.2018.08.019
Summary	CO and formic acid yield most revenue per mole of e-. (0.009; 0.015 \$/mol e-, respectively), ethylene also not too bad. Pure CO much more valuable than syngas (semiconductor industry commodity). High purity ethanol and formic acid most valuable products from CO2. Formate concentration yield of 29% must be achieved to make the system cost effective.

5. Deliverables, milestones

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

Define time: short-/medium-/long-term, x years	Short-term: 1 year
Deliverable, milestone	<ul style="list-style-type: none"> • Genome mining for 1st generation novel robust redox enzymes capable of CO₂ reduction at ambient temperature pressure (e.g. formate dehydrogenases and carbon monoxide dehydrogenases), • Selection of biocompatible electrode materials, • Selection of redox-tuned conductive interfaces, • Selection of novel 1st generation robust CO₂-reduction catalysts (CRCs), • Modelling of ET at the interfaces and enzyme catalytic centres.
Solved Challenges / Lifted barrier (in bullet points)	<ul style="list-style-type: none"> • Improved conductive interface between electrode and CO₂-reducing enzymes and synthetic CRCs,

What was necessary to solve the challenge? Did it depend on advances in other fields?	<ul style="list-style-type: none"> • Rational design of polymers for selective CO₂ reduction with CRCs that could also potentially serve as molecular wires to CO₂-reducing enzymes • Identification of ET competing pathways in the integrated CO₂-reduction biomolecular systems • Identification of biocompatible electrode materials • Identification of the 1st generation CRCs, CO₂-reducing enzymes and embedding matrices for increased O₂ tolerance of (bio)catalytic modules, • Thorough investigation of ET processes at the interface between electrode and enzymes or PRCs using STOA spectroelectrochemical approaches and kinetic modelling
TRL	2
Stability	
Energetic conversion efficiency	At least 2%
Scale	
DOI Reference	10.1002/anie.201902218 10.1021/ja508647u

Define time: short-/medium-/long-term, x years	Medium-term: 3-5 years
Deliverable, milestone	<ul style="list-style-type: none"> • Genome mining for 2nd generation novel robust enzymes, • Selection of novel 2nd generation robust CRCs, • Interfacing robust photosynthetic RCs with electrode and novel redox enzymes for CO₂ reduction, • Interfacing robust photosynthetic RCs with electrode and novel CRCs, • Interfacing whole cell biocatalysts with artificial photosensitisers; proof-of-concept devices with solar to energy efficiencies >10% with regards to target products, • Modelling of ET at the biohybrid nanoassemblies,

	<ul style="list-style-type: none"> • Nanostructuring of each module of the biohybrid nanodevices to ensure the optimisation of DET, • LCA modelling of the laboratory prototypes of the biohybrid nanoassemblies. <p>Milestones in 3-5 years:</p> <ul style="list-style-type: none"> • Libraries of 1st and 2nd generation novel O₂-tolerant dehydrogenase enzymes and CRCs, • Kinetic models of ET at the interfaces and dehydrogenase enzyme/CRC catalytic centres identifying ET competing pathways, • Medium-scale demonstrators for biomolecular carbon-based chemical production with LCA assessment, • LCA evaluation of the device performance.
<p>Solved Challenges / Lifted barriers (in bullet points)</p>	<ul style="list-style-type: none"> • Use of (bio)catalytic components with significantly improved stability, activity and O₂-tolerance • Development of redox-compatible molecular interfaces for oriented deposition of catalytic modules • Rational, ET modelling-driven design of the integrated biomolecular systems with amelioration of the competing pathways for significant improvement of solar-to-chemical product conversion efficiencies • Improved light harvesting of the biocatalytic modules (photosynthetic reaction centres)
<p>What was necessary to solve the challenge? Did it depend on advances in other fields?</p>	<ul style="list-style-type: none"> • Identification of novel robusts CO₂-reducing enzymes, CRCs and compatible interfaces for improved DET • Taking advantage of plasmonic interactions to improve photochemical activity of biocatalytic modules • Efficient molecular wiring of the light-harvesting biocatalysts, CRCs and electrode materials for improved DET
<p>TRL</p>	<p>5-7</p>
<p>Stability</p>	<p>Essential to improve it for all the working modules of the</p>

	biomolecular devices
Scale	Medium, ideally all-solid-state configuration
Energetic conversion efficiency	At least 5%
DOI Reference	

Define time: short-/medium-/long-term, x years	<i>Long-term: 10-20 years</i>
Deliverable, milestone	<ul style="list-style-type: none"> • Construction of viable solar-to-fuel/chemicals biohybrid devices of high product selectivity during CO₂ reduction, • Macroscaling of the viable laboratory prototypes based on the results of LCA modelling yielding the TRL8 of the solar C-based chemical production installations based on the best performing biomolecular systems. <p>Milestones in 10-20 years:</p> <ul style="list-style-type: none"> • Libraries of 3rd generation novel O₂-tolerant CO₂-reducing enzymes and CRCs, • Large-scale demonstrators for highly selective biomolecular solar-driven chemical production from CO₂ and water at ambient temperature and pressure, • LCA evaluation of the large-scale device performance.
Solved Challenges / Lifted barriers (in bullet points)	<ul style="list-style-type: none"> • As for medium-term challenges but also with complete LCA studies and full assessment of stability and performance of the integrated systems • Fully integrated solid-state systems operational at a large scale (10 m²) with STChemical efficiencies of a minimum of 15%.
What was necessary to solve the challenge? Did it depend on advances in other fields?	<ul style="list-style-type: none"> • No significant progress in biomolecular technologies can be made without a highly interdisciplinary approach (for rapid development of catalysts of increased stability and activity when interfaced with

	<p>electrode materials, more robust enzymes, compatible electrode materials and interfaces).</p> <ul style="list-style-type: none"> • Development of ultrasensitive STOA spectroelectrochemical and high-resolution microscopic (e.g. TUNA) approaches is vital for investigation of ET at the interfaces between electrode and (bio)catalytic macromolecular assemblies with the resolution of a single supramolecular nanoassembly.
TRL	7-8
Stability	Essential to improve the stability of (bio)catalytic components
Scale	More than 10 m ²
Energetic conversion efficiency	15%
DOI Reference	

[Link to TRL level](#)

At TRL 5-6:

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

At TRL 7-8:

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

At TRL 9:

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

6. Opportunity criteria

What are the criteria that make this technology an opportunity when ready?

Score the potential opportunity from 0 (very low) to 12 (very high).

Each contributor provides an individual score (we average afterwards).

Opportunity criteria	Individual Score
Decentralised production of solar chemicals from atmospheric CO ₂ at ambient temperature and pressure	12
Low-cost of biophotocatalytic and synthetic CRCs with the minimised use of rare or toxic elements	12
Use of light harvesting and redox active biophotocatalysts that are self assembling, self-renewing and optimised for primary solar conversion process (nearly 100% efficiency of primary charge separation)	12
Cost-effective purification of biocatalysts from large-scale cultures of extremophilic microorganisms taking advantage of laboratory evolution (for improved O ₂ -stability, activity, product selectivity and oriented nanostructuring, e.g. by genetic introduction of affinity tags, DNA origami etc.)	12

7. Feasibility criteria

What factors determine the feasibility of the final application?

Score the potential feasibility from 0 (very low) to 12 (very high).

Each contributor provides an individual score (we average afterwards).

Feasibility criteria	Individual Score
Significantly improved efficiency of the complete biomolecular CO ₂ -photoreduction systems compared to the present day technologies by optimising the stability, nanostructuring, light-harvesting and ET properties of the working modules and interfaces	12

8. Key learning points

From the exploration of the selected topic, what are the key learning points?

(Resources, enablers, barriers, decision points, knowledge gaps, risks)

Decision points	Identification of ET competing pathways Synthesis of matrices for embedding (bio)catalytic working modules that improve their O ₂ tolerance, product selectivity and stability Identification of nanostructured biocompatible plasmonic materials to boost the light harvesting and photochemical activity of the catalysts in medium-to-large scale devices
Knowledge gaps	How to rationally optimise product selectivity during CO ₂ photoconversion
Risks	

Resources

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

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

Breakthroughs in key enabling disciplines

Scale-Up	essential
System integration	Development of highly conductive interfaces that can improve DET, product selectivity and O2-tolerance of the catalytic modules.
Novel reactor designs	yes
Novel catalyst materials: earth-abundant, non-toxic, efficient, stable	Yes for CRCs and CO2-reducing enzymes
Novel absorber materials: earth-abundant, non-toxic, efficient, stable	Use of natural light harvesting properties of biophotocatalysts that can be further improved by plasmonic interactions
Standardized life-cycle assessment methodologies	Essential when developing medium-to-large scale devices
Further developments in quantitative sustainability	

analysis	
Strain robustness	
Genomic stability	
Preservation (culture collection)	

Political/societal/market barriers

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

Funding/research frameworks

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