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TECHNOLOGICAL ROADMAP

Sunrise

SOLAR ENERGY FOR A CIRCULAR ECONOMY

SUNRISE

Solar Energy for a Circular Economy

Technological Roadmap

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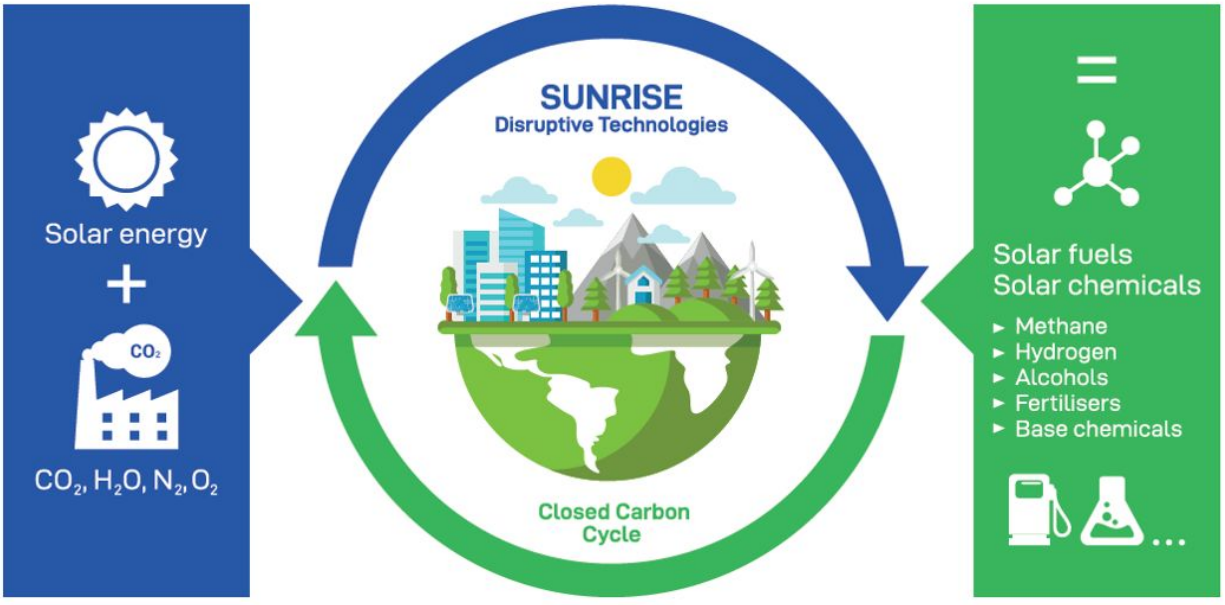
Executive Summary

Modern civilization thrives on a constant flow of energy and material goods obtained from natural resources such as fossil fuels. This leads to the production of large amounts of waste, increasingly difficult to handle. It represents a perfect example of a linear economic approach wrongly assuming that the Earth is an unlimited reservoir of resources and a bottomless dump. The ever growing increase in the consumption of fossil fuels and the ensuing release of carbon dioxide (CO_2) into the atmosphere – altering climate stability with vast environmental, societal and economic consequences – exemplifies this.

The SUNRISE action aims at promoting a large-scale research initiative to enable the transition from a linear to a circular economy: abundant molecules (carbon dioxide, water and nitrogen) are the material basis of a global economic system powered by sunlight. SUNRISE addresses the recycling of CO_2 into a variety of products, the combination of nitrogen with hydrogen to produce ammonia for fertilizers and, more generally, the direct solar-powered production of fuels and chemicals. SUNRISE will provide in a fully sustainable manner energy carriers for the transport and heating sector, the possibility of long-term storage of excess renewable energy in the power sector and fossil-free raw materials for the chemical industry. High efficiency will be necessary to make the transition economically viable and has to come out of an interdisciplinary team of scientists and engineers, handing it over to civil authorities and citizens.



SUNRISE will facilitate the transition to a circular economy and a carbon-neutral society. Abundantly available molecules – carbon dioxide, water and nitrogen (CO_2, H_2O and N_2) – replace fossil-based raw materials for the production of a broad range of chemicals and fuels. SUNRISE targets a sustainable CO_2 cycle, where the concentration in the atmosphere is decreased and then maintained at a level compatible with climate stability, committing to the sustainable use of natural resources and land.

The SUNRISE action will focus on the development of artificial photosynthesis in a broad sense, delivering important solutions for a novel energy system adapted to a circular economy:

- SUNRISE offers new options for **security of access to fuels and chemicals**, since the latter can be produced in Europe with solar energy and abundantly available resources.
- SUNRISE offers the possibility of **storing excess electrical energy at the long-term**, a growing problem with renewable electricity reaching significant shares.
- Some solar fuels, such as methane, can make **use of the existing transport and storage infrastructure** without significant modifications.
- SUNRISE aims at storing solar energy in chemicals with **yields tenfold-to-hundredfold higher than current biomass practice**. This key target allows to reduce the needed amount of land surface compared to biomass (currently the only viable renewable option for long-distance transport).

Efficiency of solar conversion	Surface per capita	Total area needed	
100 %	20 m^2	0.3 %	Thermodynamic limit
30 %	66 m^2	1 %	Artificial Photosynthesis
10 %	200 m^2	3 %	
1 %	2000 m^2	30 %	Biomass

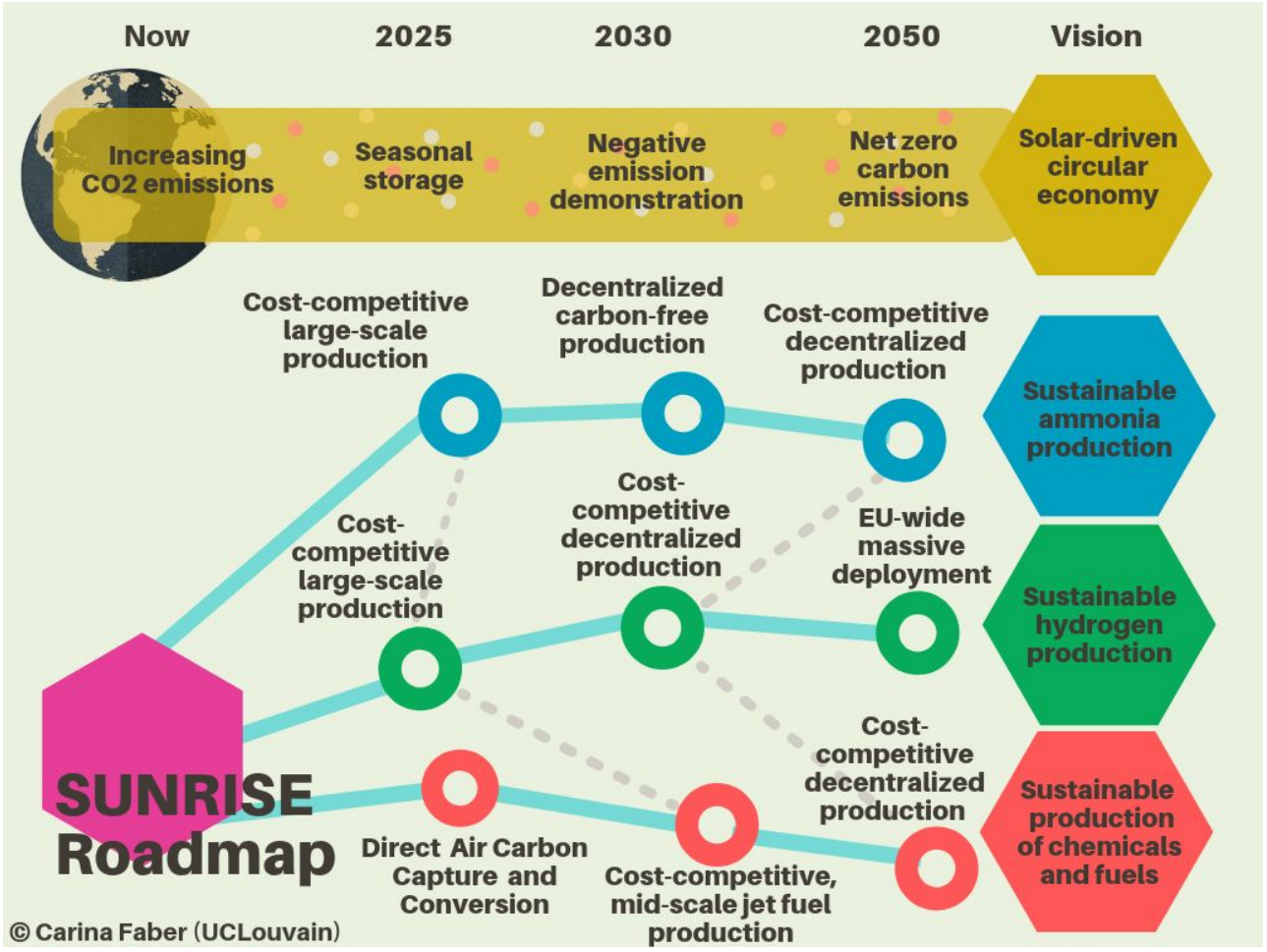
Land area required for solar fuel production at different energy conversion efficiency levels. SUNRISE aims at delivering energy at the TW scale in 2050 with a 30% conversion efficiency, representing a massive leap forward compared to current biomass practice. For 2 TW and 700 million Europeans, it translates into ~66 m^2 per capita of surface required, which corresponds to ~1% of the European surface (on average, 25 MWh per year are then provided for every citizen).

The goal of SUNRISE is to develop competitive and green production pathways. In order to efficiently tackle climate change, one needs to address the manufacturing of commodity compounds consumed or produced by the industry. Those key intermediates are hydrogen, ammonia and carbon-based compounds. To reach this ambitious objective three approaches, with different timelines and use cases, are considered:

The SUNRISE action will capitalize on the current maturity and deployment of **solar electricity and electrochemical processes**, aiming at the development of innovative technological bricks adapted to the current infrastructures and business models by 2025. This will encompass green processes for the production of ammonia and carbon-based compounds. On a longer term, the development of **photo(electro)chemical, biological and biohybrid systems** will provide the direct conversion of solar into chemical energy with milder operating conditions, more straightforward processes and better selectivity towards specific products. The capture of **CO_2 from the atmosphere** will be combined with chemical conversion processes to reach high energy efficiencies. **These direct processes will allow to go from a centralized production of solar fuels and chemicals to a more decentralized approach by 2030, bringing better resilience to regions and favouring the development of a circular economy at a local scale.** Such

technologies will be of primary interest for the development of areas where centralized infrastructures do not exist and will allow specific solutions adapted to local resources and needs. They will provide competitive prices for fuels and compounds, establishing a circular economy and, ultimately, enabling the capture of excess CO_2 in the atmosphere. Concerning fertilizers, not only a low carbon-emission production is targeted, but also a decentralized production on the small-scale, only delivering the needed amounts of ammonia and thus limiting an excessive use.

Beyond 2030, SUNRISE aims at providing a strong scientific and technological basis for negative emissions technologies, which will be then necessary to maintain the temperature increase below 2°C. Eventually, efficient solar energy conversion of carbon dioxide into long duration materials shall contribute to carbon dioxide removal, with the goal to reach a much lower land use than bioenergy-based technologies. The concomitant decoupling of economic growth from the depletion of resources is a much more appealing economical prospect than geological Carbon Capture and Storage [CCS].[1] **Finally, by 2050, SUNRISE will contribute to a CO_2-neutral circular economy, net climate neutral mobility for people and goods, as well as affordable negative emissions technologies developed at a significant scale.**



SUNRISE Roadmap: The vision of SUNRISE is a carbon-neutral society based on a circular economy driven by solar energy by 2050. The sustainable production of hydrogen, ammonia and carbon-based chemicals and fuels is key. Major milestones are e.g. the cost-competitive, mid-scale production of jet fuels in 2030 (700 000 barrels produced per year, i.e. delivering ~150 MW on 1000 ha).

[1] Since technologies for solar fuels and chemicals are an emerging field, detailed analysis comparing them with the more established bioenergy-based technologies and CCS approaches do not exist at present.

Context: what does the world look like today?

A roadmap is not an abstract object standing on its own, its purpose comes with its actual implementation and the solutions it brings to real-world challenges. It is crucial to analyze the specific context in which it will have to persist; what are today's drivers? What are the challenges we are facing? Even though it is a roadmap for research and innovation and not a business model, it is strongly dependent on non-technological enablers such as financing mechanisms, political support and social commitment. Some of the following trends will accelerate the development of the proposed solar-driven SUNRISE technologies, others will hamper them. The latter have to be anticipated and, if possible, circumvented.

Global challenges and drivers

Ecological drivers

Today's energy production system strongly depends on fossil-based energy sources and raw materials. Their intensive use over the last decades not only depleted the Earth's reservoirs, but also caused a significant increase of the carbon dioxide concentration (and other greenhouse gases) in the atmosphere. Among many worrisome consequences, a rise in the average global temperature is shattering.[2] Latest reports point out the tremendous consequences of the ongoing warming on ecosystems, resources and accordingly society in general.[3]

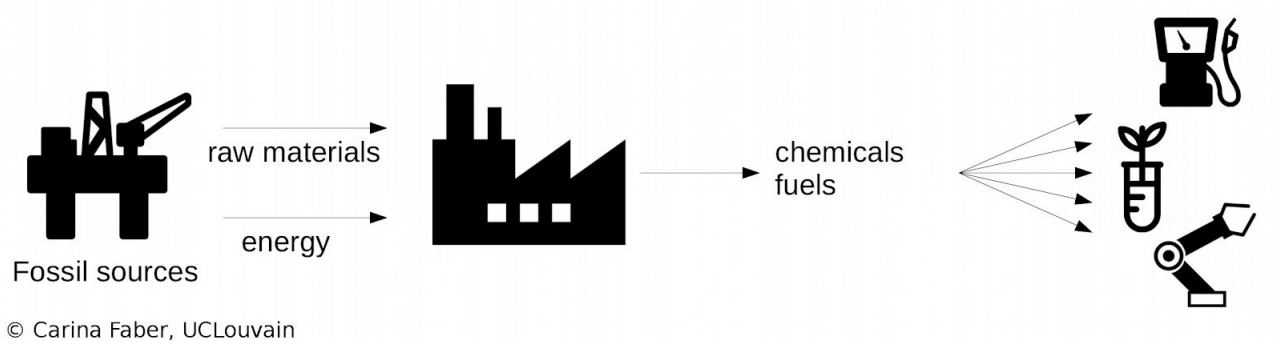
In the EU, the energy and transport sectors generate the major part of greenhouse gas (GHG) emissions, with 54% for energy-related and 24% for transport-related activities in 2016.[4] However, these sectors are central for economic growth, industrial competitiveness and quality of life. A decarbonization[5] of these sectors is urgently needed, decoupling economic benefits from the pollution of the environment. Concerning electricity production, much progress has been made in the last decade: wind and photovoltaic capacity worldwide is now an established alternative to fossil energy carriers thanks to technological developments and significant cost reductions. The electrification of society continues to grow, with the need for efficient storage solutions on the short-to-long term. For the transport and heating sectors, fossil fuels are still an unmatched energy source with a huge existing infrastructure. Chemical industry, one of the largest industrial GHG emitters in Europe, is also completely dependent on fossil-based raw materials and energy carriers.

[2] The current increase in average global temperature is estimated to 1°C as compared to pre-industrial times.

[3] See subsequent chapter on scenarios

[4] https://ec.europa.eu/eurostat/statistics-explained/pdfscache/1180.pdf

[5] Since SUNRISE proposes to make carbon-based materials, indispensable to the economy, "defossilization" will be used later in the text to better describe the goal of the transition. Defossilization is a word newly associated with the energy transition (less than 50 occurrences in google-scholar, with a first one in 2010).



Further global trends

In addition to ecological drivers, developments in politics, economy, legislation, technology and society at large are influencing the framework in which this roadmap needs to operate. An outline of the most striking ones is listed below, raising no claim to completeness:

Political: Nationalism, populism, lack of international cooperation, but overall positive political atmosphere on climate change mitigation; Sustainable Development Goals[6] adopted by all United Nations Member States in 2015 as international reference. Growing need for energy security and independence from imported energy.
Economical: Positive global economic trends, decreasing unemployment, overall EU economic growth, sinking interest rates, low employment in the oil sector, expanding global markets for sustainable technologies, policy incentives for investing in clean energy, large global business opportunities in clean energy sector, important share of the gross domestic product and jobs of energy and transport sector in Europe, decentralisation of energy production.
Societal: Rallies for climate change mitigation especially from younger generations, rising social awareness, positive Zeitgeist for global warming, democratization of knowledge, increasing standards of living coupled to increasing consumption, central role of social media.
Legislative: Paris agreement, Clean Energy for all Europeans legislative package.
Technological: Rapid developments in ICT and on-going digitalization; critical materials: research on substitution, recycling and materials efficiency; production processes: more efficient and less energy demanding.

Technologies for the transition to a low-emission society are not available for a fully sustainable, massive deployment on a global scale today.

EU climate policy

With the **Paris agreement**, the European member states engaged to mitigate global warming and to play a leading role in the fight against climate change at an international level. The necessary reduction of CO_2 emissions implies profound societal changes and technological breakthroughs. The EU is at the forefront to drive international climate policies forward and an important actor to strengthen concerted actions. The

[6] https://www.undp.org/content/undp/en/home/sustainable-development-goals.html

EU takes responsibility in the global **Mission Innovation** initiative to accelerate clean energy innovation.[7]

At the European level, the **Strategic Energy Technology (SET) Plan** is driving forward research and innovation in low-carbon energy technologies. It aligns R&I efforts between the private sector, the European Commission and the Member States. The **Energy Union** targets a sustainable, low-carbon and climate-friendly economy. It provides the regulatory framework for achieving the EU's 2030 greenhouse gas emission reduction target of 40% as compared to 1990, where cost-efficiency and the modernization of the European economy are important drivers. The **Clean Energy for all Europeans package** and the **Clean Mobility packages** are legislative frameworks that imply major market transformations in the energy and transport sector by 2030. They focus on an increase in renewable energies, efficient storage and low-carbon mobility.

A replacement of fossil-based energy sources and raw materials are crucial for Europe's vision of a zero-emission society and the global competitiveness of its industry.

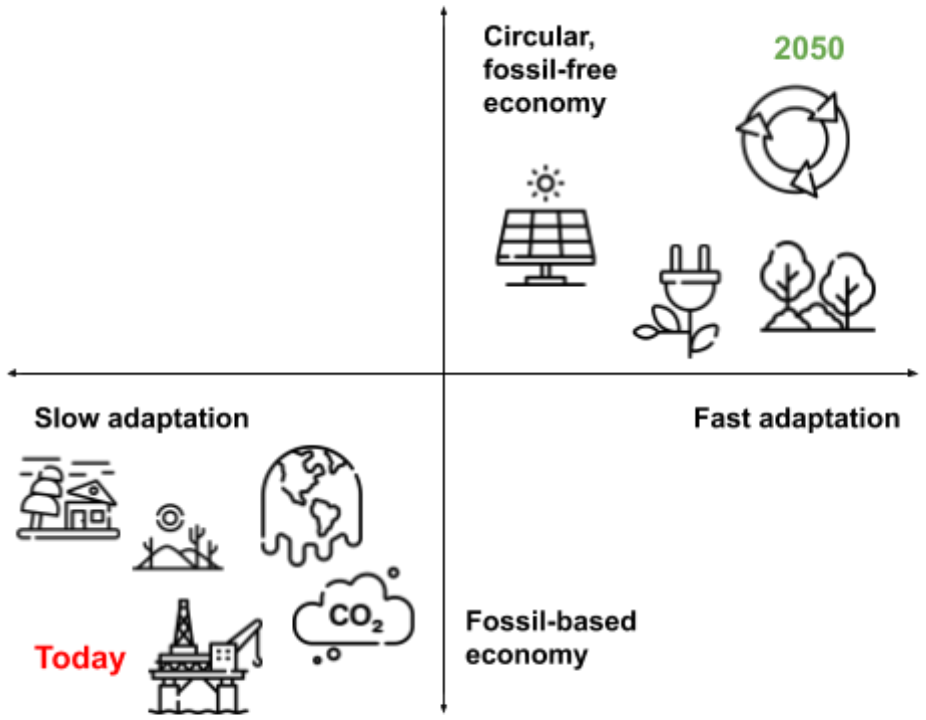
SUNRISE technologies directly address the above-mentioned challenges. They take inspiration from nature, mimicking the natural photosynthesis process. Energy from sunlight and raw materials abundantly available in the atmosphere (water, carbon dioxide, nitrogen) are transformed into green fuels and chemicals.
This allows for a defossilization of the energy and transport sector, as well as the chemical industry (including agrochemistry). SUNRISE technologies provide sustainable fuels with high energy content to the transport and heating sector, using existing infrastructure, while chemical industry profits from fossil-free raw materials and energy. Converting sunlight and electricity into chemical energy represents a safe and easy way of long-term storage for intermittent renewable energy sources. In the longer term, CO_2 is directly taken from the atmosphere and becomes a valuable raw material. When transformed into fuels and burnt afterwards, a net zero-carbon emissions cycle is established, while when transformed into long-lasting chemical products, such as polymers, net CO_2 reductions (negative emissions) are achieved.

Spurred by recent reports of the International Panel on Climate Change,[8] climate change mitigation is now increasingly recognized as one of the most pressing global challenges of our times. It necessitates an immediate coordinated large-scale effort to rapidly develop a broad portfolio of cost-effective and efficient fossil-free alternatives.

The speed for developing, upscaling, implementing and commercializing such innovative solutions strongly depends on the financial and political effort the EU R&I community will receive. It will strongly influence the EU's future economic competitiveness and is central to accelerate the transformation to a low-carbon society.

[7] http://mission-innovation.net/
[8] "Special Report: Global Warming of 1.5 ºC" 2018 and "AR5 Report Climate Change 2014"

Scenarios: what will the world look like in 2050?



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SUNRISE envisions the sustainable production of chemicals and fuels using solar energy and raw materials abundantly available in the atmosphere. Due to the high number of considered products (ranging from hydrogen to jet fuel) and the broad range of proposed technologies with different degrees of maturity, it is beyond the scope of this roadmap to model future scenarios based on current data. Instead, future needs of chemicals and fuels are estimated by analyzing different scenarios[9] described in the current literature. The scenarios described in the "2050 long-term strategy climate-neutral Europe" released by the European commission in 2018[10] play a central role. The aim of the SUNRISE roadmap is to deliver the needed technological milestones to enable the European Commission's vision for 2050. Also highly relevant for this work are recent reports of the International Panel on Climate Change.[11] A short overview of the main scenarios and forecasts as reported in these two key documents and the relevance for the SUNRISE initiative follow.

The 2050 long-term strategy climate-neutral Europe

The aim of this long-term strategy is to confirm Europe's commitment as a leader in global climate action and to present a vision for **achieving net-zero greenhouse gas emissions by 2050**

[9] More than 50 scenarios have been overviewed stemming from 11 roadmaps or strategic documents.
[10] 2050 long-term strategy climate-neutral Europe, European Commission, 2018, and support document: In-depth analysis in support of the commission communication COM(2018)773.
[11] "Special Report: Global Warming of 1.5 ºC" 2018 and "AR5 Report Climate Change 2014"

through a socially fair transition that opens up opportunities for decoupling economic growth from the depletion of natural resources.

The strategy mainly explores eight economy-wide scenarios, divided in three different categories depending on their levels of emission reductions, from 80% to 100%, in comparison to an initial baseline reflecting the 2030 European energy and climate policies and targets. The scenarios cover the potential range of required reductions for the EU to contribute its share to the Paris Agreement's temperature objectives ("*well below 2°C"* and "*1.5°C temperature change")*.

The analysed scenarios foresee the **deployment of carbon taxes**[12] and high shares of renewables in the power mix. In all these scenarios **renewables become increasingly competitive, reaching around 80% of the power mix by 2050**. Renewables deployment (wind and solar representing around 70%) is facilitated by **storage** through hydro-pumping, stationary and mobile batteries and, indirectly, in hydrogen and e-fuels as well as via demand side response. The analysis is complemented by modelling and by developing these multiple and differentiated scenarios (see table below). Especially for industry, a different model was used focusing on extremely innovative technology pathways. **In all scenarios the final energy consumption decreases, by minimum 26% to maximum 50% in 2050 as compared to 2005 values.**[13]

Economy-wide scenarios 2050

***** https://ec.europa.eu/energy/sites/ener/files/documents/ref2016_report_final-web.pdf

** In comparison to 1990 values

Economy-wide Scenarios Long-term strategy climate-neutral Europe (PRIMES-GAINS-GLOBIOM model)	
Non-changing scenario "Baseline" Based on the Reference scenario 2016 (REF 2016) *	**"Baseline scenario":** developed to reflect the current EU decarbonisation trajectory based largely on agreed EU policies or policies that have been proposed by the Commission, but are still under discussion. It keeps the macroeconomic projections, fossil fuels price developments and pre-2015 Member States policies as implemented in REF2016. It assumes the achievement of the following energy and climate targets by 2030: (a) at least 40% cut in GHG emissions (from 1990 levels), (b) at least 27% share for renewable energy, and (c) at least 27% improvement in energy efficiency.

[12] The assumed carbon price increases significantly under all scenarios, reaching 28 EUR/tCO_2 in 2030 and then increasing to 250 EUR/tCO_2 in 2050 under the 80% reduction scenarios and 350 EUR/tCO_2 under the scenarios that achieve net zero GHG emissions by 2050. Real carbon prices will depend on the deployment of other policies and how they impact technology costs and development.

[13] Final energy consumption is foreseen to be reduced already in the Baseline scenario following the European 2030 target on energy efficiency (32.5% reduction compared to 2007). In the decarbonizing scenarios, the least reductions are achieved in those including alternative zero-carbon /carbon neutral energy carriers (ELEC, H2 and P2X). Globally, baseline trends show rises in final energy consumption, although scenarios including deployment of low-carbon technologies, based on renewable energy and energy efficiency, are also compatible with final energy demand reductions by 2050. See REmap Case in "International Renewable Energy Agency, IRENA (2019), Global energy transformation: A roadmap to 2050, International Renewable Energy Agency" or Beyond 2°C Scenario (B2DS) in "International Energy Agency, IEA (2017), Energy Technology Perspectives, Catalysing Energy Technology Transformations".

1st category decarbonization scenarios: - well below 2°C ambition - 80% reduction in GHG emissions by 2050**	**"Electrification - ELEC":** electrification of the energy demand is the driver and thus higher electricity supply and high deployment of storage (6 times today's levels) will be needed to deal with variability in the electricity system.[14]
	"Hydrogen - H_2": key action is the deployment of e-hydrogen in the energy demand sectors and thus hydrogen production on the supply side, it assumes timely deployment of the necessary hydrogen infrastructure and distribution.
	"Power to X - P2X": key action is the deployment of e-fuels (e-gas and e-liquids) in the energy demand sectors and thus e-fuels production on the supply side. Hydrogen becomes mainly an intermediate feedstock and e-fuels use in transport reduces the biofuel requirements for this sector, towards 2050, hydrogen is produced by electrolysis, e-gas in methanation plants and e-liquids via various chemical routes (i.e. methanol route and Fischer-Tropsch process).
	"Energy efficiency - EE": key action is deployment of strong energy efficiency measures in buildings, industry and transport. Energy consumption is thus reduced in all final consumption sectors and particularly in buildings.
	"Circular Economy - CIRC": key action is the development of a circular economy model in the industry and transport, assuming standardization of recyclable material and improved systems for waste collection. GHG emissions reduction are driven by resource and material efficiency.
2nd category decarbonization scenarios: - 90% reduction GHG emissions	**"Combination - COMBO":** it combines the actions and technologies of the previous scenarios (except the one of circular economy, for technical reasons). In this scenario, all before-mentioned pathways are assumed to be available and GHG reductions can be achieved through all of them, including LULUCF (Land Use, Land-Use Change and Forestry).
3rd category decarbonization scenarios: - 1.5 °C ambition - Net zero GHG emissions	**"1.5ºC Technical - 1.5TECH":** aims to further increase the contribution of all the technology options, and relies more heavily on the deployment of biomass associated with significant amounts of carbon capture and storage (BECCS).
	"1.5ºC Sustainable Lifestyles - 1.5LIFE": relies less on technology options, but assumes a drive by EU business and consumption patterns towards a more circular economy, translated in lifestyle changes and consumer choices more beneficial for the climate.

[14] Electricity becomes the dominant energy carrier and its share grows strongly in all scenarios, from 22% in 2015 to 29% in 2030 and then in 2050 ranging from 41% (P2X) to 53% (ELEC) with the scenarios achieving highest GHG reductions situated within this range.

The IPCC Special Report Global Warming of 1.5ºC

This report discusses the impacts of global warming of 1.5 ºC above pre-industrial levels and related GHG emission pathways. In pathways for limiting global warming to 1.5ºC, CO_2 emissions are reduced globally to net zero around 2050. All pathways examined use Carbon Dioxide Removal (CDR), but in different amounts. Four illustrative global model pathways are presented:

- **Pathway 1**: scenario with lower energy demand up to 2050, while living standards rise in the global South; rapid decarbonization of the energy supply is enabled. The only CDR option considered is afforestation.
- **Pathway 2**: scenario with a broad focus on sustainability, including healthy consumption patterns (including healthy diets with low animal-calorie shares and low food waste), low-carbon technology innovation and well-managed land systems.
- **Pathway 3**: a middle point scenario following historical patterns. Emission reductions achieved mainly by energy production changes, followed by reductions in demand to a lesser degree.
- **Pathway 4**: a high resource- and energy-intense scenario where emission reductions are achieved by strong use of CDR, especially through the deployment of BECCS (BioEnergy with Carbon Capture and Storage).

CHANGES IN 2050 (% rel to 2010)	Pathway 1	Pathway 2	Pathway 3	Pathway 4
CO_2 EMISSION	-93	-95	-91	-97
ENERGY DEMAND	-32	2	21	44
RENEWABLE SHARE	77	81	63	70
PRIMARY ENERGY: FROM COAL	-97	-77	-73	-97
PRIMARY ENERGY: FROM OIL	-87	-50	-81	-32
PRIMARY ENERGY: FROM GAS	-74	-53	21	-48
PRIMARY ENERGY: FROM NUCLEAR	150	98	501	468
PRIMARY ENERGY: FROM BIOMASS	-16	49	121	418
PRIMARY ENERGY: FROM NON-BIOMASS RENEWABLES	833	1327	878	1137

Global indicators in 2050 for four illustrative model pathways.

Implications of the analyzed scenarios on SUNRISE

The two mentioned reports show that the energy system transition is underway, analyzing and projecting different political, social, economic and technological developments that have seen immense improvement in recent years. However, the highest ambition level can only be achieved if all mitigation options are exploited: electrification, hydrogen, bio-based feedstocks and

substitution. In several cases, carbon dioxide capture, utilization and storage (CCUS) would lead to the deep emissions reductions required in energy-intensive industries to limit warming to 1.5°C.

Current barriers to accomplish high decarbonization levels include institutional, economic and technical constraints. The hydrogen-based production of ammonia, methanol and other chemicals is hampered by high costs and infrastructure needs. **Research efforts to overcome these limitations and to develop associated processes for hydrogen production and its use as feedstock are therefore needed.** In the European strategy, the total hydrogen consumption is expected to reach approx. 30 Mtoe (around 350 TWh) for the P2X scenario and 150 Mtoe (around 1700 TWh) for the H2 scenario, as soon as consuming technologies are available (i.e. fuel cell vehicles).

2050 Long-term strategy climate-neutral Europe

Estimated consumption Europe 2050	SCENARIOS								
	Baseline	ELEC	H2	P2X	EE	CIRC	COMBO	1.5 TECH	1.5 LIFE
Mtoe*									
Hydrogen	8	15	150	30	15	15	50	70	80
Natural gas	250	125	120	125	100	100	75	60	50
e-gas**	-	-	-	90	-	-	50	40	40
e-liquids**	-	-	-	55	-	-	20	40	20

*Million tonnes of oil equivalent, approximated rounded values
** e-gas and e-liquids not produced in Baseline, ELEC, H2, EE and COMBO scenarios

Source: PRIMES-GAINS-GLOBIOM model

Consumption estimates of some energy carriers in the 2050 long-term strategy.

The SUNRISE roadmap encloses the deployment of the most advanced technologies for the conversion of renewables to electrolytic hydrogen and e-fuels by upscaling processes, aiming for cost and resources efforts alleviation. In addition, it also introduces the development of emerging research and technological alternatives based on the direct conversion of solar energy through “artificial photosynthetic” approaches. Currently, these innovative options with low technological readiness are not included in the described scenarios; however, their great impact, projected as 2 TW (17,500 TWh/year) for Europe alone, will determine the electricity demand and the decentralization for industry decarbonization.

Finally, some of the scenarios, such as the fourth illustrative pathway in the IPCC report largely rely on the deployment of BECCS, where biomass becomes an important energy carrier. The needed land area for bioenergy is expected to amount to 7.2 million km^2, globally, by 2050.[15] This

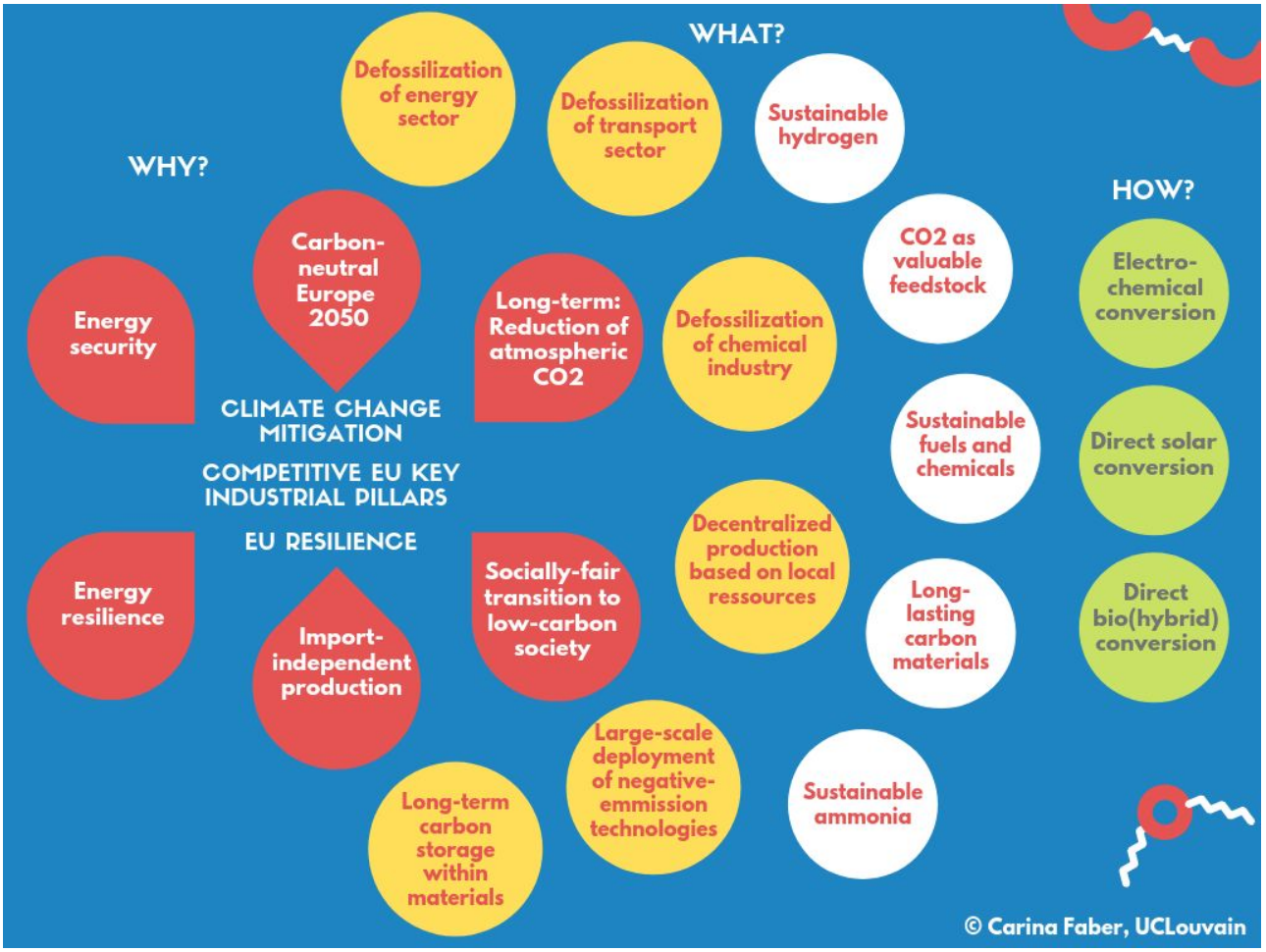
[15] For comparison, EU-28 surface is about 4 million km², geographic Europe (until the Urals) is slightly more than 10 millions km². Pathway 4 is the most extreme case: for pathway 1, land area of bioenergy crops in 2050 is estimated at 0.2, for pathway 2 at 0.9 and for pathway 3 at 2.8 (in million km²).

could have negative consequences on sustainable development, if the use of land competes with production of food or biodiversity conservation.

The development of technologies included in the SUNRISE portfolio alleviate the needs for land use, water and nutrients consumption, since they are based on decoupling of economic growth from depletion of resources, while high solar-to-fuel yields are targeted (see chapter “Needed resources and enablers beyond the scope of SUNRISE” for estimations on green electricity, land and water use).

SUNRISE Vision: how to get the future we want?

Overview



The vision of SUNRISE is to enable a circular economy of renewable fuels and chemicals on a global scale using abundant molecules as feedstocks (e.g. water, carbon dioxide, nitrogen) and, in the long term, sunlight as the sole energy source.

Urgent action is required: the latest IPCC reports underline the need to reduce anthropogenic carbon dioxide emissions to below zero within the next 30-40 years in order to reach the ambitious goals of the 2015 Paris agreement. Technologies enabling such a transition on the global level are still in their infancy. SUNRISE wants to develop artificial photosynthesis technologies in a broad sense, aiming at solar-to-products yields tenfold to hundredfold higher than current biomass practice. Using the smallest possible land area is a key objective in order to propose technologies compatible with other essential goals, in particular a sustainable food production system and the preservation of biodiversity.[16] Providing efficient devices is not enough: these devices have also to

[16] https://www.undp.org/content/undp/en/home/sustainable-development-goals.html

be conceived in accordance with society's needs, as further discussed in the "Social and environmental impact" chapter.

Why we need to act

Overarching drivers of the SUNRISE initiative are climate change mitigation, a competitive European industry and EU resilience in terms of energy and resources. From this, six high-level drivers are deduced:

- a carbon-neutral European society by 2050, in accordance with the EU policy goals,
- a socially fair and economically viable transition to a low-carbon society,
- an import-independent production for EU autonomy and sovereignty,
- energy security,
- energy resilience,
- and ultimately, reductions of the atmospheric carbon dioxide concentration.

What we can do

Six high-level solutions have been identified, promising to significantly contribute to the above-mentioned goals:

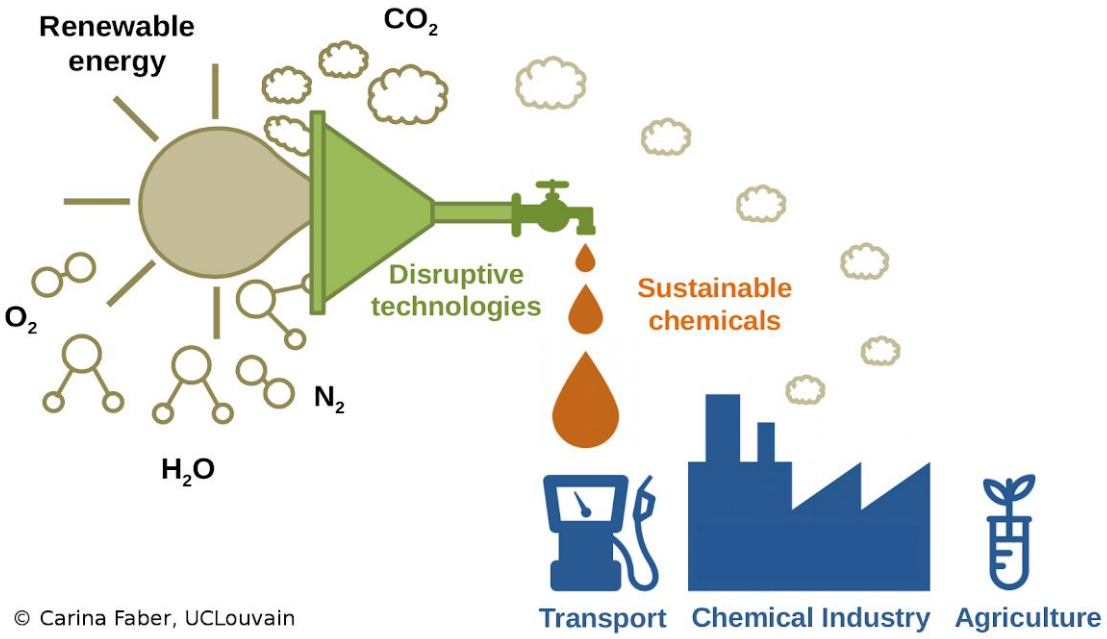
- the development, manufacturing and deployment of technologies for the long-term and large-volume storage of energy
- the manufacturing of primary energy carriers for a defossilization[17] of the energy sector, uncoupling the energy production from natural resource extraction,
- the manufacturing of feedstock for a defossilization of the chemical industry,
- the displacement of fossil fuels by renewables in the transport sector,
- a decentralized production system based on resources available everywhere
- a large-scale deployment of technologies for negative emissions combined with a long-term carbon storage within materials.

Solutions have to align with general goals of sustainability in terms of resources, land use and ecological impact. The SUNRISE vision is based on ubiquitous resources - sunlight and molecules from the atmosphere - thus enabling a purely decentralized and import-independent production system. SUNRISE will create substantial added value for all European countries by providing tailored solutions for each European region to achieve the best utilization of solar irradiance and site-specific resources.

A **sustainable production of hydrogen** with low carbon emissions is central to SUNRISE, since hydrogen is an important vector for the energy and transport sector, and a large-volume resource for chemical industry. **Turning carbon dioxide from a threat for climate stability into a valuable resource** for industry will also contribute to the defossilization of the mentioned sectors and drive the deployment of negative emissions technologies. The **sustainable production of carbon-based commodity chemicals and fuels** will provide the chemical industry with the needed energy and resources and represents a low-carbon alternative to the current use of fossil

[17] Defossilization, preferred to decarbonization, is a more recent expression now utilized by the transportation sector: e.g. the global alliance powerfuels, https://www.powerfuels.org/home, R. Schlögl, Angew. Chem. Int. Ed. 2019, 58, 343 - 348, and FVV fuel study: Options for the defossilization of the transportation sector (100 % scenarios), https://link.springer.com/chapter/10.1007/978-3-658-26528-1_1;

fuels. As carbon source, carbon dioxide from industrial processes or extracted from the atmosphere is used. Transformed into fuels and burnt afterwards, this allows to reach carbon neutrality. Transformed into **long-lasting carbon materials**, a net reduction of the carbon dioxide concentration can be achieved, achieving so-called negative emissions. With ammonia being one of the largest volume chemicals causing significant global carbon dioxide emissions, the SUNRISE vision also includes the **sustainable production of ammonia**, providing agriculture with low-carbon fertilizers.

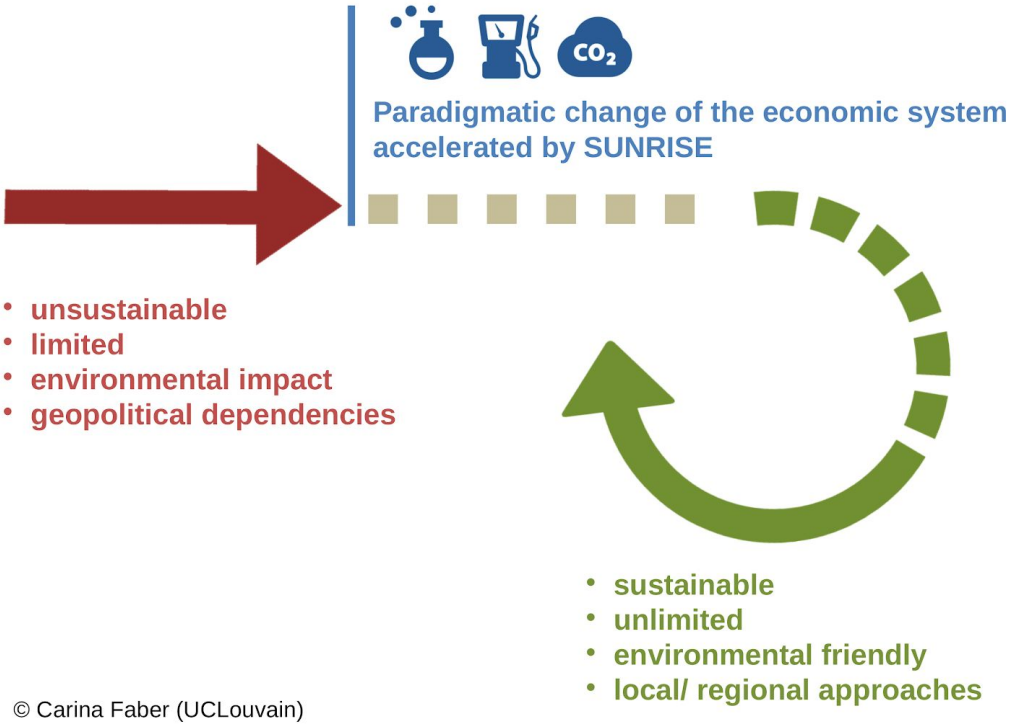


SUNRISE will foster the transition to a circular economy and a carbon-neutral society. Disruptive energy technologies will transform carbon dioxide, water, nitrogen and oxygen feedstocks into fuels, commodity chemicals and agrochemicals with the use of sunlight.

How we can do it

The production of chemicals by sunlight and widely available feedstocks (CO_2, H_2O, N_2 and O_2) is a key milestone towards a **circular economy**. In particular, we target **a sustainable CO_2 cycle**, where the concentration in the atmosphere is decreased and then maintained at a level compatible with climate stability, requiring the **sustainable use of natural resources and land**. The technology development will take into account key constraints such as the energy-return-on-investment (EROI) and the **availability and durability of critical materials**.

The transition from a civilization that is dependent on the consumption of fossil resources to one that is based on solar-powered manufacturing, and which uses ubiquitous and abundant molecules as raw materials in a circular manner, is one of the grandest scientific and technological challenges ever faced by mankind. The unifying goal of SUNRISE is to provide **disruptive technologies** to make sunlight and ubiquitous molecules the principal prime sources of energy and platform materials for modern society, and thus phase out fossil fuels.



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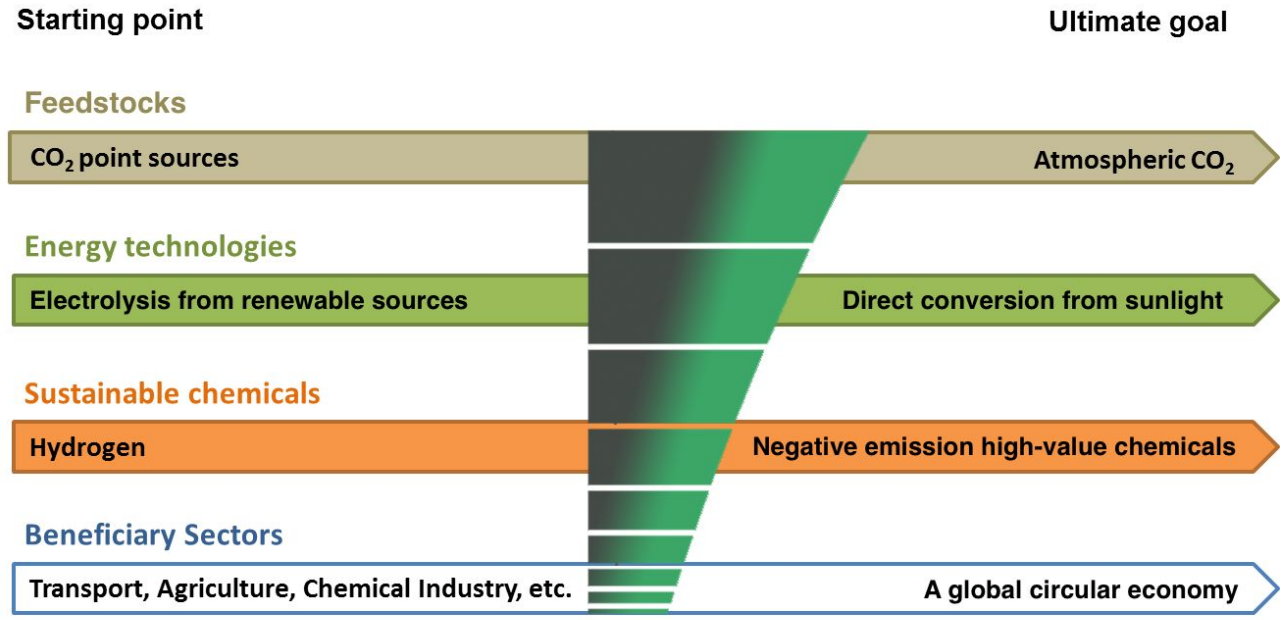
From a linear to a circular economic system.

SUNRISE focuses on three approaches to deliver solutions for the replacement of fossil resources. These work on different timescales and a detailed description of the specific milestones follows in the subsequent chapter “SUNRISE Roadmap”.

IN THE SHORT TERM, SUNRISE primarily aims at **using renewable electricity sources and waste CO_2** from industrial processes as raw material for the circular production of chemicals and fuels. The focus is on efficient and sustainable processes for the conversion and storage of **renewable power into liquid or gaseous fuels**, taking advantage of the continued growth of wind and solar electricity production. The energy return on energy invested (EROI), which is not yet maximized due to use of electricity at the intermediate stage, will be improved step by step.

IN THE MEDIUM TO LONG TERM, the energy input for the chemical processes is **directly provided by sunlight**. It drives novel technological approaches to transform CO_2, H_2O, N_2 and O_2 into fuels and base chemicals. Inspiration is taken from natural photosynthesis. Final target fuels can be concentrated to any desired level, going beyond the natural photosynthesis process with higher efficiency and a wide selection of target products. The CO_2 raw material will have to come ultimately from the atmosphere, deliberately reducing the level of greenhouse gases.



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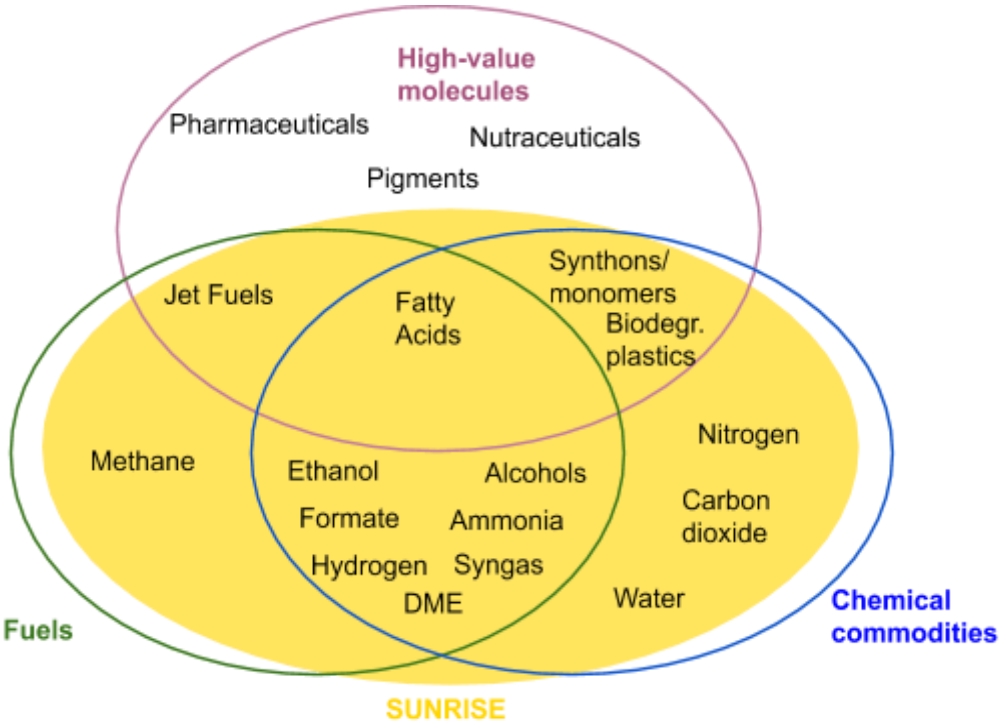
Fuels and chemicals enabling the transition to a sustainable future

Overview

The **sustainable large-scale production of solar fuels and chemicals** is key to enable the SUNRISE vision. It is based on both point and distributed sources of carbon dioxide, the ultimate goal being the extraction of carbon dioxide from the atmosphere and its long-term storage in long-lasting carbon materials.

Given the vast variety of possible solar fuels and chemicals – ranging from small molecules, such as ammonia, to complex synthetic fuels – SUNRISE has to limit its efforts to special classes of products to ensure the efficiency of such a joint large-scale research effort. The universe of identified molecules is sketched below using three intersecting domains: one for fuels and energy carriers in general, one for chemical commodities and one for complex molecules. A few concrete examples have been included in this chart. SUNRISE focuses on fuels and chemical commodities which are needed and produced in large volumes today (millions of tons per year or more on a global scale), and sold at a small price (in the range of 1€ per liter). This market reality is a major challenge, calling for very efficient, simplified and durable processes. Ubiquitous low-energy species are extracted from the environment and upgraded with abundant renewables to energy carriers such as methane or to useful versatile commodities like ammonia, syngas or ethanol. High-value molecules, such as e.g. pharmaceuticals, are low volume markets (thousands of tons or less) and high-value chemicals. They do not constitute such a challenge and thus are not included in the scope of SUNRISE, except for those who also serve as fuel or commodity chemical (jet fuels, fatty acids, biodegradable plastics, etc.).



Key molecules considered in SUNRISE are highlighted in the yellow oval area, comprising fuels and chemical commodities, but not high-value molecules per se.

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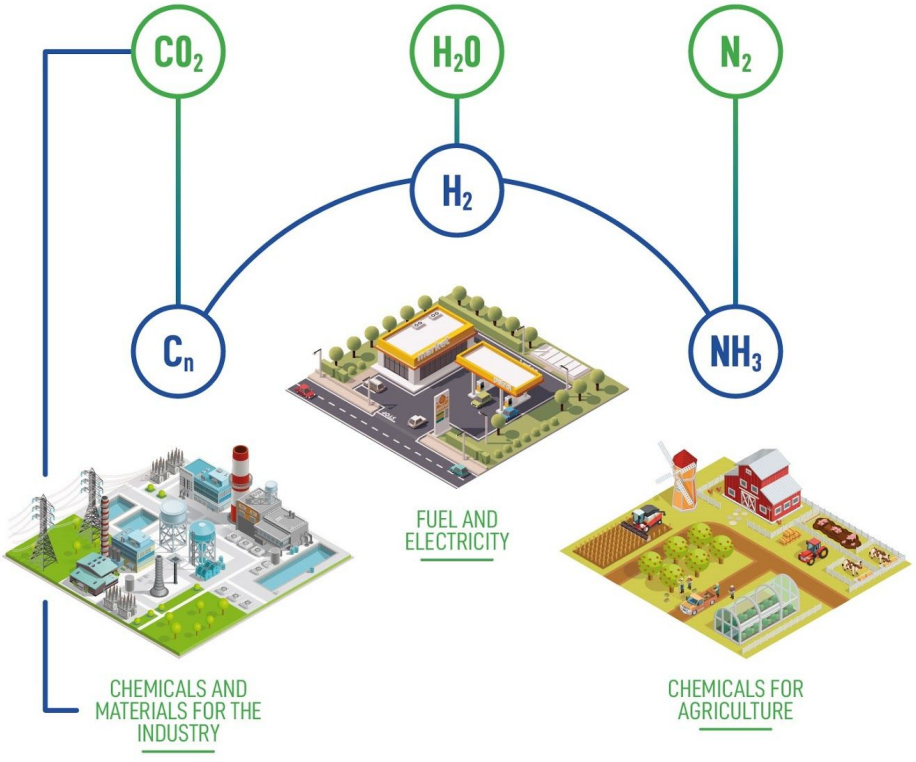
The scheme below illustrates the production and final utilization of the SUNRISE enabling chemicals, made with solar energy. For the sake of simplification, they have been grouped in three categories: hydrogen (H_2), ammonia (NH_3) and carbon-based compounds (C_n).



Hydrogen

Hydrogen is a highly important energy vector in the energy transition and in SUNRISE. Especially with respect to the transport sector, it is already a well-covered topic, with existing European large-scale structures such as the private public partnership *Fuel Cells and Hydrogen Joint Undertaking (FCH JU)* and their recently released *Hydrogen Europe Roadmap*. Therefore, in order to avoid a doubling of effort, many aspects, such as transport, storage, utilization and safety of hydrogen, are not the focus of this roadmap. Instead, we focus on the fully sustainable production from solar energy.

A sustainable, large-scale hydrogen production is central to the SUNRISE vision. As it is illustrated in the above scheme, hydrogen represents an **enabling molecule** in the production of ammonia and carbon-based fuels and chemicals. A fundamental aspect of the SUNRISE roadmap is that not only electricity-based hydrogen technologies with a high technology-readiness-level (TRL) are considered; less mature methods based on the direct conversion of sunlight into hydrogen have a prominent place. **A significant increase of the solar-to-hydrogen yield, high demands on sustainability and circularity in the systems and an economically-viable production of solar hydrogen are key drivers.**

Hydrogen Today

Hydrogen (H), the lightest chemical element, is largely abundant on Earth. Due to its high reactivity, it immediately forms bonds with other elements and thus only exists in a combined form (e.g. water or molecular hydrogen, H_2). Molecular hydrogen is a highly valuable energy carrier and in high demand in the chemical industry and for fuel-cell based transportation. However, it is scarce and its current production from fossil fuels generates large amounts of carbon dioxide emissions.

Hydrogen Impact

Today, 70 megatons of hydrogen are produced globally per year, of which 76% is from natural gas and 22% from coal, meaning that the production of hydrogen is responsible for carbon dioxide emissions of around 830 million tonnes per year. Merely 2% of the hydrogen is produced by electrolysis of water.[18] Major uses of molecular hydrogen include ammonia production via the Haber-Bosch process and fuel refining. Moreover, hydrogen is the most appealing and sustainable carbon-free solution for heavy-duty vehicles as well as personal long-range vehicles. Thus, a sustainable hydrogen production with low carbon emissions is crucial.

Beyond electricity-based routes, SUNRISE targets a large-scale production of molecular hydrogen by light-driven water splitting. Solar hydrogen can be used directly as fuel, as an energy carrier (electricity production via fuel cells) or as an intermediary step towards other molecules. Solar-to-hydrogen technologies at high efficiency will change the global energy balance. They will provide short-term as well as seasonal energy storage and thus allow for a large-scale implementation of technologies based on fluctuating renewable energy sources. Moreover, a renewable hydrogen economy can operate in both large-scale centralized facilities, as well as in small-scale distributed installations. The latter will allow on-site production and deployment without the need for a complex distribution infrastructure, with enormous economic benefits.

[18] IEA (2019), "The Future of Hydrogen", IEA, Paris, www.iea.org/publications/reports/thefutureofhydrogen/

Carbon dioxide as a valuable feedstock

Today, fossil hydrocarbons are the workhorse of our comfort, providing more than 80% of our energy supply and the major part of carbon-based chemicals and materials. Their combustion or oxidation releases almost 33 GTons of CO_2 every year in the atmosphere. This linear model being on the road to ruin, the overarching goal of SUNRISE is to establish a circular economy, focussing mainly on a closed carbon cycle.[19] In principle, such an economy is reachable and technologies to capture and convert CO_2 have been developed during the last decades. Under the name CCU (Carbon Capture and Utilization), technologies are comprised where carbon dioxide is reduced (in chemical language), turning CO_2 from a threat into a useful resource. A lot of attention is now focused worldwide on their further development, in Europe e.g. with CO2valueEurope[20], as well as in the USA[21] or Asia, gathered at the global level in the Mission Innovation Challenge 3.[22] While the technology exists or can be evaluated, the CAPEX is a major hurdle to overcome.

CO_2 utilization can first of all expand the present day industrial usage: besides direct utilization of CO_2 in food industry and agriculture, established processes include the production of urea (~110 Mt CO_2 per year), methanol (~2 Mt CO_2 per year), salicylic acid (~30 kt CO_2 per year) and cyclic carbonate (~40 kt CO_2 per year). But CO_2 uses must be taken further: in principle, every carbon-containing compound can be obtained from CO_2 from the atmosphere, ideally leading to carbon-neutral life cycles. A major obstacle towards this circular carbon economy is the high energy consumption of the processes involved: hence the insistence of SUNRISE on energy efficiency. This bottleneck has been clearly identified, for example in the ICEF roadmap,[23] which strongly recommends funding of catalysis research. Electrical, photolytic, biological and thermal catalysis are emphasized as key enablers of the CCU development,[24] both to decrease the energy needs and to allow economically viable conversion processes.

Large industrial emitters, including electricity and heat producers, are responsible for up to 20 Gton CO_2/year on the global scale. Currently, technologies for capture and utilization of CO_2 from their stationary point sources are already developed. Depending on the type of CO_2 source, CO_2 concentration can range from almost 100% (ammonia or ethylene oxide producers, hydrogen plants, biogas upgrading) to 70% for natural gas processing and down to 3-5% for gas-fired power

[19] A somewhat circular economy of carbon existed in the past, before the industrial revolution, when biomass was the main energy carrier. This was possible for a much less developed world with a global population about 10 times smaller than today. With a world-wide population soon to reach the 10 billion level, efficient conversion processes are deeply needed. CO_2 capture technologies will directly affect the performance of solar-to-energy conversion processes.
[20] Formerly SCOTproject
[21] Global CO_2 Initiative [GCI]
[22] The goal of IC3 is to enable near-zero CO_2 emissions from power plants and carbon intensive industries: http://mission-innovation.net/our-work/innovation-challenges/carbon-capture/ ; see a recent report : https://www.energy.gov/fe/downloads/accelerating-breakthrough-innovation-carbon-capture-utilization-and-storage
[23] ICEF Roadmap, Direct Air Capture of Carbon Dioxide, 2018, available online: https://www.icef-forum.org/pdf2018/roadmap/ICEF2018_DAC_Roadmap_20181210.pdf
[24] Sandalow, D., Aines, R., Friedmann, J., McCormick, C., & McCoy, S. (2017). Carbon Dioxide Utilization (CO2U) ICEF Roadmap 2.0. available online: https://www.icef-forum.org/pdf2018/roadmap/CO2U_Roadmap_ICEF2017.pdf

plants. Both the CO_2 concentration and the impurities present (e.g. NO_x and SO_x) will impact the capture process performance.

A long-term and technologically more challenging goal is to extract CO_2 from the atmosphere. Several teratons of CO_2 are available from the air, however with a low concentration of about 400ppm only. Already several industrial start-ups commercialize Direct Air Capture (DAC) units. These are integrated into projects expected to deliver in 2020-2025, where down-stream chemical processes will convert CO_2 into methanol or jet fuels.

DAC technologies[25] available today were mainly developed in view of the subsequent underground storage of CO_2 usually associated with the acronym CCS (Carbon Capture and Storage). The processes contain a final separation and concentration step, in order to deliver a concentrated gaseous stream of CO_2. However, with a growing interest for CCU instead of CCS, it seems smart to avoid this energy-intensive and costly step of CO_2 separation and concentration. Several recent research results show the possibility to produce syngas or methanol by implementing the chemical conversion process in the very medium of capture.[26,27] **Combining the capture and conversion of CO_2 in solar energy-efficient devices is one of the primary objectives of SUNRISE. Again, the goal is to demonstrate DACC (for Direct Air Capture & Conversion) overall conversion performances 10 to 100 times more efficient than today's biomass practices.**

Ammonia

Ammonia Today

Nowadays, global food production crucially depends on the use of fertilizers. Ammonia, NH_3, is by far the most used one, almost 90% of ammonia synthesized is applied in farmland; the rest serves for the production of chemicals (organic molecules such as amines). Ammonia is produced via the Haber-Bosch process using atmospheric nitrogen and hydrogen stemming from fossil fuel resources. **Although the Haber-Bosch process is highly optimized in terms of energy, it causes significant CO_2 emissions**. The annual global production of ammonia amounts to more than 150 Mtons, where 1 ton of produced ammonia generates 1.5 tons of carbon dioxide emissions.
In addition, the application of fertilizers is currently not very efficient: less than 40% of the nitrogen supplied as fertilizer is actually taken up by the cultivated crop. **Thus, the environment is heavily polluted with nitrogen compounds[28]**, resulting in extensive perturbations in the biogeochemical nitrogen balance, and consequently severe negative impacts on the environment and biodiversity.

Ammonia Impact

Reduced CO_2 emissions. The industrial ammonia production, mainly via the Haber-Bosch process, consumes 3-5% of the world's natural gas supply, contributing to around 1-2% of the

[25] ICEF Roadmap, Direct Air Capture of Carbon Dioxide, 2018, available online: https://www.icef-forum.org/pdf2018/roadmap/ICEF2018_DAC_Roadmap_20181210.pdf
[26] Li, Yuguang C., et al. "CO2 Electroreduction from Carbonate Electrolyte" *ACS Energy Letters* 4.6 (2019): 1427-1431.
[27] Kar, Sayan, Alain Goeppert, and GK Surya Prakash. "Combined CO2 capture and hydrogenation to methanol: Amine immobilization enables easy recycling of active elements." *ChemSusChem* (2019).
[28] Stevens, C. J., "Nitrogen in the environment", *Science*, **363**, DOI: 10.1126/science.aav8215

global CO_2 released into the atmosphere.[29] The proposed SUNRISE technologies providing ammonia from sunlight, air and water will save a substantial amount of fossil energy and will induce negligibly small carbon dioxide emissions. Moreover, they allow a switch from today's centralized large-scale production to a distributed on-site and on-demand ammonia production; this will also result in related savings for transport and storage. Beside its major use as a fertilizer, ammonia can play a role for storing hydrogen safely, or directly as a carbon-free fuel.

Precision farming. Approximately 90% of synthetic ammonia is used in agriculture as fertilizer, e.g. in the form of salts (such as ammonium nitrate, NH_4NO_3, or ammonium chloride, NH_4Cl). Precision farming provides a route to reduce ammonia pollution of soils and water. Nutrient management can be conducted by precise analysis of the actual resource needs of the agricultural land, by using ICT-based utilities. This allows for a targeted fertilization, limiting the amount of unused nitrogen fertilizer and leading to ecological recovery. SUNRISE technologies provide a way to a decentralized, on-site production of the needed amounts of fertilizers. Moreover, biological approaches represent a direct route to produce ammonium solutions, NH_4^+, valuable fertilizers without further transformation.

Commodity chemicals and (jet) fuels

Commodity chemicals and (jet) fuels Today

The production of fuels for the transport sector (road, rail, air, sea) consumes by far the largest share of the globally produced crude oil (about 4000 megatons per year). According to the International Energy Agency, a share of 64% of crude oil is refined into transportation fuels. Specifically, 49% of crude oil is consumed by road transport, 8% by aviation and 7% by navigation (marine shipping). This vast consumption of fossil resources directly translates into CO_2 emissions. For example, direct CO_2 emissions (from combustion of carbon-based fuels) of commercial aviation equate to more than 2% of the global anthropogenic CO_2 emissions;[30] the share in the EU amounts to even 3%.[31] This might appear small, but it has to be considered that these numbers relate only to direct CO_2 emissions from combustion, thereby neglecting the effect of non-CO_2 emissions, such as water vapour, soot and nitric oxide (NO), in high altitudes. Albeit with significant uncertainty, the effect of these non-CO_2 emissions is estimated to equal the effect of CO_2 emissions, i.e. doubling the climatic impact of aviation compared to CO_2 emissions alone.[32]

Fossil resources are not only used for energy purposes - they are also used for the production of carbon-based commodity chemicals (petrochemicals), that in turn are used to produce plastics, fertilizers, packaging, clothes and virtually everything that contains organic (*i.e.* carbon-based) compounds. About 3% of all fossil fuels (coal, crude oil and natural gas) and 10% of crude oil alone are refined into raw materials feeding the chemical industry.[33] This substantial consumption of fossil resources is naturally associated with substantial GHG emissions and other environmental

[29] Tsang et al. https://doi.org/10.1016/j.chempr.2017.10.016
[30] Air Transport Action Group (ATAG), Facts & Figures, https://www.atag.org/facts-figures.html
[31] European Commission, Reducing emissions from aviation, https://ec.europa.eu/clima/policies/transport/aviation_en
[32] Lee D. S., Fahey D.,Forster P., Newton P. J., Wit R. C. N., Lim L. L., Owen B., Sausen R. (2009) Aviation and global climate change in the 21st century. Atmos. Environ. 43, 3520–3537.
[33] Friedrich Seitz: Raw Material Change in the Chemical Industry and the Role of Biomass. In: Malte Behrens and Abhaya K. Datye (eds.): Catalysis for the Conversion of Biomass and Its Derivatives, Max Planck Research Library for the History and Development of Knowledge, 2013, ISBN 978-3-945561-19-5.

burdens. According to the BP Energy Outlook 2019,[34] the “non-combusted use” of fossil fuels, *i.e.* as feedstock for the production of petrochemicals, shows highest growth rates of all sources of types of use. This development is particularly driven by a growing demand for chemicals.[35]

Commodity chemicals and (jet) fuels Impact

Growth as a challenge: The World’s population will continue to grow and is expected to reach 9.7 billion by 2050. At the same time, the standard of living in many of today’s developing and emerging countries will rise, resulting in an increasing demand for, *i.e.*, food and feed, energy and mobility (transport in general). The need of the chemical industry for commodity chemicals will also increase to meet the demand for plastics, pharmaceuticals, agrochemicals and many goods of daily life.

The long-term development of fuel demand is difficult to predict. Accelerating the electrification of road transport could lead to a decreasing demand for hydrocarbon fuels, despite an overall growing demand for mobility and transport. However, it is clear that large volumes of hydrocarbon fuels will continue to be needed by other transport modes. Most notably, aviation will remain highly dependent on liquid hydrocarbon fuels for many decades, as technical hurdles for introducing alternative energy carriers and propulsion systems in aviation are very high. Additionally, development cycles in aviation are extremely long. Aircraft manufacturers Boeing[36] and Airbus[37] forecast a global annual growth in air traffic of 4.7% and 4.4%, respectively, for the next 20 years. Even under optimistic assumptions regarding efficiency gains, such growth rates would result in substantially increasing fuel consumption of at least 3% per year. Similar figures can be expected in navigation (marine shipping) and heavy-duty road transport.

A strong growth in demand is expected from the petrochemical sector. According to a recent report by the International Energy Agency, production of petrochemicals (including plastics) are on their way to become the largest driver of global oil consumption.[38] This sector is expected to account for more than a third of the growth in oil demand by 2030, increasing further to almost 50% of global oil consumption by 2050, surpassing heavy-duty road transport, commercial aviation and marine shipping.

In conclusion, it is certain that there will be a large need for carbon-based commodity chemicals (petrochemicals) and transportation fuels in the long-term future, even considering a high degree of electrification of the road transport sector. The development and implementation of truly renewable production pathways towards commodity chemicals and fuels are crucial to achieve a carbon-neutral and sustainable circular economy by 2050 that is consistent with the climate protection targets agreed on by the United Nations in 2015 (the “Paris Agreement”).

[34] BP Energy Outlook: 2019 edition, https://www.bp.com/content/dam/bp/business-sites/en/global/corporate/pdfs/energy-economics/energy-outlook/bp-energy-outlook-2019.pdf

[35] Persian Gulf countries are on the way to modify their refineries to make more chemicals and less fuels. See C&EN here: https://cen.acs.org/business/petrochemicals/future-oil-chemicals-fuels/97/i8

[36] Current Market Outlook 2017-2036, Boeing Commercial Airplanes, 2017.

[37] Airbus Global Market Forecast 2017-2036, Airbus S.A.S., 2017.

[38] The International Energy Agency, The Future of Petrochemicals - Towards more sustainable plastics and fertilisers, 2018.

SUNRISE Roadmap: how to go from the current state to the SUNRISE vision?

This technological roadmap is developed drawing on analysis and expert judgement to define the **activities, priorities and timelines required to reach the SUNRISE vision**. It addresses European policy makers and stakeholders from research and industry. It is conceived as a basis which will be extended later on onto the international level by the collaboration with Mission Innovation.[39]

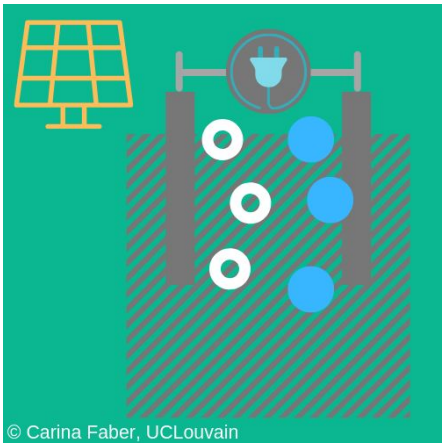
The unifying goal of SUNRISE is to provide key enabling technologies to make sunlight and ubiquitous molecules the prime sources of energy and materials for modern society, and displace fossil fuels by renewables on the terawatt scale. This objective has far-reaching consequences with global significance, such as (i) mitigating global warming, (ii) promoting the transition to a sustainable circular economy, (iii) reducing regional dependencies on energy and feedstock imports, and (iv) accelerating the phasing out of fossil fuels. SUNRISE addresses all these highly relevant issues simultaneously.

The transition from a fossil-fuel-dependent to a solar-powered, circular civilization is one of the grandest challenges of our times. Urgent action is required: the latest IPCC reports underline the need to reduce anthropogenic CO_2 emissions to net zero until 2050 to reach the ambitious goals of the 2015 Paris agreement. Technologies enabling such a transition are still in their infancy. Addressing such an enormous feat requires a multidisciplinary, intersectoral effort on a large scale with massive investment. This roadmap will serve as a guide for joint research efforts, providing a way to efficiently reach the Sunrise goals. It identifies priorities to significantly accelerate the development of solar conversion technologies.

[39] Common workshops and discussions are already scheduled.

Three main technological approaches

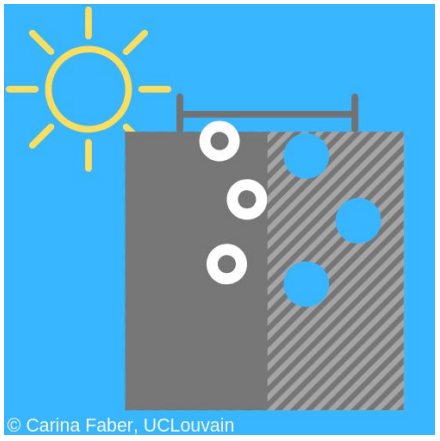
The goal of SUNRISE technologies is to enable a sustainable, low-emission production of chemicals and fuels. The proposed technologies take inspiration from nature, where - via photosynthesis - solar energy, water and carbon dioxide are transformed into chemical energy in the form of carbon-based compounds. In SUNRISE, these so-called artificial photosynthesis technologies comprise the following three approaches:[40]



Electrochemical conversion with solar power

In electrolysis, electricity provides the needed amount of energy to drive a given chemical reaction. The **electrochemical conversion of water** produces oxygen and more importantly molecular hydrogen, a key enabler in the SUNRISE vision. By using renewable electricity sources, hydrogen production becomes a sustainable source of fuel and chemical building blocks. The challenge is to scale up the production to reach the amounts needed to replace fossil-based hydrogen and also to compete with the costs of grey hydrogen (about 1-2€/kg[41] vs. 5-7 €/kg for green hydrogen produced in a centralized infrastructure).[42] It is necessary to find novel materials that can make this technology environmentally sustainable and economically feasible for a large-scale deployment.

The **electrochemical reduction of carbon dioxide** represents a promising route to convert hydrogen and CO_2 into fuels and valuable carbon-based chemicals using electrical energy. Even though the first examples of CO_2 electrolysis date from the 19th century, when carbon dioxide was reduced to carbon monoxide, this technology is still at the small scale today. A similar possibility exists to electrochemically **convert N_2 and H_2O from the atmosphere into ammonia (NH_3)**, by-passing the need for a prior H_2 production for the Haber-Bosch process. This is still in an early stage, with low efficiencies in the few demonstrated examples.[43,44]



Direct conversion via photo(electro)chemical systems

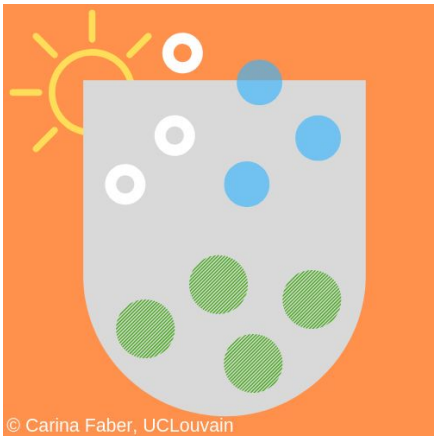
The second SUNRISE approach takes inspiration from nature. Photosynthetic organisms such as plants use the energy of the sun to produce complex chemical compounds out of simple

[40] In accordance with: “Artificial Photosynthesis: Potential and Reality”, European Commission, 2016
[41] IRENA (2019), *Hydrogen: A renewable energy perspective*, International Renewable Energy Agency, Abu Dhabi
[42] These costs only include production. However, transport and compression significantly add up to actual hydrogen production costs, leading to hydrogen prizes at the fuel station of around 10€/kg. See 2018 Progress Report for the DOE Hydrogen and Fuel Cells Program..
[43] J. Nørskov, et al., 2016, DOI: 10.2172/1283146
[44] Non-thermal plasma-assisted synthesis is an alternative for chemical conversions using electrical power. Thermochemical methods applying solar heat are on their way, reducing water and carbon dioxide to provide hydrogen or synthesis gas as building blocks for hydrocarbon fuel production.

building blocks, carbon dioxide and water. Photochemistry is a process in which the solar energy is absorbed and converted directly into fuels or other chemical compounds. Rather than using electricity from solar cells to enable the electrochemical production of hydrogen and carbon compounds, photo(electro)chemical systems combine everything necessary to go directly from sunlight to the final chemical product.

Research on photo(electro)chemical technology is still at the laboratory stage, but it bears important promises. The integration of all components into a single device can lower the total system cost and provide greater flexibility in the design. Compact, integrated devices which are independent of the electrical grid allow for a decentralized production of fuels and chemicals.

The main targets in SUNRISE are to develop novel light-absorbers and photocatalytic materials for integrated photo(electro)chemical systems and to increase solar-to-product efficiency beyond current levels. Photo(electro)chemical devices may operate as a solid state ”monolith” (buried junction cells or photoelectrochemical cells) or as a liquid phase suspensions of photochemical systems (photocatalytic nanoparticles or supramolecular assemblies).[45] Approaches hybridizing solid state and molecular active components (catalyst and light-absorber), including biological molecules extracted from living cells (bio-molecular systems) are also a promising route.



Direct conversion via biological and biohybrid systems

Photosynthetic organisms use sunlight as an energy source and raw materials such as carbon dioxide, water and mineral nutrients for the synthesis of oxygen and organic building blocks, supporting life on the planet. They do not need to be manufactured, but reproduce themselves. With the help of photosynthesis, algae and cyanobacteria can produce diverse products for industry. Dozens of genetically-engineered photosynthetic organisms hosting novel synthetic production pathways and enzymes are currently available for the production of desired chemicals.[46] Such production systems are called living photosynthetic cell factories. However, most of the available systems show low solar-to-chemicals conversion efficiencies and need significant improvements to serve as industrial-scale production platforms.

Biohybrid systems employ photosynthetic and non-photosynthetic living microbes wired to inorganic components (electrodes) to drive biosynthetic pathways. The photosynthetic microorganisms fuel the biosynthetic pathways with the energy captured from sunlight, whereas specific isolated enzymes or engineered non-photosynthetic microorganisms utilize this energy (in the form of water-derived reducing equivalents or electrons) to drive efficient CO_2 reduction into targeted organic molecules.

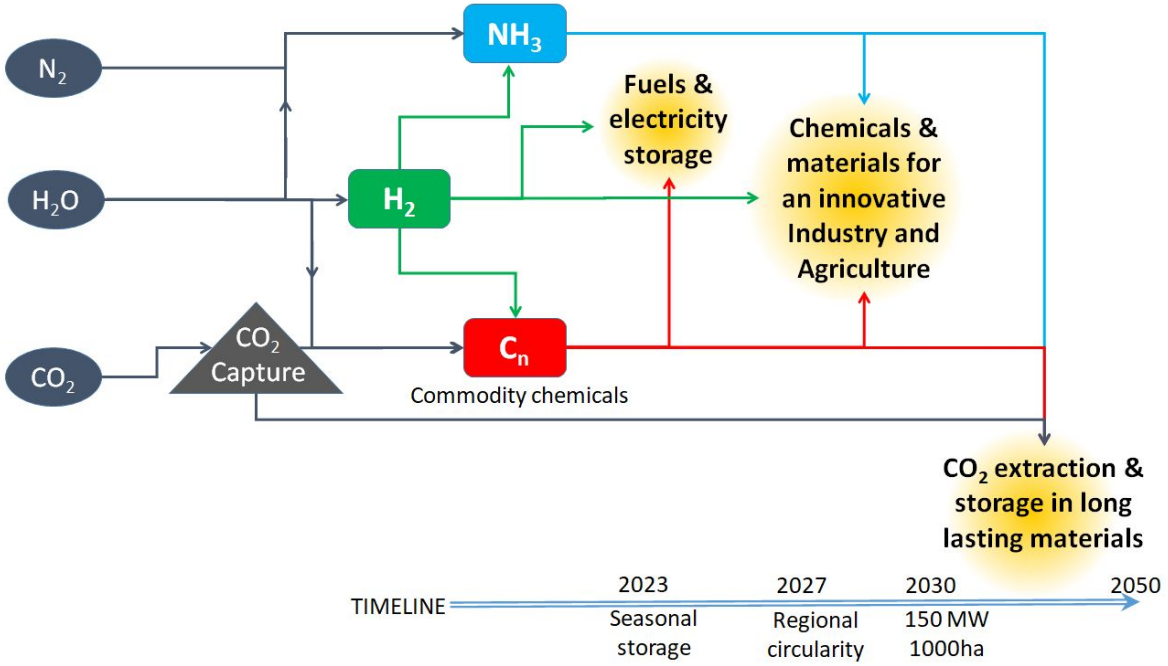
[45] Buried junction cells contain internal junctions between semiconductors, but no direct contact between the semiconductors and the catalyst/electrolyte. In photoelectrochemical cells, the light-harvesting components are directly interfaced with the catalysts/electrolyte, allowing for the catalyst to directly extract charge carriers from the excited state of the light-harvester to achieve multi-electron/multi-proton chemical conversion. The same applies in suspended or soluble photochemical systems.

[46] S. A. Angermayr et al. Trends Biotechnol., 2015, 33, 352–361.

Technological milestones to be achieved

Overview

Carbon, hydrogen, oxygen and nitrogen are the main atomic building blocks of commodity fuels and chemicals. This chapter presents a comprehensive and timely plan to unlock the path towards intermediary and final products, using atmospheric gases only as inputs, with a limited consumption of renewable energy flows. As shown in the figure below, water splitting is central, since molecular hydrogen, H_2, and water oxidation are key in the reduction of carbon dioxide and nitrogen. The timeline of future SUNRISE developments is discussed, with a first simplified time scheme in the figure below.



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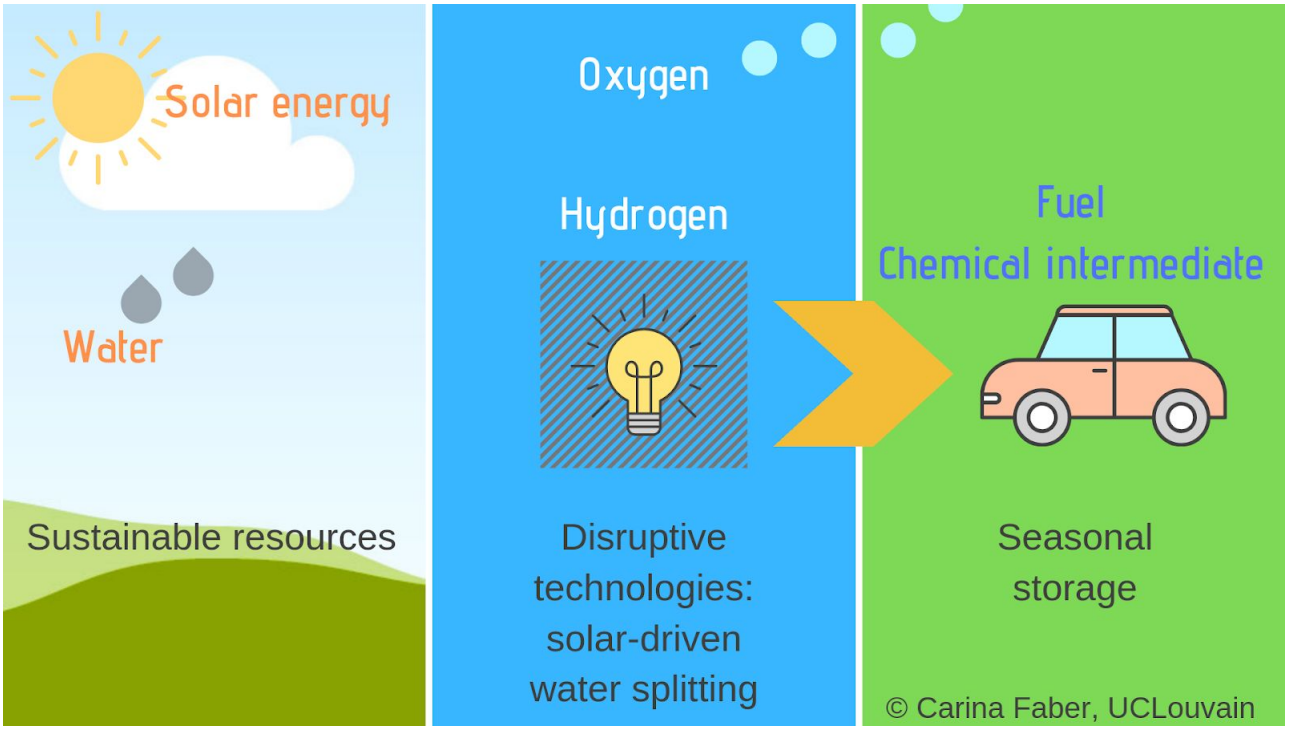
Atmospheric molecules (water, nitrogen, carbon dioxide) are converted using solar energy into hydrogen H_2, ammonia NH_3 and carbon-based chemicals C_n. H_2 is central in many processes. Carbon capture can be realized by physico-chemical devices or by photosynthetic microorganisms. Fuels and chemicals are targeted to be reached in the next decade; future progress in CO_2 and N_2 conversion will open new ways of storing atmospheric CO_2 in long-lasting carbon materials, here envisaged to reach market beyond 2030.

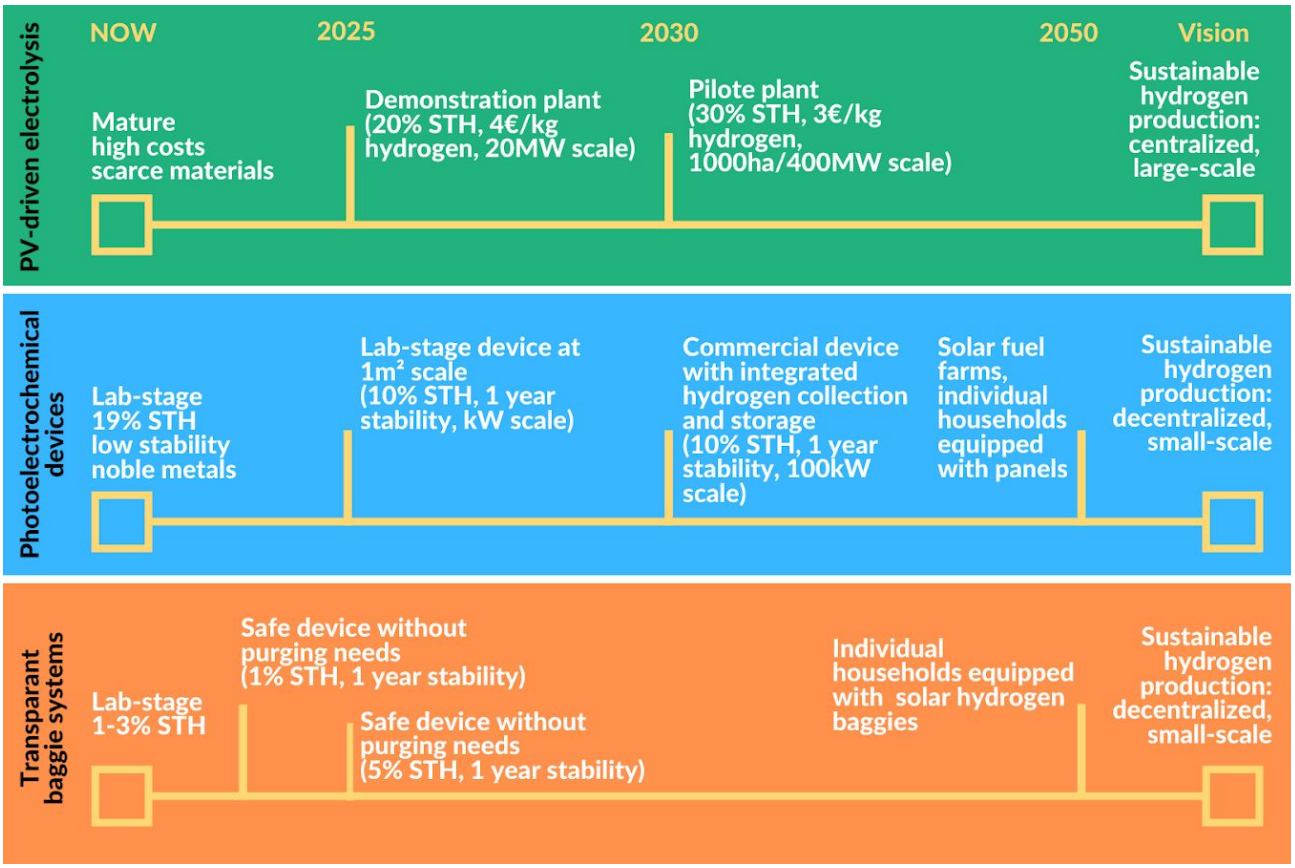
Sustainable hydrogen production

The SUNRISE vision is to produce green hydrogen in a fully sustainable and economically viable way by 2050, exclusively using solar energy and abundantly available materials and resources. Efficient solar-to-H_2 technologies will provide both short-term and seasonal solar energy storage capacity. A solar-to-H_2 transformation at a high efficiency will change the global energy balance and enable green CO_2 conversion. In addition, technological progress and achieved milestones in hydrogen production by SUNRISE technologies will directly translate into advances in solar ammonia and carbon transformation technologies.



Major milestones

Already mature technologies based on electricity-driven water splitting will provide a sustainable centralized production on the large-scale – given that system costs will significantly decrease and that bottlenecks related to upscaling will be solved. As a key milestone, an operational system of 1000 hectares to produce the equivalent to more than 90 tons per hectare per year of molecular hydrogen should be installed by 2050. Direct, light-driven approaches are currently at the lab stage, but once efficiency and stability issues are resolved, direct photo(electro)chemical technologies will provide an individual, decentralized production at the household scale. Safe and fully integrated devices (including hydrogen separation and storage) will allow for the equipment of individual house roofs or solar fuel farms and a completely local and autonomous hydrogen production. Such household equipment should also be deployable by 2050.



Major technological targets

Photovoltaics-driven electrolysis of water

Electrolyzers of different kinds are already available at advanced TRL levels (7-9). However, they show certain shortcomings: alkaline electrolyzers are available at scale, but suffer from intermittent energy supply; proton-exchange membrane (PEM) electrolyzers rely on scarce and precious metals as catalyst, which inhibits upscaling of the technology to the TW range. The most efficient high-temperature solid-oxide electrolyzers (SOE) are currently in the 20 kW range. Lifetime is always an important challenge, especially in a dynamic operation mode with rapid fluctuating power input. Current costs are high, mounting up to 1000€/kW for the electrolyzer device and 6€/kg hydrogen depending on the scale and localization of the plant. The electricity-to-hydrogen (LHV) efficiency is limited to about 60%.

Unique selling point: High technological maturity is one of the main advantages to pursue this approach and the first upscale to the MW range has been achieved. Research and discovery of new catalyst materials, based on earth-abundant elements and employed in electrolyzers, can advance and speed up the development of photoelectrochemical systems (cross-fertilization and knowledge transfer). Moreover, these systems are compact, necessitating no light management and thus enabling the stacking of the different units. They finally allow for an easy collection of already pressurized hydrogen (10-30 bars).

Vision for 2050: Photovoltaics-driven electrolysis allows for a centralized and efficient large-scale production of hydrogen. Compact systems are driven exclusively by renewable energy sources and based on abundantly-available materials and resources. Decentralized deployment of this solution at the household level will not be considered due to cost, operational and safety constraints that should not be leveraged by 2050.[47]

Working principle: The needed energy to split water molecules into molecular hydrogen and oxygen is provided by renewable solar electricity. Hydrogen and oxygen are produced at distinct electrodes coated with catalysts that are crucial to drive these chemical reactions and to avoid energy losses. Both electrodes are separated by a membrane (PEM and high-temperature electrolyzers) or a porous diaphragm (separating the electrode compartments filled with liquid alkaline electrolyte solution of potassium or sodium hydroxide in alkaline electrolysers) allowing gas separation.

Key research drivers: System costs, material scarcity, lifetime/degradation of catalyst material

Key enabling technologies: Advances in this field depend on technological breakthroughs in material science (noble-metal free catalysts and membranes, operating at different pH and impurity content), automated manufacturing technologies, system integration and upscaling.

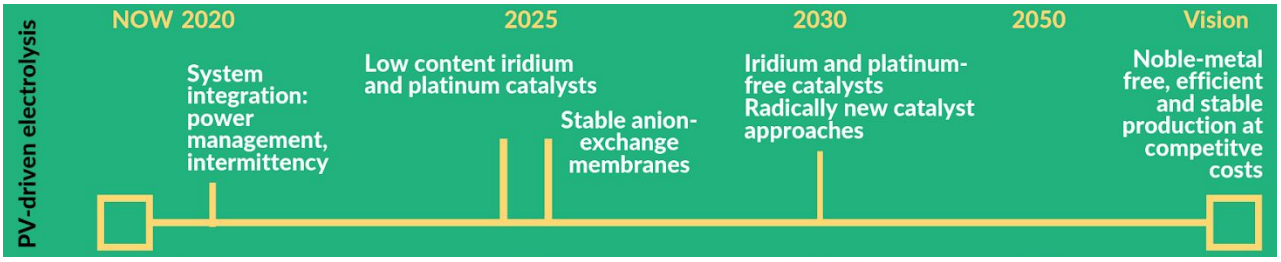
Present TRL: 4-6
TRL target 2030: 9

Major technological targets:

The goal is to provide **cost effective (100 €/kW)** and efficient electrolyzers (electricity to molecules **yield 80-90%**), where a major part can be operated **dynamically** to follow the intermittent supply of renewable energies. The required **scale of 100MW to 1 GW per unit** needs to be shown by first achieving TRL 5 and then building industrial demonstration units that go to TRL 8-9 based on an analysis of the value chain. All electrolyzers must be **user-friendly**, which means service intervals at a maximum of one year.
A challenge that needs to be solved in the polymer membrane technology is to develop **mechanically stable and highly conducting Anion Exchange Membranes** to allow the alkaline electrolyte regime to be utilized. This will also be needed for electrolyzers doing a direct conversion of carbon dioxide to hydrocarbons.
For the more dynamic neutral-acidic operation regime, a sustainable solution for replacing the scarce iridium catalyst (for the oxygen evolution reaction) and the expensive platinum catalyst (for the hydrogen evolution reaction) needs to be developed. The first approach to start demonstration will be a **dilution of the current catalyst**, e.g. on core-shell structures to reduce the catalyst loading from current 2 mg/cm² to 0.1 mg/cm². On the long-term, replacements for these materials need to be established; this will not be alternative metals or alloys, but **radically new approaches for nanostructured catalysts** using earth-abundant elements.
High-temperature solid-oxide electrolysis (SOE) will probably deliver the highest efficiencies (up to

[47] System cost analysis indicates that photovoltaics-driven electrolysis may not be competitive with electrochemical storage on decentralized (household) systems because of the high capital expenditure required for the electrolyzer, hydrogen storage system and fuel-cell.

100%), given centralized settings, where heat is available for the evaporation of the feed water. One main topic is the scaling of the membranes (currently only 100 cm²) by two orders of magnitude and increasing the dynamic operation power range. Novel ceramic technologies, such as fibre reinforcement and new construction principles to increase the stack size are promising here. Moreover, the modularity of SOE systems needs to be pushed following the example of photovoltaics to arrive at the scale needed. For both topics, the CAPEX has to be brought down by **advances in automated production technologies and power electronic environment**. In addition, **materials and interface design** will enhance performance as well as reliability and operation time (by lowering degradation) again leading to significant cost-savings.



For in-depth technical details, please refer to the technical annex (how-documents).

Photoelectrochemical devices

Techno-economic studies indicate that direct solar-to-hydrogen approaches can have both lower system costs and higher energy conversion efficiencies per active area than photovoltaics-driven electrolysis.[48] PEC systems permit a decentralized production, allowing for important savings in transportation costs (transport and compression significantly add up to actual hydrogen production costs, leading to hydrogen prizes at the fuel station of around 10 €/kg).[49] Lab-scale devices with different architectures have reached solar-to-hydrogen conversion efficiencies of up to 20%.[50]

Unique selling point:
Photoelectrochemical systems (PEC) are integrated and allow for large savings in terms of support and container as well as interconnecting electronics. As the surface of catalysis for water splitting is the same as the surface for sunlight collection, photoinduced current densities at the photoanode are up to two orders of magnitude lower than those required of classical electrolysis. This reduces the constraints on the used materials and allows for the use of abundantly available, cheap and non-toxic materials as catalysts. The overpotential losses are reduced by the integration of the PV and electrochemical stages in photocatalytic materials and components for PEC systems. In molecular systems, the very high surface to volume ratio and high extinction coefficient lead to very favourable materials efficiencies.

Vision for 2050: Photoelectrochemical devices will allow for a decentralized, local production of hydrogen, even down to the scale of single households. Systems will be fully autonomous, only depending on abundantly available sunlight. Water consumption is low.

[48] R.D. James *et al.* "Technoeconomic Analysis of Photoelectrochemical (PEC) Hydrogen Production" (2009) DOE Report, Contract Number: GS-10F-009J. Arlington, USA.
[49] 2018 Progress Report for the DOE Hydrogen and Fuel Cells Program, April 2019
[50] W.-H. Cheng et al. *ACS Energy Lett.* 2018, 3, 1795−1800.

Working principle: Photoelectrochemical cells are single devices that directly split water into hydrogen and oxygen, where the needed energy is provided by sunlight. Various architectures are possible but all of them combine light-harvesting materials (inorganic and organic semiconductors, molecular dyes or biological pigments) and catalysts for the hydrogen and the oxygen evolving reactions. Both reactions occur at separate (photo)electrodes or on different sides of a membrane allowing for easy gas separation.

Key research drivers: stability, efficiency, scalability. Total system cost, exclusive use of affordable and earth-abundant materials for light harvesting, charge separation and catalysis, ease of hydrogen collection. When mature, knowledge transfer to systems that produce other molecules than hydrogen.

Key enabling technologies: Advances in this field depend on technological breakthroughs in photon management technologies, nonadiabatic conversion of reactants into products, catalyst and semiconductor materials science and development. This field will largely profit from bio-inspiration (control of auto-assembly and charge photo-accumulation and transfer processes, development of responsive matrices and interfaces, development of self-repair/self-healing processes, discovery of noble-metal free and non-toxic catalysts inspired by enzymes, function-based systems engineering across length scales) resulting in devices with an increased efficiency.

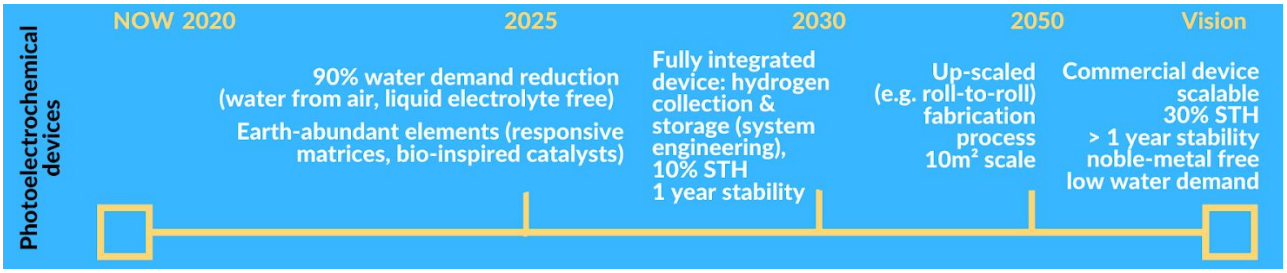
Present TRL: 2-4
TRL target 2030: 5-8

Major technological targets

Starting from the state-of-the-art, the first milestones (2025) will consist in (i) reducing the water demand of the devices by implementing components for water collection from the air and gelified membranes as the sole electrolyte in photo(electro)chemical devices; (ii) improving the stability of the devices (currently 1-30 days) through the development of improved interfaces as well as self-healing/self-repair processes for the active components responsible for light collection and conversion or catalysis; and (iii) achieving breakthroughs in materials research to design active components solely based on earth-abundant elements.

In parallel, efforts in chemical engineering shall allow to design a fully integrated system with 10% solar-to-hydrogen efficiency combining light-collection and hydrogen collection/storage at the m^2 scale and 1 year stability. Upscaling (e.g using roll-to-roll or equivalent processes) should allow the production of such devices at >10m^2 scale by 2050. Further optimization and full exploitation of the bioinspiration potential will allow to ultimately develop commercial devices at 30% solar-to-hydrogen efficiency.

For in-depth technical details, please refer to the technical annex (how-documents).



Transparent baggie systems (microorganisms and photocatalytic systems)

Techno-economical analysis have shown that suspended or surface coated systems in transparent baggies have the potential for competitive cost for hydrogen evolution.[51] Photosynthetic microorganisms (green algae and cyanobacteria) and inorganic photocatalytic systems (nanoparticles) are both able to directly produce molecular hydrogen from water under sunlight irradiation.
Solar-to-hydrogen conversion efficiencies are usually in the range of 1%. In such systems, oxygen, the co-product of the water-splitting reaction, is generally mixed with hydrogen in the output gas.

Unique selling point: Extremely low system cost, fast regeneration and long-term production capacity of living organisms (high stability) are the major advantages of this technology.

Vision for 2050: Transparent baggie systems allow for a decentralized, local production of hydrogen for single households and niche applications. Systems are fully autonomous, only depending on abundantly available sunlight. Preferably waste water is utilized.

Working principle: Very easy and cheap system consisting of transparent plastic bags, permitting solar energy to enter the system and to drive (bio)chemical reactions. Microorganisms (biological and biohybrid approach) or synthetic photocatalytic systems (e.g. nanoparticulate systems or supramolecular assemblies) are floating in water or attached to solid polymers (solid-state cell factory) and surfaces and split water into hydrogen and oxygen.

Key research drivers: Hydrogen separation, safety issues and production efficiency: currently with specific production protocols and with genetically-engineered algae, efficiency can be increased to 4% in lab scale,[52,53] while the theoretical limit of natural photosynthesis is 10-13%;[54] photocatalytic systems are currently limited by recombination processes (in the bulk of the materials and at their interfaces) and by unfavourable optical absorption profiles.

Key enabling technologies: Advances in this field depend on technological breakthroughs in system engineering for the separation, collection and storage of hydrogen, photobioreactor design, photon management, fundamental understanding of natural photosynthesis and cell metabolism, enzyme chemistry and material science and development, advanced theoretical and experimental techniques, synthetic biology toolboxes and other molecular technologies.

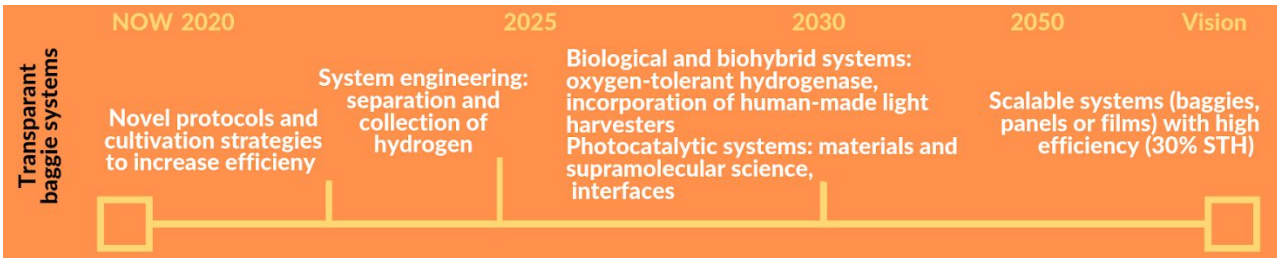
Present TRL: 3-4
TRL target 2030: 6-8

Major technological targets

A major milestone regards the separation of hydrogen from oxygen and overall safety. These issues can be fixed through efforts in chemical engineering by 2023-2024 (with e.g. membrane

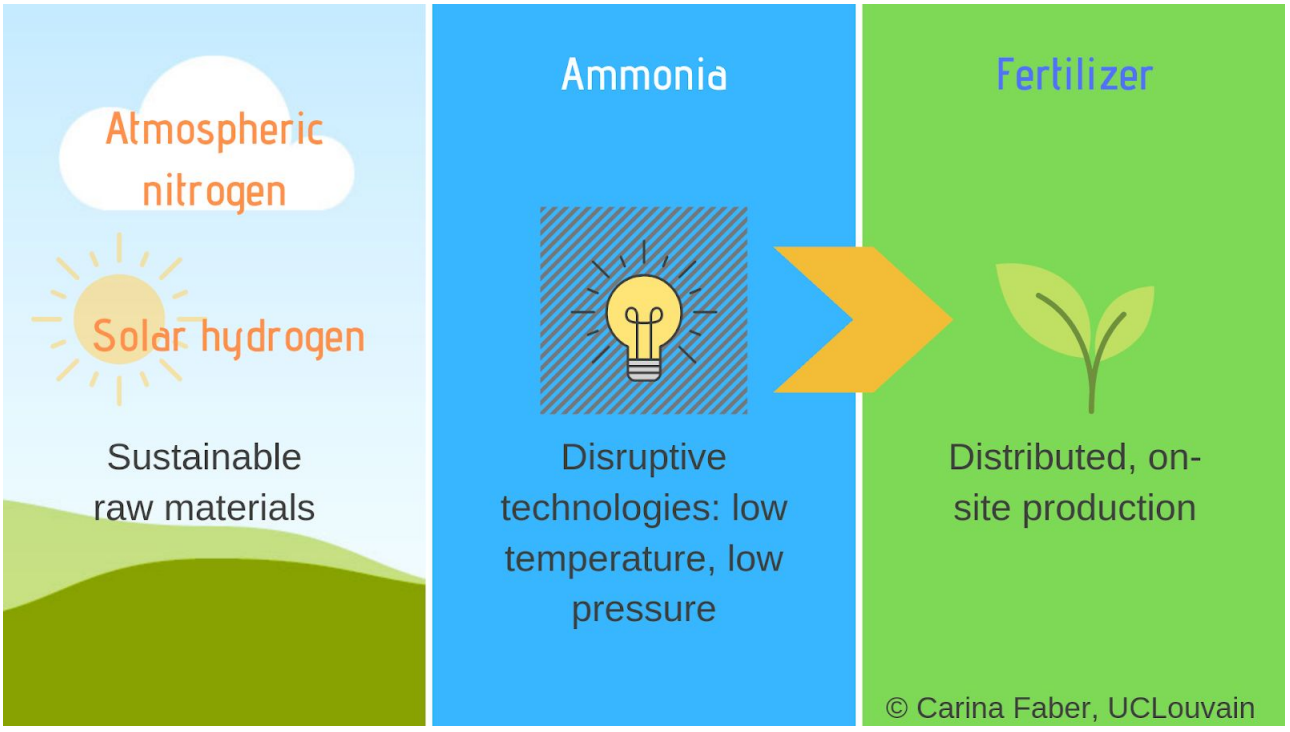
[51] Technoeconomic Analysis of Photoelectrochemical (PEC) Hydrogen Production 2009 DOE report; Domen et al., Nature Materials Vol. 15, 611-615 (2016); Domen et al., Joule Volume 2, Issue 3, 2018, 509-520
[52] Kosourov S. et al., Energy Environ. Sci. 1, 1431-1436 (2018)
[53] Nagy V. & Tóth SZ (2017) Photoautotrophic and sustainable production of hydrogen in algae, European Patent Application 17155168.2
[54] Torzillo, G. et al. (2015), Crit. Rev. Biotechnol. 35, 485-96

technologies). The development of more efficient systems is a second milestone, which will require breakthroughs in: (i) unlocking photosynthetic control to funnel more electrons to hydrogen-producing enzymes; (ii) synthetic biology to incorporate and develop efficient and stable enzymes and photosensitizers in microalgae; (iii) materials sciences to develop highly efficient photocatalytic systems that overcome recombination losses.



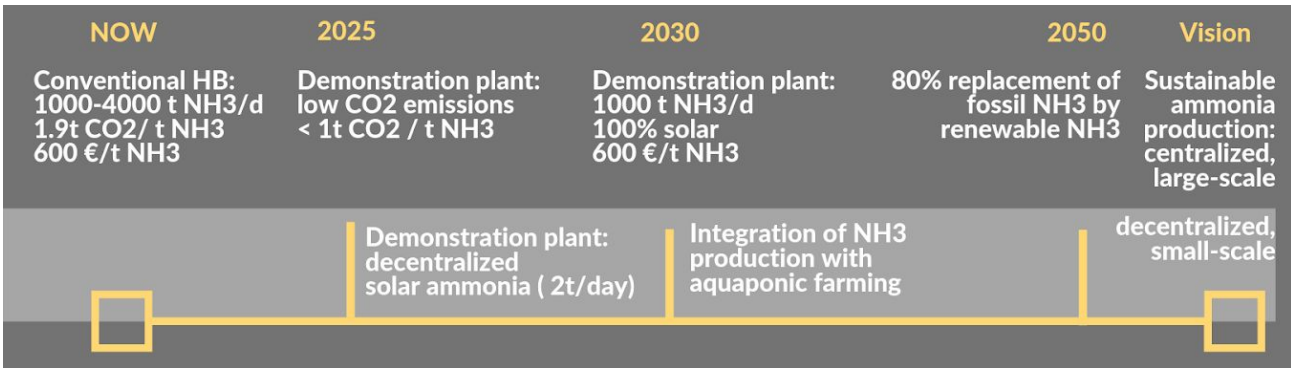
Sustainable ammonia production

SUNRISE aims at a sustainable production of ammonia by converting atmospheric nitrogen and sustainably produced hydrogen. One direction is to minimize carbon emissions related to the conventional production. This low-carbon Haber-Bosch process works at lower temperature and pressure and profits from the possibility to use already existing large-scale infrastructure. Another route is the decentralized, on-side demand production of ammonia using photo(electro)chemical and biological technologies. Within 2030, SUNRISE plans to set up pilot plants for a CO_2-neutral, centralized and decentralized solar ammonia production.

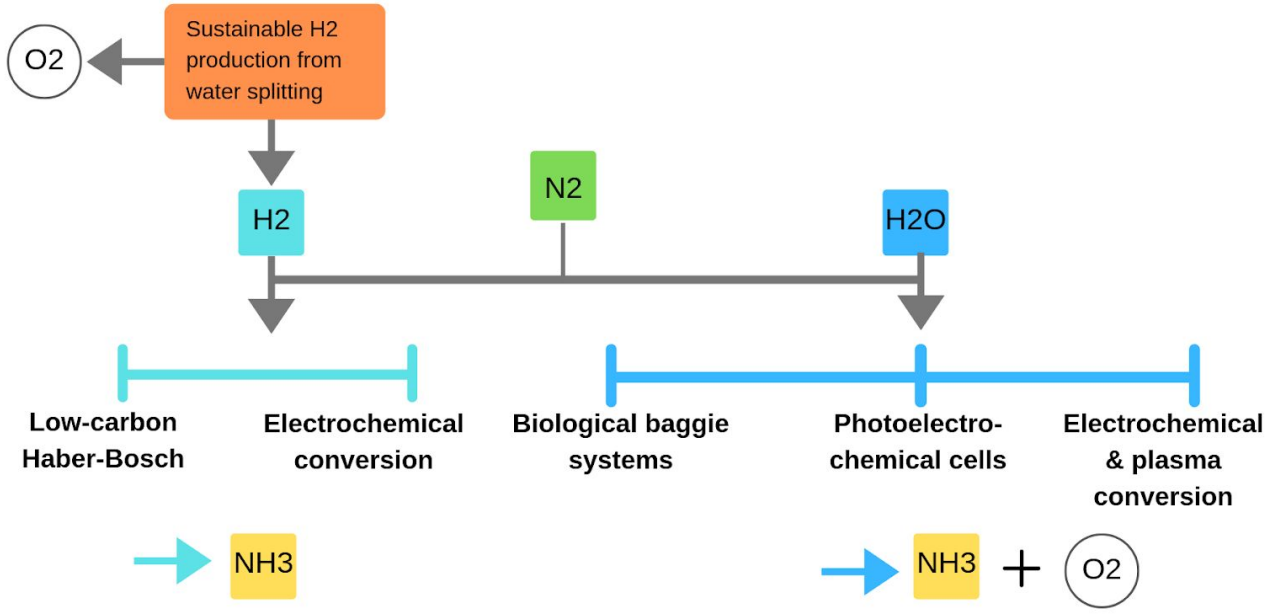


Major milestones

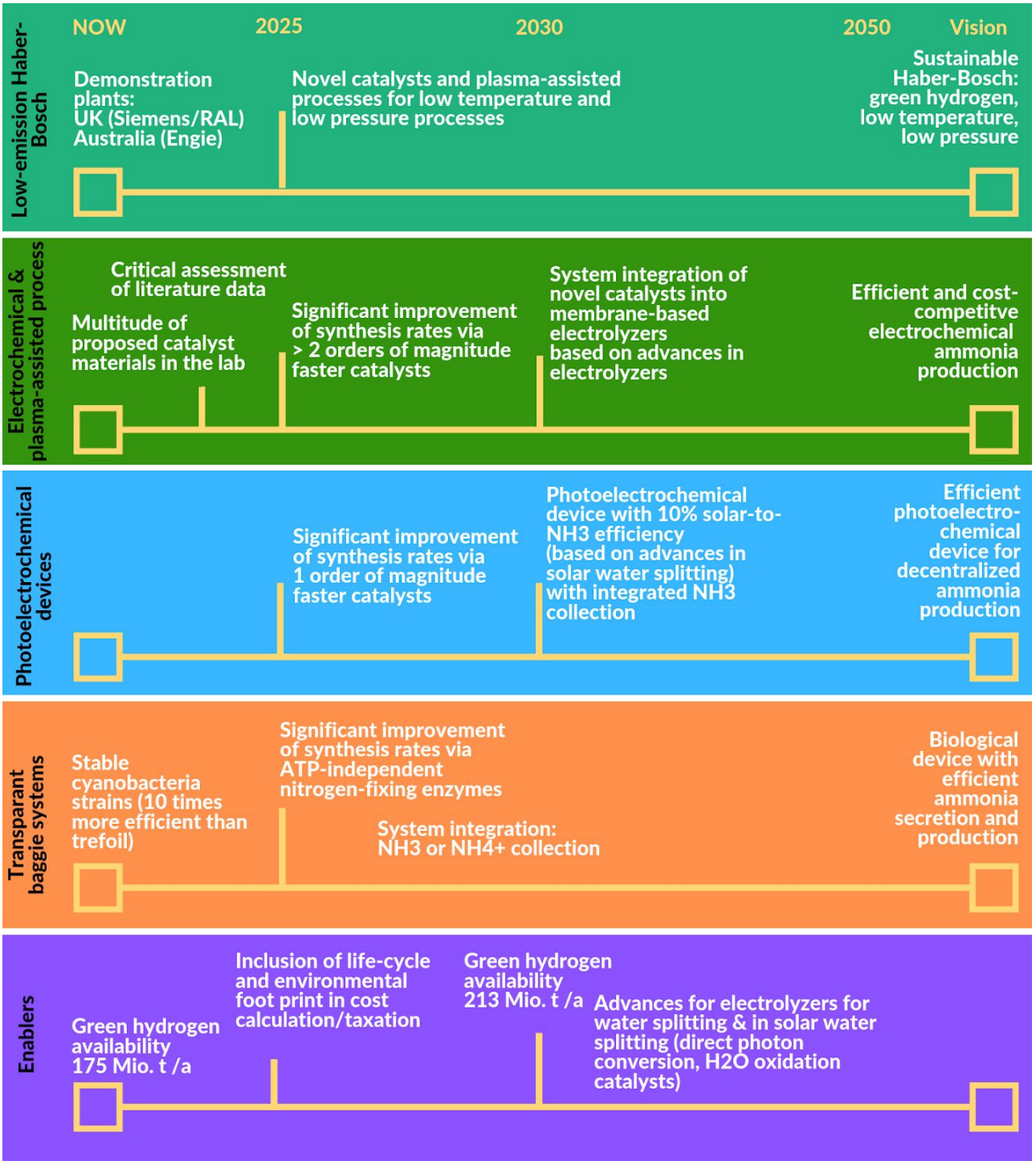
The SUNRISE vision is to produce green ammonia without CO_2 emissions and to enable an on-side production. This reduces CO_2 emissions caused by transportation and allows the integration of fertilizer production with aquaponic farming and precision farming. Starting from the currently deployed Haber-Bosch process, a first milestone consists in adapting it to the use of significant amounts of solar hydrogen so as to reduce its carbon footprint. A reduction by 50% of CO_2 emissions is targeted for 2025 and full decarbonization is expected for 2030. In parallel, the development of small ammonia production devices working at lower temperature and lower pressure will allow their tailored implementation and integration in sustainable agricultural practices. These two routes combined will allow for the replacement of >80% ammonia produced from fossil resources by renewable ammonia by 2050.



The following scheme summarizes the different technologies for ammonia production considered in this roadmap. Approaches using molecular hydrogen as a raw material include the low-carbon Haber-Bosch process and the electrochemical conversion. The large-scale deployment of these technologies strongly depends on the availability of sustainably produced green hydrogen. This possible risk is circumvented by approaches taking water as hydrogen source (transparent baggie systems with microorganisms, photo(electro)chemical cells, as well as plasma conversion).



Major technological targets



Low-emission Haber-Bosch

The conventional Haber-Bosch process is very efficient in terms of energy consumption. However, it currently relies on hydrogen produced at high pressure from natural gas or hydrocarbons and results in high CO_2 emissions (around 1.9 t CO_2 per 1 t NH_3). The use of renewable (solar) hydrogen produced on-site as input will allow the progressive defossilization of this process. In order to be fully compatible with green hydrogen production, it is necessary to bring down pressure

and temperature demands of the Haber-Bosch technology from 300 bars and 600°C to <30 bars and <100°C, therefore reducing the needs for compression and heating.

Unique selling point: Technological maturity and the possibility to use existing infrastructure, together with the existing solutions to produce solar hydrogen, are the main reasons to pursue this approach.

Vision for 2050: Low-emission Haber-Bosch allows for a centralized, low-carbon large-scale production of ammonia. Existing infrastructure from conventional Haber-Bosch plants can be used. If the process is adapted to work at lower temperature and pressure, decentralized production of ammonia could also be deployed.

Working principle: The Haber-Bosch reaction (N_2 +3 H_2 ⇒ 2 NH_3) needs catalysts to proceed at an appreciable rate. The reaction is exothermic, but low conversion is obtained even at T=600° and p=300bar due to kinetic issues; Lowering the temperature and pressure is beneficial for thermodynamics, but detrimental to kinetics.

Key research drivers: catalyst development to drive processes at ambient temperature and pressure; combine catalysts with non-thermal (cold) plasma techniques to assist the cleavage of the N_2 molecule; decrease energy consumption of air supply unit for nitrogen extraction from the air.

Key enabling technologies: advances in green hydrogen production, high-throughput computing for materials science and development. Rational design of bioinspired catalysts for N_2 reduction derived from nitrogenases that operate at ambient temperature.

Present TRL: 5-6
TRL target 2030: 9

Major technological targets:
Two demonstration plants are under development, in Oxford, UK (Siemens/RAL) using wind as a primary energy and in Pilbara, Australia (Engie/Yara, to be commissioned in 2021 at the earliest) with a target of > 80 t of ammonia produced per day using a 50-60 MW electrolyzer coupled to a PV field and producing 10% of the hydrogen required. These plants use conventional high-temperature, high-pressure Haber-Bosch technology and it is expected that such plants can use up to 100% renewable hydrogen so as to cut direct carbon emissions. To further improve the energy efficiency of carbon neutral ammonia production, it will then be required to develop alternative catalysts working at lower pressure and temperature, possibly with the assistance of non-thermal (cold) plasma techniques to ease the cleavage of the N_2 molecule.
For technical details, please refer to technical annex (how-documents).

Electrochemical and plasma-assisted ammonia synthesis

The use of renewable electricity to produce ammonia encompasses two technological solutions. The first one relies on N_2 co-electrolysis with either water or solar hydrogen and requires the development of novel, possibly bioinspired, electrocatalysts for proton-coupled N_2 reduction

(Nitrogen reduction reaction, NRR; the second one uses plasma techniques to cleave the very stable N_2 molecule and allow for its conversion in the absence of catalysts.

Unique selling point: These technologies have the potential to allow for carbon-free ammonia production. They do not require high pressure or high temperature and can then be developed in a decentralized production system.

Vision for 2050: These technologies will allow a decentralized, low-carbon large-scale production of ammonia in field and even possibly at the foot of the plants.

Working principle: At the anode of electrochemical cells, water or renewable hydrogen will be oxidized delivering protons and electrons to the cathode electrocatalysts (solid-state materials, nitrogenases or molecular mimics of their active sites) to achieve the 6-electrons/6-protons reduction of N_2. The anode and cathode compartments are separated by a proton-permeable membrane to allow for easy separation of the ammonia product. A reduced (0.2-0.4 V) electrical potential is required when H_2 is used instead of water (>2.5 V) at the anode. The plasma-assisted process uses electrical power to create a cloud of atoms from a mixture of N_2 and water. These atoms then react together to form ammonia and oxygen. Water consumption is low but purification of nitrogen from atmospheric oxygen will be required.

Key research drivers: NRR catalyst discovery and non-thermal plasma assisted process development, proton conducting electrolyte developments.
Key enabling technologies: Regarding membrane and anode catalysts, electrochemical nitrogen reduction will strongly rely on advances in electrolyzers and fuel cells for hydrogen production and utilisation.

Present TRL: 1-2
TRL target 2030: 4-5

Major technological targets
The field of NRR catalysts seems nowadays very prolific but recent reports[55] by experts in catalysis seriously question the methodology used so far to assess NRR catalytic performances. A critical assessment of literature data is then needed urgently to establish the field on solid ground. The discovery of novel catalysts of NRR with performances at least two orders of magnitude higher than currently reported (i.e. allowing current densities of >100 mA/cm2) is required and will then be implemented into electrolysis cells, thanks to the knowledge gained in electrochemical hydrogen production and CO_2 valorization. Plasma processes will be developed in parallel with the aim of improving the yield of ammonia production and the energetic yield of the process.

Photoelectrochemical devices

Similarly to direct solar hydrogen production, photoelectrochemical systems have the potential to allow for decentralized ammonia production at lower cost compared to other techniques.

[55] "A rigorous electrochemical ammonia synthesis protocol with quantitative isotope measurements" S. Andersen et al., Nature 570, 504–508 (2019); "Role for Standardization in Electrocatalytic Ammonia Synthesis: A Conversation with Leo Liu, Lauren Greenlee, and Douglas MacFarlane" C. MacLaughlin ACS Energy Lett. 2019 46 1432-1436 and references herein.

Unique selling point: Photoelectrochemical systems are integrated and allow for large savings in terms of support and container as well as interconnecting electronics. As the surface of catalysis for water splitting is the same as the surface for sunlight collection, current densities at the photocathodes (10 mA/cm^2) are up to two orders of magnitude lower than those required for cost-effective electrolysis. This reduces the constraints on the used materials and allows for the use of abundantly available, cheap and non-toxic materials as catalysts. For the supramolecular photochemical systems, the intrinsically high surface to volume ratio leads to favourable materials efficiencies.

Vision for 2050: Photoelectrochemical devices will allow for a decentralized, on-site and on-demand production of fertilizers, down to the scale of greenhouses or fields. Systems will be fully autonomous, only depending on abundantly available sunlight. Water consumption is low, but purification of nitrogen with air-separation units will be required.

Working principle: Photoelectrochemical cells are single devices that directly split water and N_2 into ammonia and oxygen, where the needed energy is provided by sunlight. Various architectures are possible, but all of them combine light-harvesting materials (inorganic and organic semiconductors, molecular dyes or biological pigments) and catalysts for the ammonia-forming and the oxygen-evolving reactions. Both reactions occur at separate (photo)electrodes or in molecular reaction cascades embedded in membranes allowing for easy separation of the products. A flow of the cathodic electrolyte might be needed to recover the ammonia product.

Key research drivers: NRR catalyst discovery
Key enabling technologies: relies on advances in the development of photo(electro)chemical devices for direct solar water splitting and electrochemical NRR (see above);

Present TRL: 1-2
TRL target 2030: 4-5

Major technological targets
Although photoelectrochemical nitrogen fixation is still at its very infancy, rapid progress can be expected when actual catalysts for nitrogen fixation will have been discovered and 10% solar-to-ammonia efficiencies can be achieved in photo(electro)chemical devices with integrated collection of aqueous ammonia solution before 2030.
For technical details, please refer to technical annex (how-documents).

Microorganisms for direct fertilizer production

Some photoautotrophic microbes use solar energy to fix atmospheric N_2 to ammonia via a nitrogenase enzyme. The enzyme is oxygen sensitive, therefore oxygenic photosynthetic microbes known as cyanobacteria (e.g. trichome) produce ammonia in specialized micro-oxic cells, called heterocysts, or in micro-oxic niches inside of the cells. This enables the O_2-sensitive nitrogenase to perform N_2 fixation during photosynthetic oxygen evolution and under ambient air. In principle, a similar approach can be developed for synthetic photocatalytic systems.

Unique selling point: Different from Haber-Bosch, this process does not demand high temperature, high pressure or purified resources (N_2 and H_2). Green ammonia is produced from solar cultures of photosynthetic microbes, simultaneously with CO_2 sequestration. The living organisms are self-replicating which lowers system costs. The product can be directly used in precision farming and aquaponic culture (NH_4^+).

Vision for 2050: Precision agriculture (or organic farms and greenhouses) with co-cultivated cyanobacteria acting as N_2-fixing biocatalysts producing and secreting NH_4+.

Working principle: Baggie or photobioreactor systems allowing a decentralized, local production of ammonia for single households and niche applications**.** The technology will include newly identified and engineered photosynthetic microbes acting as N_2-fixing cell factories: the cells produce NH_4^+ from atmospheric N_2 and excrete it out**.** Integrated crop/ algae co-culturing in organic farms and greenhouses will enable a closed loop of nutrient cycling.

Key research drivers: high cultivation costs, low product efficiency, bottlenecks in product separation; fast assimilation of ammonium by cyanobacteria should be avoided, toxicity of the product at high concentrations, robustness of production strains.

Key enabling technologies: synthetic biology tools, special photobioreactor design and optimization, product separation, collection, modelling and development of control tools, scale-up modelling.

Present TRL: 1-2
TRL target 2030: 4-6

Major technological targets
Engineered cyanobacterial strains currently exist which produce and excrete ammonium ten times more than trefoil.[56] Application of new metabolic engineering strategies to develop novel and efficient ammonium producers, identification of efficient, low energy-demanding (or ATP-independent) and O_2 resistant nitrogenases via mining and introduction of these enzymes in living systems through synthetic biology will allow a significant improvement of productivity by 2025. System integration efforts will then be needed to design photobioreactors with integrated ammonia or ammonium separation and collection. Such photobioreactors should be able to be installed in field and greenhouses and supply fertilizers in a decentralized manner.
For in-depth technical details, please refer to the technical annex (how-documents).

[56] Bui et al. 2014 Isolation, improvement and characterization of an ammonium excreting mutant strain of the heterocytous cyanobacterium, Anabaena variabilis PCC 7937. Biochem Engineer J. 90: 279-285

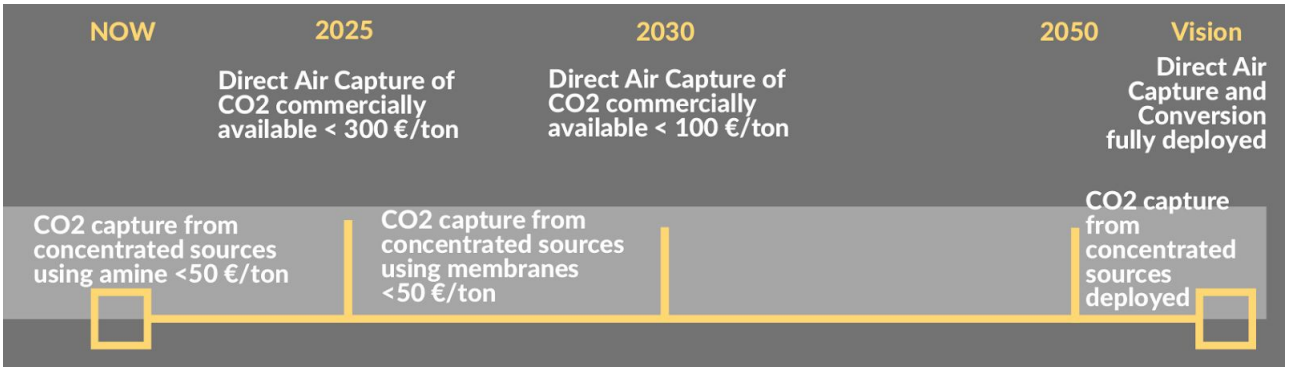
Sustainable carbon capture

Many policy and industrial drivers exist to activate the deployment of already mature carbon capture technologies. CCU actors and CCS promoters push for a large scale adoption and most of the effort will go on disconnected from SUNRISE S&T development. However, one topic will be directly impacted by SUNRISE ideas and is thus addressed in more details: the research towards combined processes of capture and chemical conversion.

Today, a large range of potentially attractive CO_2 sources is available, which can be divided into CO_2 point sources and atmospheric CO_2. The largest emitters are fossil-fuelled power plants. Other point sources include cement plants, the first largest industrial emitter (3.8 Gton CO_2/year), followed by the iron and steel industry (2.8 – 2.9 Gton CO_2/year), pulp and paper, refineries, steam crackers and chemical plants. Depending on the type of CO_2 source, CO_2 concentration can range from nearly 100% for ammonia / ethylene oxide / hydrogen plants and biogas upgrading, up to 70% for natural gas processing[57] and down to 3-5% for gas-fired combustion processes. Not only CO_2 concentration but also the impurities present will impact the performance of the capture process. Besides, the atmosphere is a potentially huge (teraton scale) CO_2 reservoir for decentralized systems, but with a concentration of only about 400 ppm. This will require highly efficient separation from oxygen and nitrogen, especially for electrochemical and photo(electro)chemical methods.

Different types of carbon capture technologies can be applied depending on the source of CO_2: for point sources, the most mature technologies consist in separating and concentrating CO_2 by chemical or physical absorption (e.g. utilizing amine solvent) or by adsorption (using a solid sorbent or membranes). Capturing from the atmosphere is termed Direct Air Capture (DAC).

Major milestones



CO_2 capture from concentrated sources

Among the different technologies existing for capturing CO_2 from industrial point sources, the most mature one is by chemical absorption (amine, ammonia…). This technology will likely develop at industrial scale (400000 ton CO_2/year for a large scale plant) with reasonable economics (capture cost < 50 €/ton CO_2) within the next 3 years. However, chemical absorption will have to face different challenges: reduction of the energy consumption (currently at 3.5 – 3.8 GJ per ton of CO_2

[57] Natural gas processing refers to dehydration and cleaning to make pipeline grade natural gas.

from point sources)[58], management of the environmental impact (risk of aerosols formation / amine emissions, solvent stability, chemical waste handling), scaling-down for smaller point sources. In the next 5-10 years, improvement in process design and solvent development (e.g. amino acids, demixing amines, ionic liquids, enzymes, …) can bring down the energy consumption to 1.5-2 GJ/ton CO_2 from point sources.

Concentrated point sources ([CO_2] > 20%) offer early opportunity for membrane capture deployment with performances equivalent to the amine process. Membrane technology presents the advantages of being modular and affords a smaller footprint, fully electrified, flexible, lower CAPEX, especially at small scale. Membrane capture is probably one of the best candidates for small scale, decentralized CCU. Its maturity is probably 5-10 years behind amine absorption. In the coming years, membrane development (e.g. facilitated transport, nanocomposite membranes or systems with higher permeability and selectivity) and better process integration (e.g. pre-treatment, configuration) can further increase their industrial application.

Besides post-combustion capture, other capture technologies such as oxyfuel combustion (*i.e.* with pure oxygen or oxygen enriched air), Calix's technology (development for cement industry: indirect heating of the limestone in the calciner in an enveloping vessel, allowing pure CO_2 release from the limestone calcination) or Smelting Reduction Process in the steel industry (Hirsana) will allow to obtain pure CO_2 without significant energy penalty. Industrialization of these latter processes are expected by 2030-2035.

Unique selling point: The high maturity and availability at short-term of these technologies are one of the main advantages to pursue this approach. Moreover, they produce a CO_2 stream with a high purity.

Working principle: CO_2 in the flue gas is separated and concentrated by chemical absorption/regeneration (amine technology) or by membrane technology using a physical or chemical mechanism.[59]

Key research drivers: Improvement of energy efficiency, environmental impact, scale-down, cost.

Key enabling technologies: Advances in this field depend on technological breakthroughs in new solvents development and process optimization to reduce the energy requirements and the environmental impact (higher stability of solvent, control of emission …).

Present TRL: 6-7
TRL target 2030: 9

For technical details: refer to technical annex (how-documents)

[58] A useful comparison for this energy by weight is obtained by considering how much energy is obtained while producing the waste CO_2. If this CO_2 is released from methane burning, about 19.6 GJ are obtained per ton, whereas about 13 GJ are gained in case of oil burning, and about 8 GJ only from the combustion of coal.
[59] Transport through a membrane can also be based on a chemical reaction.

Direct CO_2 Capture from the atmosphere

Direct Air Capture (DAC) can be applied for centralized or decentralized systems but mostly, it can deal with mobile sources, such as automobiles, ships, aircraft and other non-stationary sources.

Unique selling point: Technological maturity and the possibility to use this technology for decentralized systems are the main advantages to pursue this approach.

Working principle: Direct Air Capture (DAC) is the physical or chemical separation of CO_2 from ambient air. There are currently two main technologies in development: Absorption with a liquid strong base, referred to as High temperature DAC (Carbon Engineering), and adsorption on solid sorbent, referred to as Low temperature DAC (Climeworks, Global Thermostat, Antecy).[60]

Key research drivers: cost, energy demand, material stability and kinetics

Key enabling technologies: Advances in this field depend on technological breakthroughs in material science (improvement of sorbent/solvent (kinetics, stability and lower regeneration energy), process integration and identification of renewable sources of heat.

Present TRL: 6
TRL target 2030: 8-9

Major technological targets

At present, major challenges are (i) the high cost (today 300-600 €/ton CO_2, some technology providers have announced cost reduction down to 100 €/ton CO_2 on the short term, but this still has to be demonstrated) and (ii) energy consumption (today, 5-9 GJ/ton CO_2). This is mainly due to the low concentration of CO_2 in the atmosphere, roughly 0.04%. In order to be successful, DAC technology will need to achieve low total cost and high amounts of net CO_2 removal (reduce energy consumption[61] and use of low carbon energy). To reach these goals, research is needed for sorbent/solvent development (low regeneration energy, high CO_2 selectivity, fast reaction times and low degradation rates), process integration with low-carbon heat, improved process design and air contactors. This needs to play together with the size increase of the systems (economy-of-scale).

On the short-medium term (5-15 years), R&D to improve process design and integration will support reducing the cost and energy consumption of DAC. It is also foreseen that the number of demonstration projects will increase and confirm the scale-up potential (up to several hundred kton CO_2/year), establishing references systems, integrating the use of low carbon energy sources, validating cost and performance. By 2030-2035, a commercial portfolio of DAC systems with potential capacity of 100 Mton CO_2/year can be expected. Regarding the cost, according to providers, improved design and better solvent/sorbent development can reduce it to < 300 €/ton

[60] Solvent regeneration necessitates high temperatures (about 700°C), whereas solid sorbents can be regenerated at low temperatures (ca. 100°C).
[61] There is a lot of room for improvement, the thermodynamic limit being more than 10 times lower than present energy consumptions. See e.g. K.S. Lackner, *Energy*, **50** (2013) 38-46.

CO_2 on the short term (< 5 years) and with the expected deployment and mass production, it can be further reduced to < 100 €/ton CO_2 by 2030.

Direct Atmospheric CO_2 Capture & Conversion (DACC)

CO_2 capture technologies have in common one major challenge: the energy use. Most of the energy use is linked to the regeneration step where pure, gaseous CO_2 is released. The best strategy is to avoid this step and to develop a technology allowing the direct conversion from the captured CO_2 solution. This is called Direct Atmospheric CO_2 Capture & Conversion (DACC).

Unique selling point: Such a system will have the advantage to combine in one single-step the capture and conversion of CO_2 and in the long-term will enable the decentralized production of chemicals and fuels with highly efficient solar energy devices.

Working principle: CO_2 capture often uses alkali or amine solution and CO_2 is captured under the form of carbonates or carbamates. Captured CO_2 can serve as electrolyte or intermediate for direct reduction to CO or hydrocarbons. Such an approach has been found in different recent studies. Sargent et al have studied[62] the reactivity of K_2CO_3 solutions using an Ag catalyst for the direct conversion to syngas. Prakash et al. on the other hand have studied[63] the possibility of using amines grafted onto solid supports for tandem CO_2 capture and conversion to CH_3OH using homogeneous hydrogenation catalysts.

Key research drivers: reactivity of carbonates / carbamates, development of CO_2 selective catalyst, direct conversion of atmospheric CO_2 to syngas by thermochemical and photo(electro)-chemical routes.

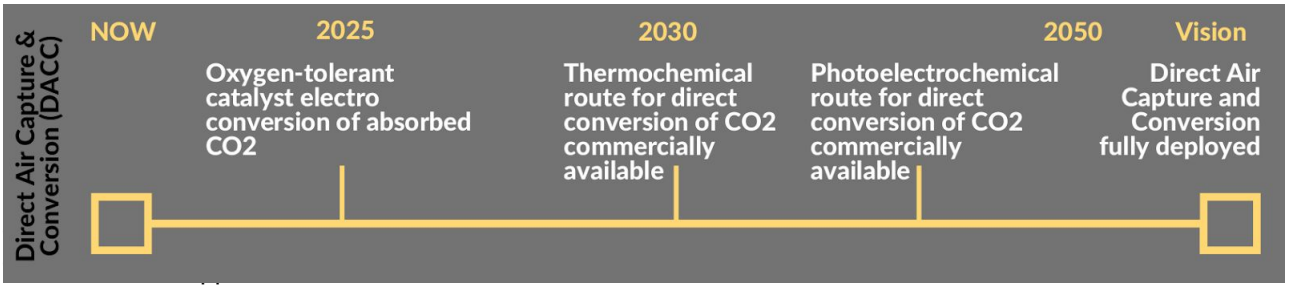
Key enabling technologies: Advances in this field depend on technological breakthroughs in material science (catalysts) to increase the selectivity and reactivity of carbonates / carbamates.

Present TRL: 1-2
TRL target 2030: 5-7

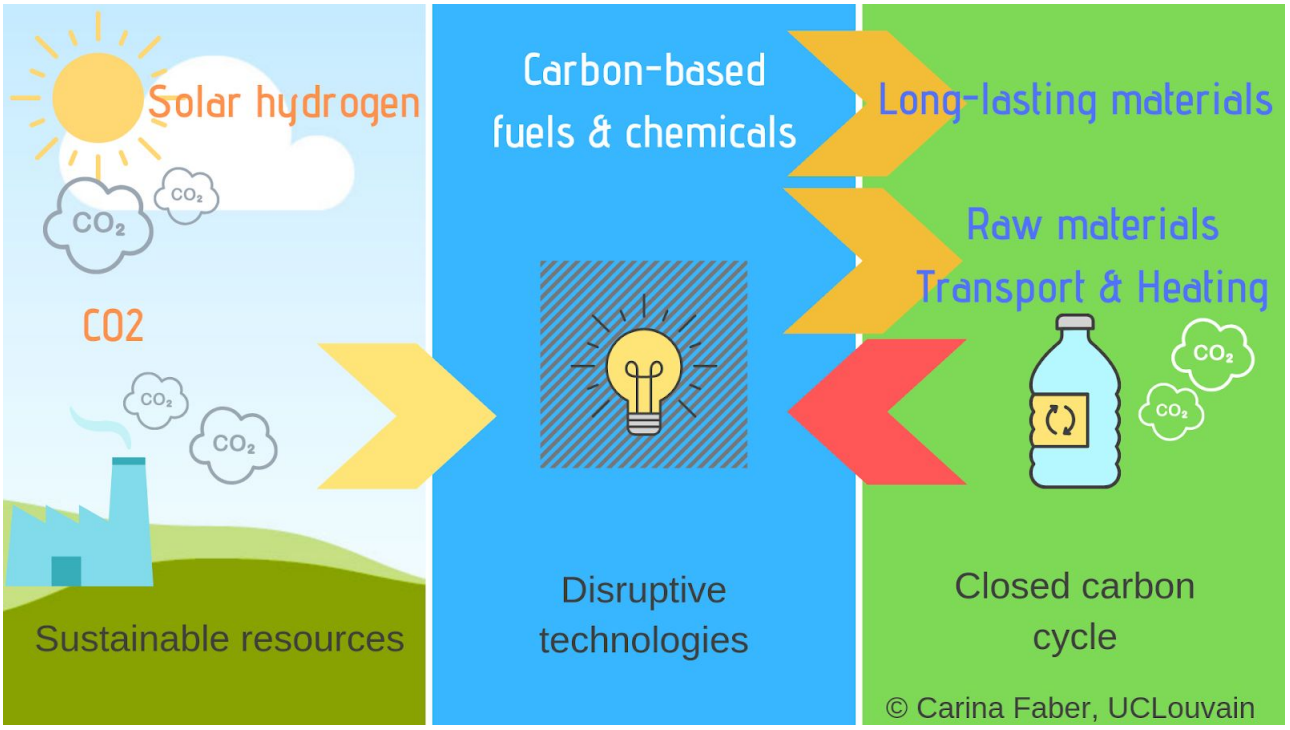
The following timeline is expected to achieve by 2035-2040 commercial solutions for DACC:

- In the next 5 years, study of oxygen-tolerant catalyst for photo/electro-reductive conversion of carbonates/carbamates: existing and development of new systems.
- Thermal chemical conversion route: direct conversion of atmospheric CO_2 to syngas TRL 5 in 2025, commercially available by 2030.
- Photo(electro)chemical conversion route: direct conversion of atmospheric CO_2 to syngas TRL 3 in 2025, TRL7 by 2035, commercially available by 2040.

Major technological targets



Sustainable production of commodity chemicals and (jet) fuels



Today, the overwhelming majority of carbon-based fuels and chemicals has fossil origin. Upon their combustion and utilization, large amounts of CO_2 are generated, contributing to global warming.

For many application scenarios, alternatives are currently developed. For instance, battery-electric and fuel cell vehicles are designed for road-based transportation. In certain cases, however, 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. CO_2 emissions account for about one third of the total adverse effect of aviation on the climate (with the other two thirds being caused by water vapor, NO_x-induced ozone production and induced cloud formation)[64]. By using renewable solar fuels, the effect of aviation on global warming could therefore be significantly reduced. In SUNRISE, we aim at the cost-competitive, mid-scale production of sustainable jet fuels (700 000 barrels produced per year, i.e. delivering ca. 150 MW, on 1000 ha) for 2030.

In principle, it is possible to produce and use carbon-based fuels and chemicals without net CO_2 emissions. This requires CO_2 capture from the air or industrial processes, followed by the synthetic production of carbon-based fuels and chemicals. Carbon dioxide is then either stored in long-lasting carbon materials on the long term (negative emissions) or directly released when the products are e.g. combusted using conventional technology. In the following, four different technological routes are detailed: Power-to-Liquid, solar-thermochemical conversion,[65] direct photo(electro)chemical conversion and bio-catalytic production.

[64] Lee et al., Atmos. Environ. 43, 2009, 3520-3537

[65] Solar-thermochemical conversion processes are not originally part of the three Sunrise approaches, yet they are a promising option for producing carbon-based compounds,They are thus briefly described in the following as additional approach in the SUNRISE Roadmap.

Power-to-Liquid: Electrochemical processes

Power-to-Liquid production pathways represent a group of processes converting water and CO_2 into liquid carbon-based products. They involve electrochemical reactions, typically the splitting of water into hydrogen and oxygen and/or the reduction of CO_2. Diverse organic compounds, such as formic acid (HCOOH), methanol (CH_3OH), ethylene (C_2H_4), methane (CH_4) and carbon monoxide (CO) can be produced via the electrochemical reduction of carbon dioxide, forming a versatile basis for a broad range of chemical products and fuels. Higher-order alcohols, such as ethanol and *n*-propanol, could be highly promising under future conditions.[66] Heavier hydrocarbon products, such as synthetic fuels, can be generated based on the primary electrochemical production of syngas (mixture of hydrogen, H_2, and carbon monoxide, CO), which is then converted into hydrocarbons via the thermochemical Fischer-Tropsch synthesis. This is a very attractive production route to liquid hydrocarbon fuels for the aviation sector, which will remain strongly dependent on such fuels for decades.

Power-to-Liquid pathways are often based on the electrochemical splitting of water generating hydrogen, which is then used for a subsequent chemical (thermocatalytic) conversion of CO_2. Alternatively, production pathways can also involve electrochemical reduction of CO_2. Both options will be briefly described in the following.

Electrochemical water splitting and thermocatalytic conversion of CO_2

Unique selling point: Hydrogen electrolyzers in the 1-10 MW are current industrial standard (see previous chapter). Thermocatalytic reactors and processes that use hydrogen to reduce CO_2 into energy containing molecules exist and are already used on a similar scale. Demonstrators to generate synthetic fuels are currently built and operate at the MW scale.[67] Given that these technologies are scaled-up and improved in efficiency, they will become the first available technology path for green fuels.

Working principle: The process basically consists of two steps. The first step is an electrochemical one, where renewable energy is used to generate high-energy intermediate products. This can be H_2 from electrolysis of water or CO/H_2 mixtures (known as synthesis gas, yielded from electrolysis of CO_2/water mixtures). The energy is stored in chemical bonds.
The second step consists of one or multiple thermo-catalytic reactions at elevated temperatures and pressures. Various reaction schemes are known: Dependent on the target product, this can be direct reaction of H_2 and CO_2 to e.g. methanol. The latter is a valuable intermediate product that can be used as a commodity chemical or further processed via thermo-catalytic reactions to olefins, gasoline or middle-distillates, such as jet fuel. The reaction can be steered towards methane (CH_4) as green replacement of natural gas. As an alternative to the production of methanol as an intermediate product, synthesis gas[68] can be converted into medium and

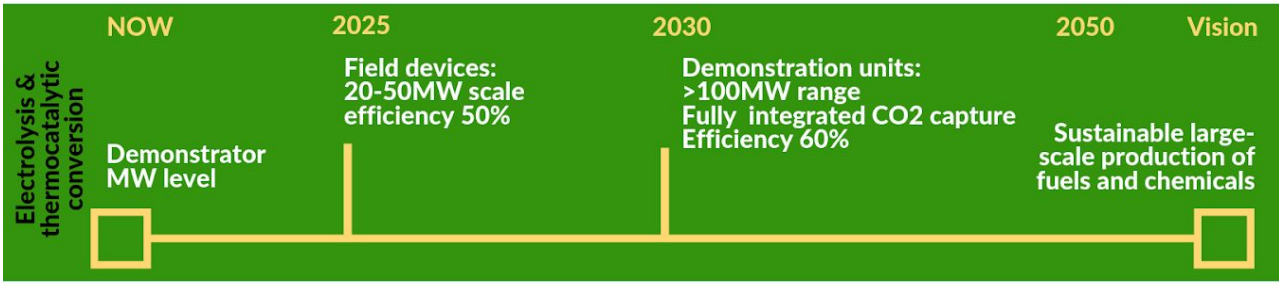
[66] Jouny, Matthew; Luc, Wesley; Jiao, Feng (2018-02-14). "General Techno-Economic Analysis of CO2 Electrolysis Systems". *Industrial & Engineering Chemistry Research*. **57** (6): 2165–2177. doi:10.1021/acs.iecr.7b03514
[67] e.g. The SPIRE project http://www.mefco2.eu/
[68] A mixture of H_2 and CO directly generated from co-electrolysis of water and CO_2 or from water electrolysis with subsequent reverse water gas shift.

long-chain hydrocarbons by a thermo-catalytic reaction (Fischer-Tropsch synthesis). The products can subsequently be refined into (jet) fuel.

Key research drivers: Scale-up of electrolysers, optimization of thermo-catalytic reactions with catalysts showing improved energy efficiency and stability towards contaminations of the input, new and energy efficient thermo-catalytic reactions (e.g. direct electric heating with renewable energies), optimised product separation and purification technologies, process intensification e.g. by coupling reaction and separation and agility of the process (conventional chemical processes are run in steady state, they have to be modified to follow the intermittent supply of renewable energy sources).

Key enabling technologies: Catalysis research with ab-initio modelling and high-throughput screening, multi-scale modelling for thermo-chemical electrically heated reactors, systems engineering for dynamic life-cycle cost analysis, advanced manufacturing for new reactor concepts, systems engineering.

Present TRL: 6, first demonstrators built at the MW level
TRL target 2030: 9



Vision for 2025: Within the SUNRISE initiative, the technology will be fully demonstrated in field devices that work at the 20-50 MW scale. They will demonstrate the feasibility for scaling together with the dynamic integration of electrolysis and thermochemical processes and show the desired stability of the catalysts against possibly unavoidable concentrations of contaminants in the feed stream coming from a coupled CO_2 capture system. At this stage, an overall energy conversion efficiency (electrical energy to chemical products) of at least 50% is targeted with the agile process.

Vision for 2030: Fully engineered and designed demonstration units in the >100MW range that show the full dynamic and chemical robustness expected from an industrial system that is already fully integrated with a suited CO_2 capture system. By thermal integration and media management an energetic efficiency of >60 % will be obtained. This fully operable industrial demonstrator is expected to trigger investment decisions for the large-scale deployment of the technology.

Direct electroreduction of CO_2

Unique selling point: The direct electroreduction of CO_2 to hydrocarbons at low temperatures (<80°C) is the most simple process chain, with a homogeneous technology doing the full job. It

promises to deliver already C_2-C_4 components with higher efficiencies compared to a two-step conversion with a subsequent thermochemical process (with high-temperature steps involved).

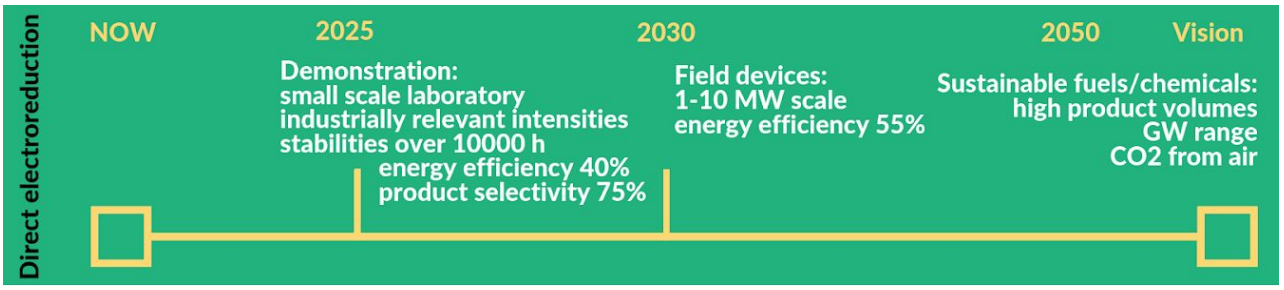
Working principle: CO_2 is fed together with water into a low-temperature electrolyzer at the cathode side. A special catalyst is employed that limits water reduction to hydrogen, while promoting CO_2 reduction. This catalyst has a high overpotential for water reduction and a low one for CO_2 reduction, driving the selective reduction of CO_2 to CO in a first step. The catalyst then needs to be able to keep the intermediate reduction product at its surface, allowing further reduction of the CO to hydrocarbon components; further, it needs to allow diffusion of the intermediate products on the surface to allow C-C bond formation to generate C_2-C_4 compounds.
Most promising in technical terms is to distribute the first step (generation of CO) and the second electrochemical step (further reduction of the CO to C_2-C_4 components) in separate cascaded electrolyzers to freely optimize both reaction parameters.

Key research drivers: Discovery of alternative catalysts for the reduction of CO_2 to hydrocarbons, overcoming the instability of copper-based catalysts (the surface morphology on atomic scale needs to be overcome by self repair or short regeneration pulses); understanding and modelling of processes in gas diffusion electrodes towards chemomechanical stability and media transport; development of alternative electrolyzer architectures; integrated system engineering of stacked gas to gas/liquid electrolyzers.

Key enabling technologies: Catalysis research with ab-initio modelling and high-throughput screening, in-operando analytical tools, multi-scale modelling, systems engineering, life-cycle cost analysis.

Present TRL: 3
TRL target 2030: 6

Major technological targets
Current research at laboratory-scale shows that mainly copper-based compounds are able to generate hydrocarbons and enable the C-C coupling. However, most of this work is done at current densities of 10-30 mA/cm²; this is two orders of magnitude below any practical application and nearly all experiments show severe degradation within a few hours. Stable catalysts need to be developed (several 1000 hours of operation, >80% product selectivity, 0.5-1 A/cm² current densities).
Moreover, novel electrolyzer architectures have to be developed that allow a sufficient supply of CO_2 to the catalyst. Ohmic losses in the electrolyte dissipate valuable renewable energy and have to be minimized. Pressurized electrolyzers that directly generate products at 30-50 bar have to be implemented to cut energy costs for a afterwards compression of products needed for further processing and storage. The electrolyzers need to have a high turnover referring to their volume to limit the CAPEX (capital expenditure), so they need to be able to work with industrially relevant current densities of (500-1000mA/cm²).



Vision for 2025: Demonstration of the feasibility of this efficient approach by long-term experiments at small-scale laboratory level (100 cm² electrode surface) that need to operate at industrially relevant intensities (current densities of 0.5 - 1 A/cm², temperature 70°C). They will prove the principle by obtaining stabilities over 10000 hours without degradation, showing product selectivities to hydrocarbon components of about 75% and a related energetic conversion efficiency of about 40%.

Vision for 2030: Within the SUNRISE initiative, the technology will be fully demonstrated in field devices that work at the 1-10 MW scale. They need to be fully engineered and designed in terms of thermal and media management. By optimisation of ohmic dissipation in the conduction channels, energetic efficiencies of about 55% will be reached.

Vision for 2050: These systems will be scaled up to the GW range in a dynamic system integration with volatile renewable energy supply and CO_2 capture from air and deliver product quantities matching volumes of future markets of fuels and chemicals. Intermediate C_2-C_4 products will be fed into refineries, where established petrochemical techniques are applied to convert them into transport-grade fuels and other marketable products.

Direct solar-thermochemical conversion of water and CO_2

As an alternative to the electrochemical options described above, an appealing pathway for CO_2 and H_2O 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.

Unique selling point: The combined thermochemical reduction of CO_2 and water is highly efficient, since solar heat is directly fed to the process instead of converting it to other energy forms such as electricity before. The intermediate products are manifold (composition and hydrogen/carbon ratio), enabling the production of all conceivable hydrocarbon products.

Working principle: The thermochemical cycle typically consists of two steps at different temperatures, mediated by an oxygen-carrying material (typically a metal oxide) as key element:

1. Oxygen release from the material: At high temperature (1350-1700°C), the material releases some of its chemically-bound oxygen. The energy required for this reaction is provided by solar heat.
2. H_2O/CO_2 splitting: At lower temperatures (600-1200°C), the oxygen-deficient material reacts with water (H_2O) and CO_2 by splitting these molecules and taking up oxygen from them, thus being re-oxidized. Thereby, H_2O is converted into molecular hydrogen and CO_2 to carbon monoxide (CO). This mixture of hydrogen and carbon monoxide is called syngas and can be used to produce hydrocarbons, such as jet fuel.
The process is entirely reversible, meaning that the mediating oxygen-carrying material is not consumed.

Key research drivers:
The two main factors to consider are efficiency and cost: in practice, large heat losses decrease process efficiencies drastically. A large amount of oxygen exchanging 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. Besides low efficiencies, 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.
This technology is still far from being economically competitive, compared to conventional (fossil) production, but also to today's Power-to-Liquid technologies. Larger-scale demonstration projects are required to show realistic potentials of this intriguing approach.

Key enabling technologies: Materials engineering, materials research with ab-initio modelling and experimental screening, solid particles technologies, membrane technologies, smart process control and interfaces.

Present TRL: 4-5
TRL target 2030: 6

Major technological targets
The targeted design of optimized solar-thermochemical materials includes:

- Solid-solid heat recovery rate > 60 %
- Steam heat recovery rate > 95 %
- Scale-up to improve efficiency
- Improved separation of products and reactants

Vision for 2025: Demonstration of the feasibility of this efficient approach by increasing the solar-to-fuel efficiency for solar-thermochemical hydrogen production to 15 % while demonstrating it at a scale of 250 kW (thermal) in a solar simulator or at a solar tower.

Vision for 2030: To reach competitiveness, a substantial decrease in cost per kg of jet fuel produced needs to be realised. Increasing the overall process efficiency is crucial for this capital-intensive technology, e.g. through reduced reaction temperatures and effective heat recuperation. Use of less expensive materials for reactor design and a decrease in cost of solar-thermal technologies (heliostats, towers) due to the implementation of concentrated solar power plants on a larger scale are also important drivers for overall cost reduction.

Vision for 2050: Commercialization of this technology through further efficiency increase to achieve lower cost. This is done by further optimizing solid-solid heat recovery (target: 80%), by decreasing temperature differences between reduction and oxidation through further materials optimization, by scale-up and therefore decreased component cost and by process optimization using experience from existing pilot plants.

Photo(electro)chemical devices

Similarly to direct solar hydrogen production, photo(electro)chemical systems have the potential to allow for a decentralized CO_2 valorisation at lower costs compared to PV-driven electrolysis.

Unique selling point: Photo(electro)chemical systems are integrated and allow for large savings in terms of support and container as well as interconnecting electronics. As the surface of catalysis is the same as the surface for sunlight collection, catalytic turnover is up to two orders of magnitude lower than that required for cost-effective electrolysis. This reduces the constraints on the used materials and allows for the use of abundantly available, cheap and non-toxic materials as catalysts. The large surface used for photon collection can also be used for atmospheric carbon capture.[38]

Vision for 2050: Photo(electro)chemical devices will allow for a decentralized, on-site and on-demand production of formic acid and hydrocarbons (methane etc.). In centralized facilities, products necessitating additional considerations on safety and utilization, such as CO, syngas or ethylene, will be obtained. Systems will be fully autonomous, only depending on abundantly available sunlight. Water consumption is low, but purification of CO_2 from atmospheric oxygen will be required.

Working principle: Buried junction cells and photoelectrochemical cells are single devices that directly split water and CO_2 into C-based products and oxygen, where the needed energy is provided by sunlight. Various architectures are possible, but all of them combine light-harvesting materials (inorganic and organic semiconductors, molecular dyes or biological pigments) and catalysts for CO_2 reduction and the oxygen evolving reactions. Both reactions occur at separate (photo)electrodes allowing for an easy separation of the products. A flow of the cathodic electrolyte might be needed to recover products if they are soluble in the electrolyte (as formic acid for example). Alternatively, photocatalytic reactor containing liquid phase suspensions of photochemical systems (photocatalytic nanoparticles or supramolecular assemblies) can be used. In that case, additional separation of the products from oxygen will be required.

Key research drivers: CO_2 reduction catalyst discovery (O_2-tolerant catalysts are required if CO_2 is to be captured from the air), Direct Air Capture and Conversion technologies

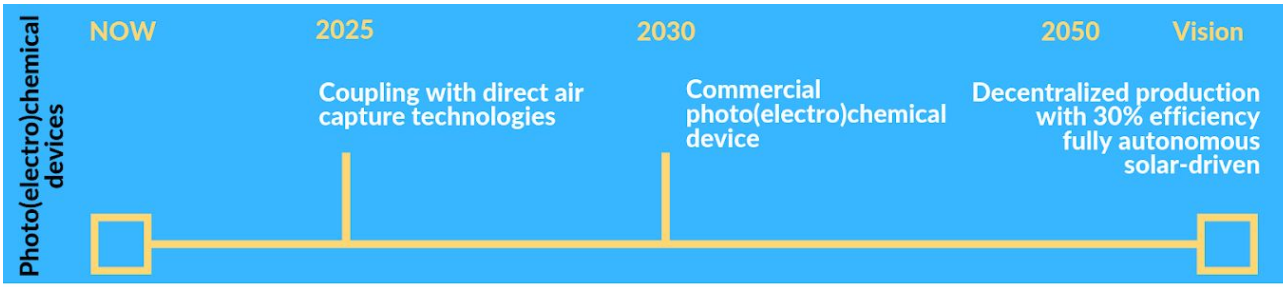
Key enabling technologies: relies on advances in the development of photo(electro)chemical devices for direct solar water splitting and electrochemical CO_2 reduction (see above);

Present TRL: 1-3
TRL target 2030: 6-7

Major technological targets

Photo(electro)chemical cells for CO_2 valorization into CO or syngas are at the same stage of development as those for H_2 production and similar targets are expected in terms of the reduction of the water demand, the improvement of stability, breakthroughs to design active components solely based on earth-abundant elements and collection of gases. An important milestone will concern the coupling with direct air capture technologies by 2025 with commercial PEC devices with 10% solar-to-syngas efficiency available by 2030. Further optimization and upscale will allow to ultimately develop commercial devices at 30% solar-to-chemical efficiency.

For in-depth technical details, please refer to the technical annex (how-documents).



Biocatalytic production of carbon-based solar fuels and chemicals

Share of renewable bio-based raw materials for chemical industry is set to target 25% of the total volume of feedstock used by the chemical industry in 2030 in Europe.[69] Importantly, photosynthetic microorganisms, such as microalgae and cyanobacteria, are considered as third generation feedstock for the chemical and petrochemical industry. The photosynthetic microorganisms use sunlight, water and CO_2 to produce organic compounds and are also capable of hosting novel synthetic production pathways that allow the cells to function as living cell factories producing the desired carbon-based solar fuels and chemicals.

There are already dozens of proof-of-the-concept for direct production of chemicals in photosynthetic microbes.[70] Some production systems are functioning at TRL 4-5 (e.g. Photanol for lactic acid production). For new products, one needs to design metabolic pathways from scratch and engineer new strains. Moreover, obtained cells producing specific compounds can be further engineered to make the system more efficient and stable.

Unique selling point: Photosynthetic microorganisms are capable of synthesising complex organic compounds with high efficiency and selectivity, combined with the ability of self-replication (recovery) and of long-term operation under physiological conditions.[71] The biosynthetic products are excreted from the cells into the cultivation medium, from where they can be collected and subjected to downstream processing when necessary.

Working principle: By application of the techniques of synthetic biology and metabolic engineering, photosynthetic microorganisms can be designed to produce and excrete a wide range

[69] RoadToBio chemicals roadmap for the European Chemicals industry https://www.roadtobio.eu/uploads/publications/roadmap/RoadToBio_action_plan.pdf

[70]Santos- Merino et al. 2019 New applications of synthetic biology tools for cyanobacterial metabolic engineering. Front. Bioengineer Biotechnol, v 7, article 23

[71] D. Lips et al. Many ways towards 'solar fuel': quantitative analysis of the most promising strategies and the main challenges during scale-up (2018) *Energy Environ. Sci.* 11. 10

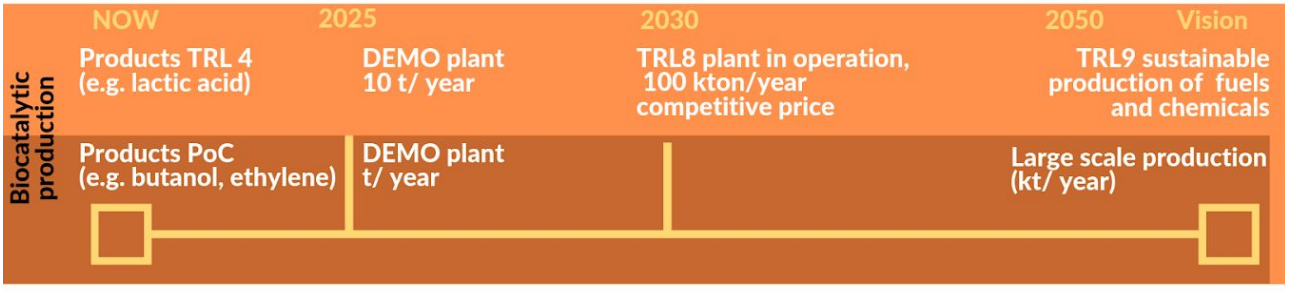
of chemicals and fuels (such as long-chain wax esters, fatty acids and hydrocarbons). The engineered microorganisms can be cultivated in photobioreactors. But also solid-state production platforms (artificial biofilms) are developed. In biohybrid approaches, inorganic photoelectrodes or light absorbers will transfer energy or reducing power to metabolically engineered organisms for the valorization of CO_2.

Key research drivers: High cultivation costs, tight regulation of photosynthetic apparatus that results in loss of absorbed solar energy into protective mechanisms, complexity of metabolic pathways that serves to cell fitness rather than product efficiency, instability of the production strains and losses in production efficiency.

Key enabling technologies: Efficient engineering and synthetic biology tools, combined with strain characterization and optimization. Engineered new strains with enhanced metabolic pathways for the synthesis and excretion of various chemical and fuel products. Construction of cost-efficient dedicated photobioreactors for cultivation and production phases. Improvement of photosynthetic performance and carbon metabolism; upscaling, including cheap bioreactor construction and operation as well as downstream processing.

Present TRL: 1 (for newly designed chemical pathways) to 6 (e.g. lactic acid production)
TRL target 2030: 4-9

Major milestones



Technological targets for 2025:
Selection and characterization of robust strains with high photosynthetic efficiency
Automated tools for fast and cheap construction of microbial cell factories
Scale-up challenges solved for several chemicals
Proof-of concept for newly developed production strains
High volumetric productivity and light-to-product conversion efficiency established
Redesign of photosynthetic apparatus for high yield
Novel strategies to avoid contaminations of production cells from foreign strains

Technological targets for 2030:
Engineering tools for a wide-range of natural organisms
Detailed theoretical models of fundamental photosynthesis established

Technological targets for 2050:
Automated DNA synthesis and construction (“cell designer”)
Dozens of large-scale demonstration plants

Long-lasting carbon-based materials

Energy carriers, like methane, or commodity chemicals, like ethylene, will eventually release their carbon in the atmosphere in the form of CO_2, on timescales of a few months or years. These two kinds of CO_2 utilization are high on today's agenda to accelerate the phasing out of fossil fuels. By inventing new efficient and optimized ways to convert CO_2 into fuels and chemicals, and also by mastering nitrogen conversion, SUNRISE will develop catalysis concepts, skills and processes which will also be instrumental in the area of Negative Emissions Technologies (NETs).[72,73] Within NETs, which are crucial in most scenarios complying with the Paris agreement, CO_2 should be stored for long durations, *i.e.* centuries or more. Depending on the success of emissions reduction policies and on the targeted climate goal, NETs need to be ready for a global scale deployment by 2040 or 2050. Considering the long time necessary to validate and optimize technologies, it clearly appears that new processes should be ready on the market in the course of the 2030s.
Up to now, the main long-term disposal considered in scenarios is underground storage of gaseous CO_2 (CCS). This storage technology bore very high promises in the 2000s, but developed slowly, due to the limited availability of underground suitable sites i.a. requiring pipeline infrastructure from large CO_2 point sources to large storage reservoirs, and mainly economic and societal obstacles. A safe and reliable long-term storage can be provided when CO_2 enters a mineral composition. Such processes have been studied by reacting CO_2 with minerals (mined for themselves, mainly silicates rocks or found in mining or industrial wastes).[74] The resulting materials, where carbon is usually in a fully oxidized state, need a limited amount of energy to be produced, and are very interesting as aggregates[75] in concrete. CO_2 can also be utilized to improve the curing of cement, as demonstrated for example by the company *CarbonCure*[76]. Both utilizations are seriously considered by the construction industry, with very promising perspectives to use and store CO_2 on the Gigaton level in the next decade, according to recent roadmaps on CO_2 utilizations.[77]

When CO_2 intended for these exothermic mineralization reactions is captured directly from the atmosphere, the energy consumption of the capture process strongly impacts the overall performance of the product. As already mentioned earlier, one must optimize the process by combining steps and possibly by preparing CO_2 under the best chemical form for the reaction. Since CO_2 must be activated (thermally, with physical pressure or by any form of chemical activation), there is a clear interest in developing combined capture and conversion, associated with the mineralization processes.

Keeping in mind that large CO_2 volumes could be stored in structural materials, like aggregates in concrete, we foresee that there would be a major progress if those materials would need no input

[72] Minx, J. C., et al. 2018; Negative emissions - Part 1: Research landscape and synthesis. Environmental Research Letters **13**(6):063001. https://doi.org/10.1088/1748-9326/aabf9b
[73] National Academies of Sciences, Engineering, and Medicine 2019. Negative Emissions Technologies and Reliable Sequestration: A Research Agenda. Washington, DC: The National Academies Press. https://doi.org/10.17226/25259
[74] Sandalow, D., et al. (2017). Carbon Dioxide Utilization (CO2U) ICEF Roadmap 2.0. available online https://www.icef-forum.org/pdf2018/roadmap/CO2U_Roadmap_ICEF2017.pdf
[75] See for example Carbon8 aggregates, now O.C.O. Technology Ltd: https://c8a.co.uk/our-process/
[76] See https://www.carboncure.com/
[77] See the contribution of CO_2 Sciences & Global CO_2 initiative, Global Roadmap for Implementing CO2 Utilization, November 2016, for the ICEF project. https://www.icef-forum.org/platform/upload/CO2U_Roadmap_ICEF2016.pdf

from mining at all, i.e. if their synthesis could be obtained by capturing raw materials in the local environment only. Such a prospect seems today beyond our programming horizon, but its potential contribution to NETs, needed by 2040, justifies its mention here. In the year 2030 and beyond, with atmospheric N_2 and CO_2 being readily, efficiently and commercially transformed to useful products, new processes could emerge to obtain structural polymers, able to replace mineral carbonates as long term storing materials.

In the long-run, SUNRISE technologies could also help another type of NET by a new form of artificial photosynthesis: Soil Carbon Sequestration[53]. The decentralized solar-driven synthesis of nitrogen- and carbon-based products could deliver materials for soil enrichment, thus contributing to the conversion of arid surface into fertile soils by performing long term storage of a significant amount of CO_2.

SUNRISE key enabling technologies

The future deployment of SUNRISE technologies at scale, providing net global GHG reductions, necessitates enabling resources, technologies and analyses.

Upscaling, i.e. bringing novel technological solutions from the lab to a global industrial scale, is a significant challenge for mature SUNRISE technologies. The overall sustainability, the availability of needed resources on a large scale and economic viability have to be ensured.

Novel materials will allow cost-competitive, efficient and durable solutions across the three proposed technological SUNRISE approaches.

Product separation, i.e. the conversion of a mixture of chemical substances into distinct products, is a crucial step once the desired solar fuel or chemical is produced by the artificial photosynthesis device; in most of today's devices product separation, purification and collection represent one of the major bottlenecks due to the energy consumed for production and operation.

The SUNRISE toolbox comprises advanced computational modelling, quantitative sustainability assessment, advanced experimental techniques and emerging concepts. **Computational materials modelling** guides experiment, avoiding tedious sequences of trial and error in the lab, and thus significantly speeds up the innovation process. Thorough **life-cycle, techno-economic and social impact analyses** will ensure the establishment of a sustainable carbon economy, viable business models and social acceptance of SUNRISE technologies. **Synthetic biology** opens enormous perspectives for the realization of an efficient algae/cyanobacteria-based production of fuels and chemicals. **Emerging concepts** transfer insights from nature to artificial systems and will be key for developing the next-generation efficient solar-to-fuels energy conversion processes based on molecular engineering.

Upscaling

The transformation of current laboratory-scale solar energy conversion devices into widespread, efficient industry-grade systems and installations is a grand S&T challenge that requires both scientific and technological breakthroughs. Laboratory experiments are in Watt scale, whereas the TW scale is needed for the energy system. This difference of 12 orders of magnitude outgoes the

scale where physical effects can be easily described within the same methodology. To overcome this gap, two main approaches need to be undertaken :

The technologies need to be scalable. The use of *scarce or expensive materials* (like iridium or other rare chemical elements) has to be limited as much as possible and ways have to be investigated to produce these technologies in *highly automated factories* using controllable processes. The energy return on energy invested *(EROI)* has to be preferably above 10; moreover it has to be verified that *processing of huge areas* is feasible (e.g., nanostructures over 1000 km² done by photolithography are hard to imagine). Devices must not use toxic materials (like significant amounts of lead or mercury) in a chemical form that allows dissipation into the environment.[78] *Appropriate scaling concepts* have to be developed that might evolve as scale of individual devices, as well as use a high degree of modularity (example: today's photovoltaics production). Also the effect of the law of large numbers on production costs has to be estimated.

Scale-up is orders of magnitude more expensive compared to lab research and needs to be financed. A necessary investment in the billions euros range is unlikely to be financed by a single research program or national subsidies. These kinds of instruments are usually adapted for the MW range. On the contrary, upscaling projects need to be financed by investors, believing in the proposed technology. In order to attract investors, intermediate business cases have to be attainable with the SUNRISE technology. This might be the creation of some high-value green products, where the molecule value is higher than the energy content or – as alternative – a product where customers are willing to pay a higher price. This way, the technology can be scaled to the 100 MW to GW range; it matures, it demonstrates its sustainable potential and reliability and it attains bankability. When this step is finally reached, the investors' trust is available to propel the technology in the TW range.

An example: Photobioreactor design. The scale up of biological applications requires design, construction and easy operation of open or closed photobioreactor systems for algae and cyanobacteria cultivation and production stages. Large-scale closed photobioreactors at TRL 5 - 6, operating with engineered cyanobacteria for direct production of e.g. ethanol have already been reported.[79] By way of example, Ecoduna GmbH (Austria) operates 1 hectare vertical photobioreactors (total length 230 km) with an annual capacity of 100 tons of algae biomass production. The feasibility of upscaling the production of bio-based chemicals needs to address yet unsolved issues: Concerning EROI, the energy for producing/building/recycling the reactors, plus operation (pumping), plus the energy for product separation and cleaning has to be at least one order of magnitude below the energy content of the products. Moreover, contamination by predator bacteria, as well as the genetic stability of the engineered algae and bacteria needs to be researched and positively solved.
For further technical details, please refer to the technical appendix on Upscaling.

Novel materials

An important challenge is the development and optimization of materials for artificial photosynthesis. Today's catalysts and photo-absorbers have to be significantly improved in terms

[78] Lead glass or piezoceramics for example contain lead, but in a chemically bonded way that inhibits release.
[79] J. Dexter et al. *J. Appl. Microbiol.*, 2015, 119, 11–24

of efficiency and durability; novel materials are crucially needed that are earth-abundant and non-toxic in order to allow for a sustainable upscaling of the proposed technologies. Once efficient materials are found, these outcomes have to be tested in real device conditions and the nanoscopic scale has to be bridged to the macroscopic world.
The challenge is the intrinsic complexity of the considered thermo- and electrochemical, photoelectrocatalytic or bio-inspired systems, where one deals e.g. with complicated surface reactions, complex thermodynamic properties, the interplay between electrodes and electrolyte, photoabsorption and catalysis. Employed materials have to fulfill diverse requirements which are often competing and where a compromise has to be found. In order to allow for an efficient and targeted materials development, it is crucial to understand the underlying fundamental principles and reactions.

Product separation, purification and collection

Generating valuable and energy containing products from sunlight is one side of the trophy, separating and cleaning them into a state that allows further use is the other one. The energy required for the separation must not be underestimated. This is relevant for the refining of fuel components into fuel, and it is especially hard for commodity chemicals (such as ethylene, aromatics, propylene and alcohols), where usually a high purity is required.

The energy for separation cannot approach zero – even with the ideal technology – due to thermodynamic reasons. In existing, already optimized processes of the chemical industry, the relation of the energy needed for separation and the energy content of the products can vary from almost zero to more than 40%. It is thus crucial for the efficiency chain of SUNRISE products to consider the energy needs for separation.

Amongst possible options, distillation (especially cryogenic) is a powerful, but energy consuming process and may be limited to well mixable substances. Membrane separation – an energy efficient tool – is already employed in volume processes, but the selectivity needs to be improved. Temperature and pressure swing separation is mighty but restricted to several tasks. There is no universal technology for product cleaning in view of the varying output of the SUNRISE technology and the broad range of usable product options. Product separation must be optimized individually for the intended use cases of SUNRISE developments.

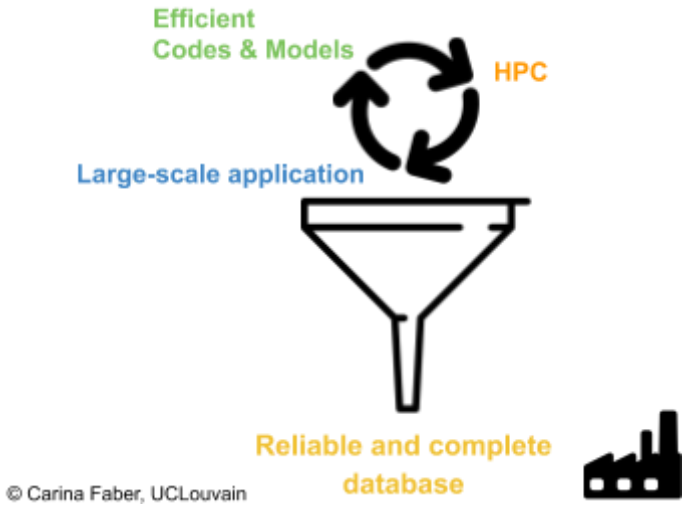
SUNRISE tool box

Advanced computational modelling: from novel materials to solar fuel devices

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

[80] Mission Innovation 6, Clean Energy Materials:
http://mission-innovation.net/our-work/innovation-challenges/clean-energy-materials/

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



Efficiently predicting the performance of materials and processes and translating these findings on the device level necessitates different dimensions which inherently depend on each other:

1) The development of theoretical models accurately describing complex, real-life processes in a simplified manner has to be pursued, as well as the improvement of computer codes solving equations in the most efficient way; this allows for the calculation of material properties both efficiently and accurately and to ultimately simulate real solar fuel device structures. Interfaces need special focus, since materials with an optimum property do not necessarily show the best performance in a device.
2) Innovation in high-performance computing facilities and the development of new algorithms and software with respect to these infrastructures allows to use resources in the best possible way and consequently to approach more complex systems, higher reliability and millions of calculations of material properties.
3) Simulations of artificial photosynthesis systems and the calculation of material properties on a large-scale will prove the reliability of the developed methods and deliver key quantities for experimental studies; machine-learning algorithms allow for automated calculations and the study of millions of novel materials (combined with high-performance supercomputers). The lack of understanding of how to profit most effectively from artificial intelligence approaches for materials discovery and especially artificial photosynthesis has to be overcome. New big data analyses and high-throughput screening based on interoperable complex workflows will retrieve the most promising candidates instead of only predicting properties.
4) Reliable and complete databases are the prerequisite of modern research and especially for machine-learning approaches. The establishment of a SUNRISE database with reproducible data on the most promising materials for artificial photosynthesis allows to

select the best candidates and prevents a doubling of research efforts. The establishment of commonly agreed on criteria (for data formats, the quality of results, details on how data is obtained) permits to easily search in multiple existing databases and to find suitable materials using artificial intelligence.

For further technical details, please refer to the technical appendix on Materials Modelling.

New methods and software tools for early quantitative sustainability assessment: bridging environmental, economic and social impacts

The rapid pace of technology development requires the development of new methods and software for the fast assessment of the environmental, economic and social impacts of emerging technologies. Life-cycle assessment (LCA) is a powerful tool to evaluate total energy requirements, net carbon emissions and overall environmental impacts (far beyond just carbon footprinting). It goes hand in hand with techno-economic analyses (TEA) which determine the technical and economic viability of a new technology and social impact assessment (SIA) studying the societal acceptance of a new technology.

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

Nevertheless, current technology assessments frequently do not provide the needed level of transparency, consistency and accessibility.[81] Existing methods lack integration and advances in technology evaluation tools need to take place in parallel with the development of SUNRISE technologies. Today's methods are able to assess existing, well-defined technological systems, but could be improved when emerging technologies need to be assessed and recommended. This is mainly due to two major gaps: first, there is a lack of data coverage for e.g. processes, environmental exchanges, market dynamics, social implications of technology diffusion or technology transition monitoring; second, all models assess emerging technologies only with existing methods, data and software tools.

For further technical details, please refer to the technical appendix.

Synthetic Biology

Synthetic biology is an emerging technology that aims at the genetic redesign of biological organisms to build up novel living systems, not existing in nature. Synthetic biology combines engineering, digitization, robotics and biology. This enables the reprogramming of living cells to function in a way that benefits the economy. The genetically engineered organisms act as *living cell factories* producing desired fuels and chemicals ranging from e.g. lactic acid to jet fuel.

Recent breakthroughs in plant science demonstrated that crops engineered with a synthetic photorespiratory shortcut are 40% more productive than natural plants in real-world agronomic

[81] Gaseous Carbon Waste Streams Utilization: Status and Research Needs, 2019, National Academy of Sciences

conditions.[82] A proof of principle for the highest 1-butanol production (a maximal rate of 0.3g/L/d) was recently reported in engineered cyanobacteria.[83] This offers realistic opportunities for further improvement in the near future. Importantly, besides the conventional CO_2 fixation pathway of oxygenic photosynthetic organisms, there are many more efficient CO_2 assimilating pathways recently discovered in other microbes.[84] Utilization of these previously unknown catalytic principles of CO_2 assimilation will allow for the development of even more efficient synthetic routes to convert CO_2 into complex organic molecules of industrial interest.

Robust and efficient modelling, systems biology and automatization of the synthetic biology tools (encompassing the design-build-test-learn cycle) are necessary to drive both photosynthetic and heterotrophic microorganisms towards commercially profitable cell factories. The current challenge is to fuse existing information and ongoing research to generate more efficient standardized synthetic biology practices for a wide array of robust microorganisms.
For further technical details, please refer to the technical appendix.

Emerging concepts

Plants and algae use natural photosynthesis to convert light energy into energy-rich organic building blocks. While replicating the photosynthetic apparatus in artificial systems is not viable, research on natural photosynthesis reveals physical quantum phenomena that enable e.g. highly efficient light harvesting. It also provides novel design principles for developing artificial photosynthetic systems.

Bottom-up molecular engineering of bio-inspired artificial photosynthetic assemblies will be a key enabling technology in SUNRISE for developing next-generation solar-to-X energy conversion processes and systems. Breakthroughs in the development of molecular-based artificial photosynthetic systems could be accomplished by combining fundamental concepts of natural photosynthesis and by applying them onto synthetic (supra)molecular or polymeric systems, molecular materials, nanomaterials, membranes, matrices and interfaces (including molecule-nanoparticle and molecule-semiconductor electrodes). This research will be based on three guiding principles: (i) independent building blocks (ii) vibration-assisted charge separation and transport (inner coherence), and (iii) responsive matrices.

Work on molecular design of artificial photosynthesis systems will reveal new ways of function-based systems engineering of biomimetic materials hierarchies with active cofactors incorporated in molecular units (such as the recently developed quantasomes) and extend the "quantum design" principles from natural photosynthesis to synthetic systems of considerably higher efficiency and stability. This research, together with developing new molecular materials, will lead to next-generation artificial photosynthesis technology to be developed in the SUNRISE project. Some of its aspects will have an impact beyond SUNRISE, e.g. in quantum technologies.
For further technical details, please refer to the technical appendix.

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[82] P. South et al. (2019) Synthetic glycolate metabolism pathways stimulate crop growth and productivity in the field, Science 363, eaat9077

[83] X. Liu et al. (2019) Modular engineering for efficient photosynthetic biosynthesis of 1-butanol from CO_2 in cyanobacteria. *Energy Environ Sci* DOI: 10.1039/C9EE01214A

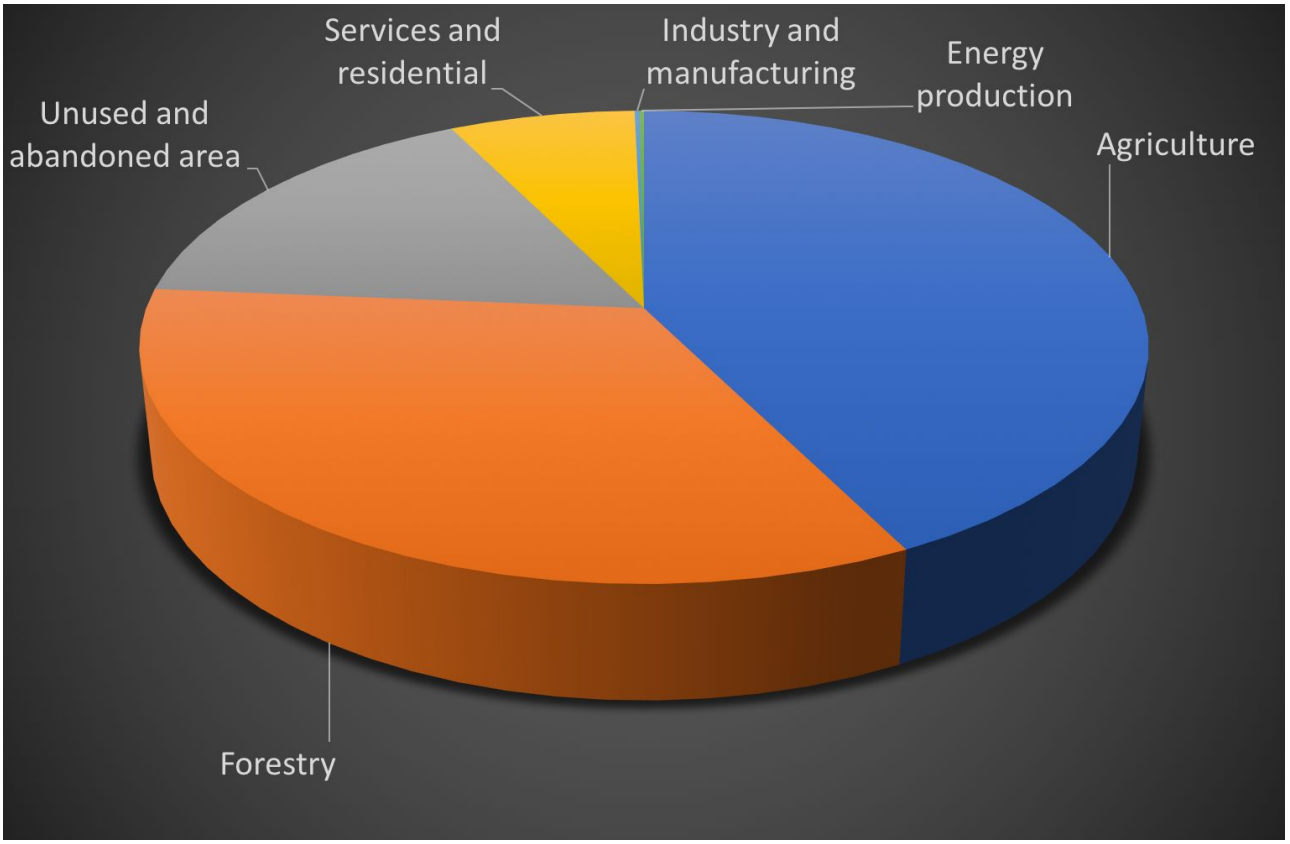
[84] T. Erb (2011) Carboxylases in Natural and Synthetic Microbial Pathways, *Appl Environ Microbiol* 8466-8477

Needed Resources and enablers beyond the scope of Sunrise

Social and environmental impact

Land use

The European soil is one of the most intensively exploited in the world. With up to 80%, Europe has the highest proportion of land used for settlement, production systems (in particular agriculture and forestry) and infrastructure (European Energy Agency - Land use). Agriculture is the most common primary land use category in the EU-28, followed by forestry, unused and abandoned land, and services residential. Only a small portion is dedicated to energy production and industry/manufacturing. **The deployment of any new technology should carefully consider the additional land use demands in this context.**



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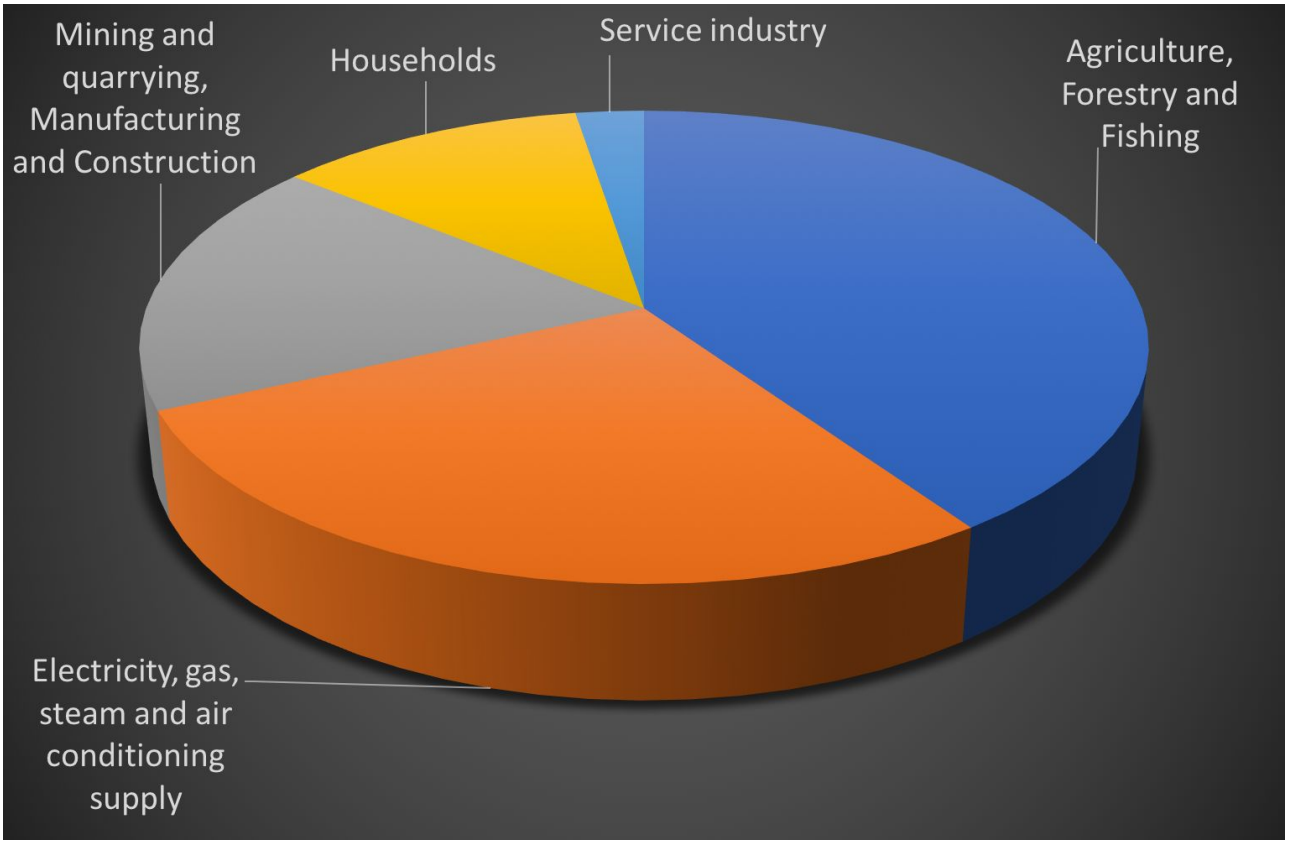
Agriculture has the highest land use (41%, ca. 1 800 000 km^2), followed by areas used primarily for forestry (33%, 1 400 000 km^2), services and residential (7%, 295 000 km^2), along with unused or abandoned land (16%, 690 000 km^2), data from EUROSTAT - land use statistics. About 7 000 km^2 are dedicated to energy production and 7 700 km^2 to industry/manufacturing, 0.16% and 0.17% respectively.

Freshwater demand

Freshwater represents another precious resource. Water is essential for life, it is an indispensable resource for the economy and plays a fundamental role in the climate regulation cycle. The management and protection of water resources is one of the cornerstones of environmental protection. Water is provided either by public water supply (public or private systems with public access) or is self-supplied (for example, private drills). In Europe, around 223 000 megatons of water were abstracted in 2015 as off-stream to meet the demand of the European economy, 90 000 megatons were used and 142 000 megatons were returned back to the environment with a certain level of physical or chemical deterioration.



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Around 40% of total water use is accounted for by agriculture, forestry and fishing (38 000 Mt), followed by 28% (26 000 Mt) for electricity, gas, stream and air conditioning, and for mining and manufacturing (17 000 Mt, 18%). Public water supplies mounts to 14% (12 500 Mt), accounting for households (11.6%, 11 000 Mt) and service industry (2.6%, 2 400 Mt); European Energy Agency - Water use.

SUNRISE: estimated impact on land use and freshwater demand

SUNRISE targets the production of fuels and carbon-based chemicals, using abundant molecules as feedstocks (e.g., H_2O, CO_2, N_2) and sunlight as the primary energy source. As an example of how the SUNRISE technology would impact on the freshwater and land use scenario, the paradigmatic case of hydrogen is considered: its production, as envisaged by the SUNRISE vision, requires the highest freshwater demand among the targeted molecules.

Nowadays, the global hydrogen demand is around 70 Mt/y, which is almost entirely obtained from fossil fuels (ca. 76% from natural gas, 23% from coal) and <2% from water electrolysis. As a consequence, **the global production of hydrogen generates about 830 Mt/y of CO_2 emissions**, slightly lower than the total CO_2 emissions of Germany in 2015 (930 Mt/y). For comparison, EU-28 emits about 4 500 Mt_{CO2}/y. Assuming that the total current hydrogen demand is supplied through water electrolysis (using water as feedstock), this would result in an annual electricity demand of about 3 700 TWh and a freshwater requirement of about 630 Mt_{H2O}/y. This is roughly one third of the current European freshwater use by the service industry (2 400 Mt/y), and 0.7% of the EU-28 annual global consumption. **If we consider that the hydrogen demand of Europe is about 15% of the global demand, it is evident that the electrolytic production of molecular hydrogen will not significantly impact on the availability of freshwater.** On the other hand, **if the electricity needs were provided by PV, it would require the deployment of 22 500 km^2, roughly corresponding to the surface of Slovenia (20 273 Km^2) or ⅔ of Belgium (30 528 km^2).**[85]

The situation is different when considering the **direct solar conversion of fuels and chemicals using photo(electro)chemical cells** as proposed by SUNRISE. Here, a yearly production of hydrogen of 52-130 tons/ha (average 90 tons/ha) is targeted. Based on this, a land use of <8000 km^2 (corresponding to a surface with a radius of 50 km) can be envisaged for the production of 70 Mt_{H2}. **Although this surface represent <0.2% of the total land use in Europe, it compares to that presently devoted to energy production and industry/ manufacturing, but is still much smaller than service & residential (see above). The aspect of land area has to be carefully taken into account, since it can potentially limit the deployment of SUNRISE technologies. A way not to limit SUNRISE technologies and to increase their social relevance resides in the development of decentralized devices deployed in urban or agricultural environments, meeting the needs of the inhabitants.**

The estimated environmental impact, in terms of land usage and freshwater demand, of the SUNRISE associated technologies is summarized in the table below, where the global annual production of the relevant product is taken into account. The European demand represents a fraction of these values.

Impact of SUNRISE technology on the environmental resources

	Today global production [a] [Mt / y]	Production potential [b] [tons ha^{-1} y^{-1}]	Land use [km^2][86]	Freshwater use [c] [Mt / y]
Hydrogen	70	52 - 130	13 500 - 5 400	630
Formic Acid	< 1	1 182 - 2 956	8 - 3	< 0.5
Formaldehyde	52	386 - 964	1 350 - 540	30
Methanol	75	274 - 686	2 700 - 1 100	85
Ethanol	95	197 - 494	4 800 - 1 900	110
Ammonia	176	308 - 772	5 700 - 2 300	280

[85] Considering an average PV output in Europe of 1 100 KWh/y per KWp and an average power density of 150 Wp/m^2 per PV panel;

[86] Land use is calculated following this example: for a production potential of, e.g., 52 ton/ha/y and an annual demand of 70 Mton/y, one needs a surface of (70000 / 52) ha of land.

[a] Hydrogen data from *IEA Hydrogen*; Formic acid data from *ULLMANN's Encyclopedia of Industrial Chemistry*; Formaldehyde data from *Merchant Research & Consulting ltd* (https://mcgroup.co.uk); Methanol data from *The Methanol Institute* (https://www.methanol.org); Ethanol data from *OECD-FAO AGRICULTURAL OUTLOOK 2018-2027*; Ammonia data from *World fertilizer trends and outlook to 2018*, FAO-UN. [b] Estimates for chemicals production are obtained under the following assumptions: (a) systems absorbing 90% of the photons and converting 80% into products (SUNRISE target); (b) two photons per electron transfer; and (c) maxima and minima based on average annual solar irradiation in Malaga (Spain) and Stockholm (Sweden), respectively. [c] Net usage, since some reactions considered by SUNRISE use hydrogen as a feedstock, obtained from water electrolysis, and produce water as product.

Overall, the impact on freshwater availability of SUNRISE is expected to be minimal (thus sustainable). However, depending on the local situation, it can become important to be able to use waste water or water vapor from the atmosphere. Therefore this sustainability criterion has been considered in the technological targets for the proposed approaches.
On the contrary, land use could be a key criterion and must be carefully assessed. From this side, actions should be put in place in order to increase the social adaptability of SUNRISE-based technologies. SUNRISE technologies target a ten to hundred times smaller land use than current bioenergy: the local deployment must be thought through wisely together with pertained communities. Since CAPEX is a major hurdle to overcome, co-culturing for reaping the benefits of high economic efficiency in urban and rural zones cannot be excluded.

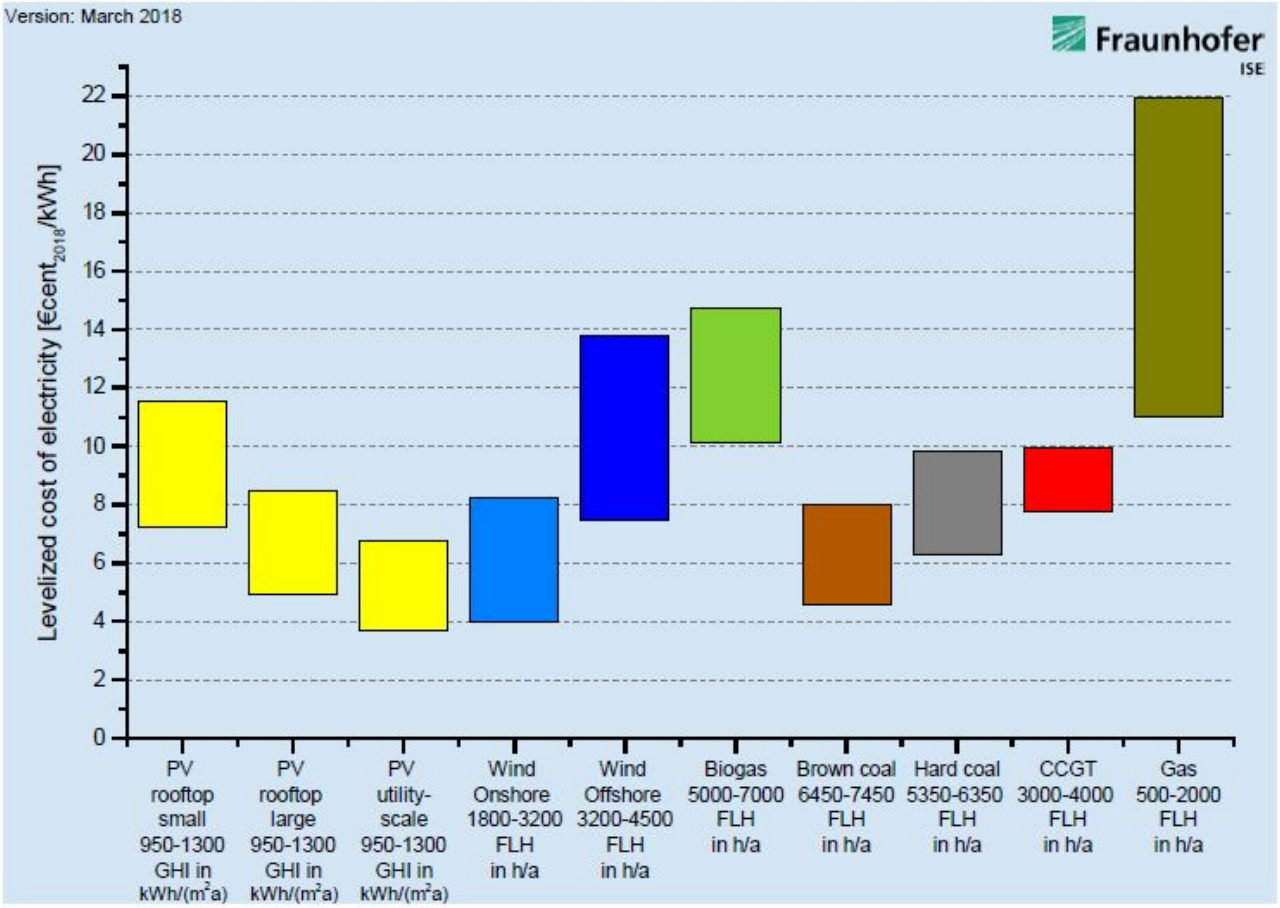
Green electricity

The share of renewables in the production of electricity is increasing at a constant rate. DNV-GL estimates that renewables will ultimately dominate the electricity production (photovoltaics, onshore wind, hydropower, and offshore wind, in the given order). Already mainstream today in many countries, these renewable energy sources will together account for 85% of the global electricity production in 2050.[87]

At the same time, the levelized cost of electricity achieved by those technologies (<22 €/MWh in 2018) already competes with the current price of production from fossil resources and will continue to decrease.[88] Depending on the location and weather conditions, this situation is already achieved, even in Europe.[89] This clearly emphasizes the need for efficient storage solutions to compensate production intermittency. SUNRISE technologies provide a promising way to chemically store intermittent renewable surplus energy on the medium and long term. Storage in chemical energy carriers complements the short-term storage provided by battery technologies and enables a loss-free long distance transport of energy using the already existing infrastructure of fossil fuels.
For SUNRISE technologies, the question arises if there will be enough renewable electricity to drive the proposed electrolyzer approaches. PV is the renewable energy growing at the fastest rate with wind being complementary in supply timing. Again, the case of hydrogen can serve as a valuable example. As stated above, today'sglobal hydrogen production through water electrolysis would result in an annual electricity demand of about 3 700 TWh. This is about 15% of the global

[87] DNV-GL "RENEWABLES, POWER AND ENERGY USE FORECAST TO 2050" Energy Transition Outlook (2017).
[88] IRENA "The Power to Change: Solar and Wind Cost Reduction Potential to 2025" (2016).
[89] C. KOST *et al.* "LEVELIZED COST OF ELECTRICITY RENEWABLE ENERGY TECHNOLOGIES", Fraunhofer Institute For Solar Energy Systems ISE, March 2018. (link)

annual electricity production (ca. 25 000 TWh), and more than the annual EU-28 production (3 100 TWh). If this energy would have to be generated entirely by PV, the installed power demand would be 3 400 GW, that is almost 7 times the global installed PV power at the end of 2018.[90] **Thus, the production capacity of the photovoltaics-driven electrolyzer approach will be severely limited by the availability of installed PV power. The SUNRISE approach based on direct conversion using photo(electro)chemical cells and ultimately photocatalysis can overcome these limitations.**



Levelized cost of electricity (LCOE) of renewable energy technologies and conventional power plants at locations in Germany in 2018. The value under the technology refers in the case of PV to the global horizontal irradiance (GHI) in kWh/(m²a), for the other technologies to the annual full load hours (FLH). Specific investments are taken into account with a minimum and maximum value for each technology. Ref.: C. KOST *et al.* "LEVELIZED COST OF ELECTRICITY RENEWABLE ENERGY TECHNOLOGIES", Fraunhofer Institute For Solar Energy Systems ISE, March 2018 (link).

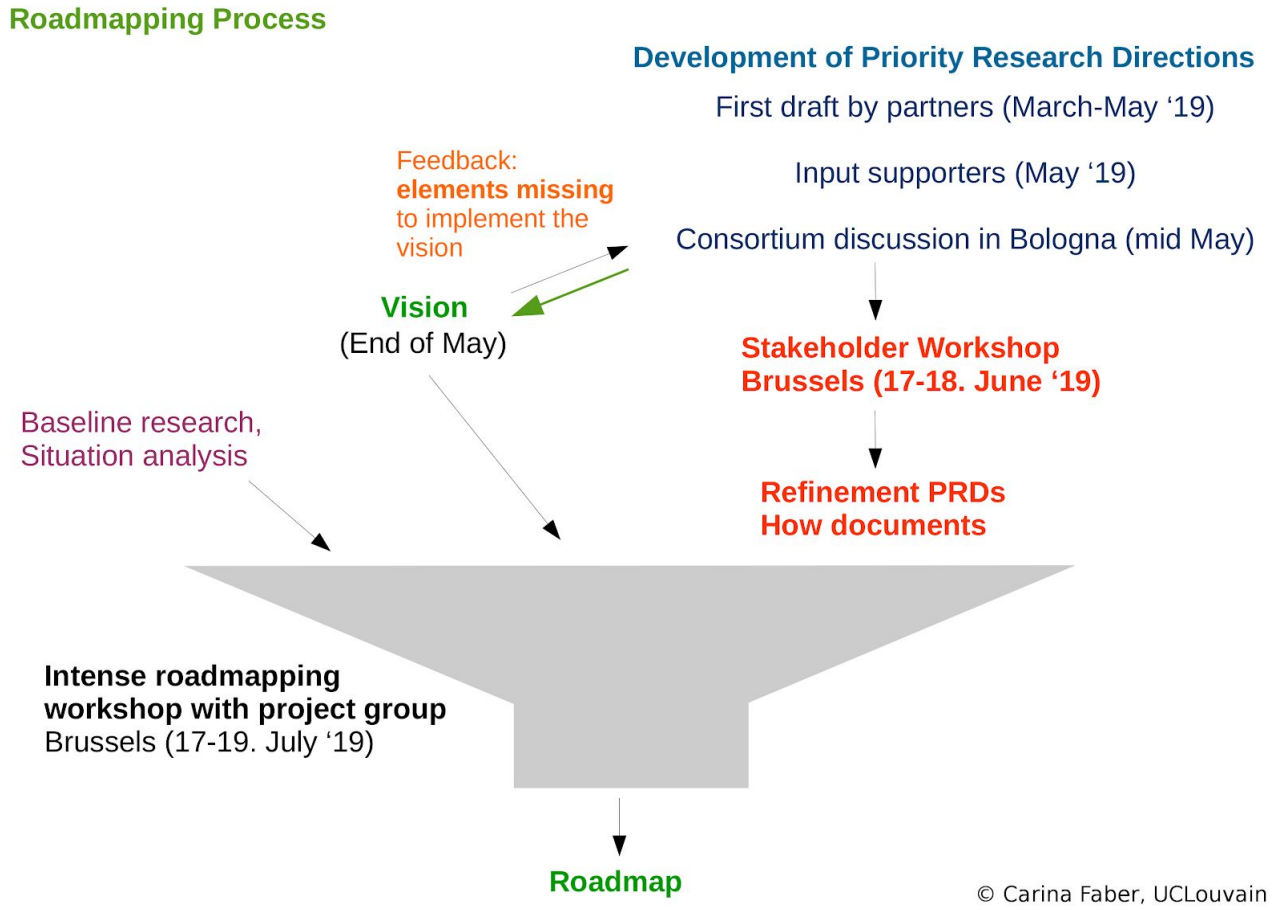
Supply chain optimization

The proposed technologies create the need for a regional and temporal optimization of supply chains, since the availability of all resources can change significantly (e.g. solar irradiation, water, CO_2 sources, N_2 sources and possibly O_2 sources). These decentralized solutions have thus to be coupled with electric and gas grid infrastructures on a wider scale to guarantee production security and higher efficiency in supply chains. In the future, networks of diverse energy carriers and material resources have to couple together to optimize consumption.

[90] REN21 Report, 2019

SUNRISE roadmapping process

This technological roadmap is developed drawing on analysis and expert judgement to define the **activities, priorities and timelines required to reach the SUNRISE vision**. It has been elaborated by the SUNRISE consortium, involving the entire SUNRISE stakeholder community. It addresses European policy makers and stakeholders from research and industry. It is conceived as a basis which will be extended later on. In particular the solar fuel topic shall be consolidated at the international level by the collaboration with Mission Innovation Challenge on Solar Fuels (Innovation Challenge 5).[91] As it is the nature of a roadmap, it is not a final document, but a dynamic process revisiting the set targets on a regular basis. It is a structured visual framework to understand dependencies and manage complexity.



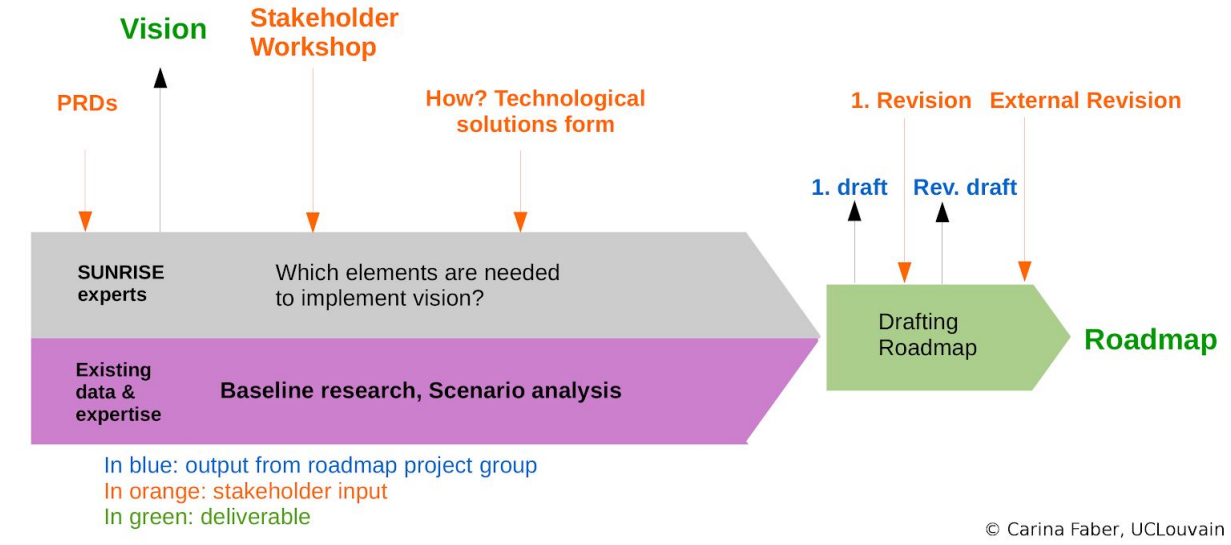
The roadmapping process identifies which technological elements are crucial to reach the SUNRISE vision. The latter has been established starting from the so-called Priority Research Directions (PRDs),[92] drafted by the SUNRISE partners from March to May 2019 and extended later on by the SUNRISE stakeholder community. Our ambition is to have a **consensus-based document** resulting from intense discussions between partners, stakeholders and policy makers.

[91] A common workshop is already scheduled for October 2019.
[92] https://sunriseaction.com/category/prd/

This is especially important in view of the lack of direct high-level political support and the missing prospect of a large-scale funding to implement the elaborated roadmap.
It is the creation of the roadmap where real insights lie, through discussions and the structuring of ideas. The roadmapping process included a dedicated workshop taking place on the second day of the general SUNRISE stakeholder workshop (17-18. June, Royal Academy of Science, Brussels).[93] This was followed by an intense 3-days workshop of the roadmapping project team.

Boundaries: from 2020 to 2050, in line with the European Commission's Climate Strategy for a Zero-carbon Europe in 2050
Scope: Artificial photosynthesis technologies, including electrochemical conversion for the short-term, photo(electro)chemical conversion and biological approaches for the mid- to long-term; biomass-based approaches are excluded because of the elevated demand for available land surface;

Process and involvement



Stakeholder roadmapping workshop

The SUNRISE stakeholder event in Brussels has been an important opportunity for mining completely new approaches and ideas among the 170 participants. Two hours of this general ramp-up meeting of the project had been dedicated to roadmapping. After a short general introduction into the roadmapping process, the plenum has been asked to split into three groups as regards content: Hydrogen and ammonia, CO_2 capture and electrochemical conversion, and Direct conversion via bio-, biohybrid- and integrated photo(electro)chemical cells.
The first hour of the workshop was dedicated to a **landscaping exercise**. In small groups of around 10-15 people, the goal was to develop coherent storylines including major technological milestones to reach the vision (with discussion leaders from the SUNRISE partners). For this, the

[93] https://sunriseaction.com/if-you-missed-sunrise-stakeholder-workshop/

following questions served as a guideline, with the obligation to follow a timeline and to give quantified targets:

Drivers & Trends: *Why do we need to act? What is the need?*

Example: in 2050, carbon-neutral Europe

Abstract solution: *What can we do? What do we want to deliver to reach the vision?*

Example: Carbon-free ammonia production by 2030

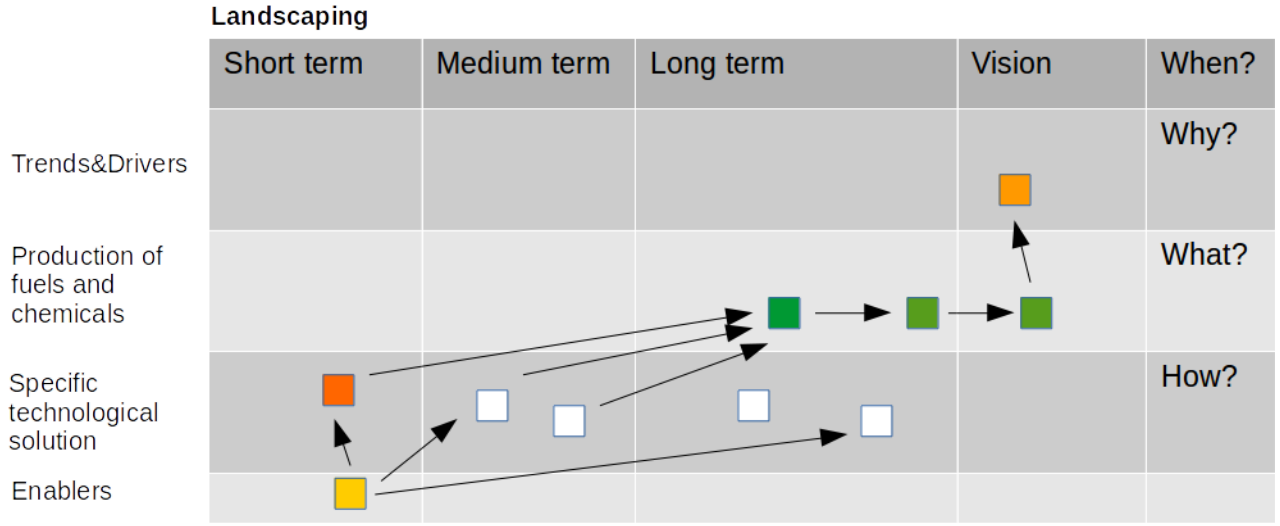
Concrete technological Solution: *How can we do it?*

Example: Low-carbon Haber-Bosch process at ambient temperature and pressure

Enablers: *What are the enablers? Which resources are needed?*

On the technological level, but also political (legislation), societal (acceptance), ..

After free brainstorming, similar ideas have been clustered and narratives leading to the vision have been created.



The second part was dedicated to **topic roadmapping**: groups of 2-3 people have been asked to choose one particular technological solution (how?) that needs to be unpacked to explore its potential. The goal was to articulate the *vision and potential application*, as well as the *current status and state-of-the-art*. Most importantly, a set of *deliverables* that provide a series of stepping stones from the current state to the future application/vision had to be defined, including an associated time dimension. Participants have also been asked to note their key learning points during this exercise and to provide a summary narrative of the technology using a Narrative Feedback template.

The postprocessing of the workshop results consisted in an in-depth analysis of the collected stakeholder input in the form of landscaping and topic roadmapping exercises and narrative feedback documents by the project leader. In general, various solutions for hydrogen production technologies have been provided, whereas a lack of input for CO_2 conversion via photo(electro)chemical approaches can be stated. The quality of the results was extremely varying from one working group to the other, sometimes missing a coherent storyline. However, one has to keep in mind that it has been a complex task for the groups to channel widespread ideas into common vision, given the very limited amount of time and the inhomogeneity of participants. In

our opinion, this roadmapping exercise has been a rich experience and we state a fruitful exchange of knowledge and ideas among different communities. We are confident that it contributed to reach consensus and to strengthen the SUNRISE goals. The received feedback was very positive and the provided contact list helped to further exchange with those interested in continuing the exercise.

The detailed analysis resulted in:

* the **mind map** (see chapter “SUNRISE vision”)
* a rich **basis for milestones and technological targets** (see chapter “SUNRISE roadmap”)
* the development of standardized technological solutions forms (so-called **How-documents**, see subsequent chapter).

SUNRISE stakeholder event (17.-18.06.2019, Brussels), roadmapping workshop.

Roadmapping workshop for the project team

During three days (17-19 July 2019), the project team met in the EERA premises in Brussels for an intense roadmapping workshop. This small group (14 people) mirrored the SUNRISE community with senior researchers for all three technological approaches and representatives from Siemens, Engie, Johnson Matthey and EMIRI. As workshop preparation, the PRD leaders had been asked beforehand to transfer and complete the content of the PRD they are responsible for into multiple How-documents. They have been free to engage experts outside the consortium and stakeholders. The PRDs are in general on the "what?"-level, containing diverse technological solutions and thus necessitating several How-documents (e.g. PRD "Sustainable hydrogen production" contains among others PV+electrolysis and bio-molecular PEC with quite different milestones and targets). This was an important step in order to obtain a collection of data and content as complete as possible. It represented an agreed-on basis the roadmapping team could efficiently analyze, filter and structure into a coherent roadmap.
The workshop followed a tight schedule: after a short introduction to the roadmapping process and the applied tools by the project leader, the team finalized the mind mapping. How-documents were analyzed, discussed and completed, missing elements and weak points identified. A thorough landscaping on hydrogen, ammonia, carbon-based fuels and chemicals, and CO_2 capture has been carried out in the plenum and later on in small experts groups, respectively. Moreover, the scenario analysis to estimate the future state and a STEEPLE[94] exercise for the current context have been initiated. This fruitful work has been continued afterwards via several virtual meetings in August and beginning of September for the actual drafting of the roadmap.

Revision

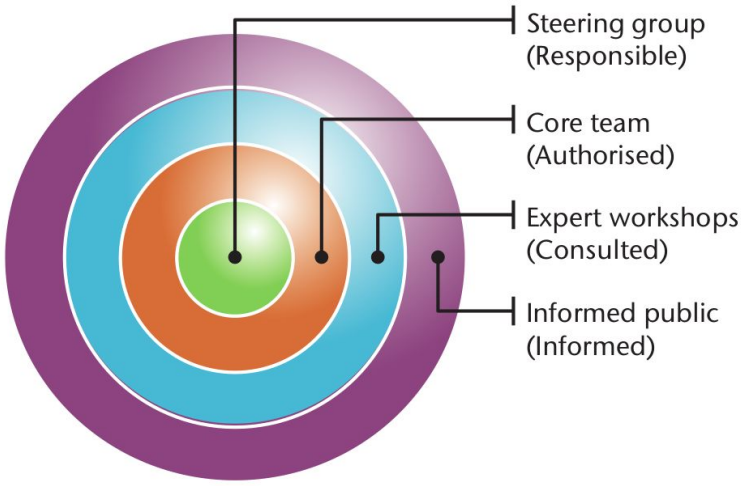
The first draft of the roadmap is revised by the SUNRISE managing board and the Quality and Impact Assurance team. Afterwards, an external review is planned based on a close-to-final document, by a group not having been involved so far (e.g. the SUNRISE advisory board).

Types of organisations and individuals participating

From the SUNRISE proposal it follows that UCLouvain coordinates the task, involving companies (Siemens, Engie, Johnson Matthey), research and technology organisations (CEA, Fraunhofer, Forschungszentrum Jülich) and associations (EMIRI, EERA) with consolidated experience in preparing scientific and industrial roadmaps. In addition, CNR is involved as leader of the entire work package. The University of Uppsala, Imperial College and the University of Warsaw volunteered to join forces given their involvement in Mission Innovation and their leading role in the SUNRISE Quality and Impact Assurance team, respectively. ICIQ is of precious help for the scenario analyses and dissemination activities related to the roadmap. Input from the policy side is provided by DG RTD which will also insure a close link to the roadmap development within Mission Innovation. As an additional dimension, the project team covers expertise for the three SUNRISE approaches.

The roles and responsibilities of organisations and individuals have been identified using a RACI [95] chart.

[94] STEEPLE stands for: Social, Technological, Economic, Environmental, Political, Legal and Ethical
[95] Responsible, Accountable, Consulted and Informed



Stakeholder involvement strategy following a RACI chart; taken from *Energy Technology Roadmaps, A guide to development and implementation, 2014, IEA*;

Steering group SUNRISE managing board Industry: Jan Mertens (Engie) Policy: Philippe Schild (EC, DG RTD)	This group is composed of senior representatives from policy, industry and research to assure the actual implementation.
Project team **Project leader: Carina Faber (UCLouvain)** Hervé Bercegol, Vincent Artero, Juliette Jouhet (CEA) Hélène Lepaumier, Han Huynhthi, Laurent Baraton (Engie) Max Fleischer (Siemens) Andrea Barbieri (CNR) Yagut Allahverdiyeva-Rinne (Turku University) Laura Lopez (ICIQ) Arne Roth (Fraunhofer) Anita Schneider (EERA) Robert Potter (Johnson Matthey) Leif Hammarström (Uppsala University, MI5) James Durrant (Imperial College, MI5) Marcel Meeus (EMIRI)	Core team that is actually undertaking the vast majority of the work on the roadmap; mirrors the composition of the steering group;
Consulted **SUNRISE Priority Research Direction Leaders** → lead Ann Magnuson (Uppsala University) **SUNRISE Quality and Impact Assurance Team** → lead Stefan Baumann (FZ Jülich), Joanna Kargul (Warsaw University)	This group channels the input from stakeholder experts participating in the writing of PRDs and workshops and insures the quality of the input; it typically includes expert representatives; Mandate: Attend workshops, provide reports, review roadmap drafts;
Informed SUNRISE community not actively participating.	More than 200 supporters from policy, research and industry.

Technical appendix: technologies and milestones

Separate documents

Sustainable hydrogen production

1. Large-Scale hydrogen production using PEM electrolysis
2. Hydrogen production using photoelectrochemical cell devices
3. Hydrogen via buried-junction photoelectrochemical cells
4. Hydrogen production by photosynthetic microorganisms
5. Hydrogen photoproduction by biomolecular technologies
6. Baggies with particulate systems

Sustainable ammonia production

1. Renewable Haber-Bosch process
2. Electrochemical ammonia synthesis
3. Direct photoelectrocatalytic ammonia synthesis
4. Ammonium production by photosynthetic microorganisms
5. Plasma-assisted ammonia synthesis

Sustainable carbon-based chemicals and (jet)fuel production

1. Dark electrochemical reduction of CO2 to C1/C2/C3 products
2. Electrochemical production of hydrocarbon fuels
3. Thermochemical production of hydrocarbons and jet fuels
4. Biocatalytic production of chemicals by microorganisms
5. Carbon-based fuel production by biomolecular approaches

Carbon capture technologies

1. Amine-based carbon capture
2. Polymeric membranes based carbon capture
3. Low-Temperature Direct Air Capture
4. High-Temperature Direct Air Capture

Enabling technologies

1. Computational materials modelling: from novel materials to solar fuel devices
2. Development of new methods and software tools for early quantitative sustainability assessment of emerging SUNRISE technologies: bridging environmental, economic and social impacts
3. Redesigning photosynthesis for the biocatalytic production of chemicals and fuels
4. Synthetic Biology
5. Bottom-up chemical engineering of bioinspired artificial photosynthesis reactor materials and cascades
6. Upscaling artificial photosynthesis systems for a sustainable larger scale production of energy carriers
7. Oxygen evolution (Water oxidation)