Green Chemistry

PERSPECTIVE

View Article Online
View Journal | View Issue

Cite this: *Green Chem.*, 2021, **23**, 1584

Chemical energy storage enables the transformation of fossil energy systems to sustainability

Robert Schlögl[a,b]

The quest for the sustainable energy transition requires replacing fossil fuels by renewable electricity (RE). Systems of energy supply consist of both electrons and molecules as energy carriers. It is thus essential to interconvert both types of carriers. Capitalizing on the intrinsic efficiency of using electrons it is desirable to electrify in the sustainable system more end energy applications than in the fossil system being fully based upon molecular carriers. This does not eliminate the need to retain molecules as energy carriers in a substantial fraction of a whole energy system. The application "energy storage" as example compensates the volatility of RE and is thus critical to any energy transition. Chemical energy conversion (CEC) is the critical science and technology to eliminate fossil fuels, to create circular energy economies and to enable global exchange of RE. This paper describes generic structural features and dimensions of CEC.

Received 18th September 2020,
Accepted 7th December 2020

DOI: 10.1039/d0gc03171b

rsc.li/greenchem

Structure of the energy challenge

The states of Europe have ratified the Paris agreement and intend with the "Green Deal" to transform within the next 3 decades their energy systems towards carbon neutrality on a yet to be defined trajectory. In many states this is legally binding as a contribution to global climate protection. The first consequence of this is that the question is no more if this is possible but only how this can be achieved.[1] In the present debate it would be a substantial achievement if this fact would be accepted generally. Techno-economic comparisons of critical technologies needed in this trajectory should then no longer be related to the continuation of fossil options as they do no longer exist.

Another consequence is that the primary source of energy in the future will be RE. This energy is local (within the range of a power transmission grid) and volatile (incompatible with baseload requirements). It can (in contrast to the present situation) only be traded inside its grid and cannot be distributed globally and it needs to be used at the instant of its generation. This is in strong contrast[2] to the quest for a demand-driven secure supply. At present in Europe up to half of the average electrical load can be supplied by volatile RE supplemented by the other half from fossil and nuclear sources. Fig. 1 gives an illustration of the complexity of the power sector of the actual German electrical grid. The absence of a baseload structure is evident as is the critical function of import-export substituting national energy storage capacities of relevant dimensions.

On a higher integrated scale, it is not easy to see that more RE in an electrical grid will automatically reduce the CO_2 emission. Fig. 2 illustrates this for Germany. The steady increase in RE fraction is not mirrored by a steady reduction of CO_2 emission. Variable power consumption and fluctuations in the primary energy mix both strongly affected by economic boundary conditions are made responsible for this effect. The figure reveals that an energy transformation based upon subsidised influx of RE alone will not automatically defossilize the power system nor will it transform the system into a sustainable future.

The span of volatility in the power generation that has reached in Germany now about 80% of the average load (Fig. 1) indicates a technical hindrance in removing conventional power generation. The economics of these critically required installations are compromised by the rapid reduction in full load hours leading to severe conflicts with neighbouring electricity grids by import/export as well as in the regulatory and economic system. Recognizing the need to provide synthetic fuels to the combustion power industry would not only remove much of the conflict potential but could speed up the defossilization of the power sector. The important role of natural gas as an intermediate solution is not seen clearly enough by stakeholders and might soon be compromised by the emerging trend to refurbish the gas transmission system into a hydrogen transport system. These phenomena urgently call for a roadmap with a realistic timeline to avoid conflicts between energy sectors that prevent a fast and economically viable transformation of the fossil energy system with its infrastructures.

[a]*Max-Planck-Institut for Chemical Energy Conversion, Stiftstr. 34–36, 45470 Mülheim an der Ruhr, Germany*
[b]*Fritz Haber Institute of the Max Planck Society, Faradayweg 4–6, 14195 Berlin, Germany*

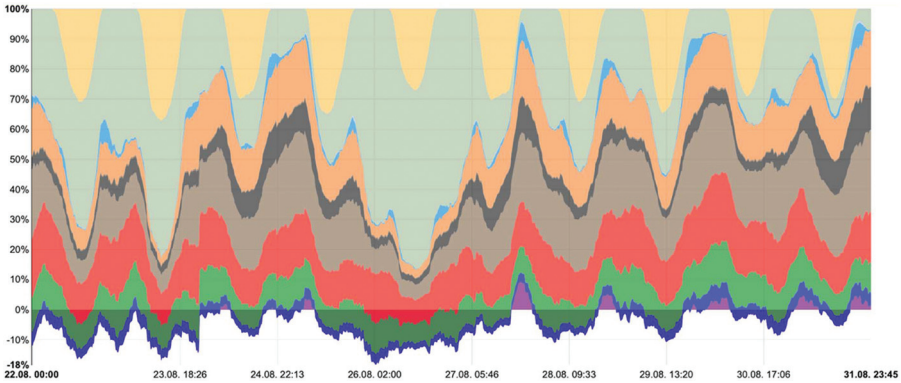

Fig. 1 Energy mix of the German power grid throughout August 2020 in fractions of the total demand. The maximum power demand was 74 GW. The negative values represent the export, the purple elements the net import of power. Colour coding: yellow solar, light green wind, light blue pumped hydro, orange gas, dark brown coal, light brown lignite, red nuclear, green biomass, dark blue hydro. (Source: Fraunhofer ISE, Energy Charts.)

The situation is complicated by the unclear definition of "sustainable energy system". Some assume that nuclear fission options are part of the trajectory whereas others do not. Others accept the pyrolysis of fossil fuels into the chemical elements hydrogen and carbon as a contribution to the transformation, despite of the finite nature of this resource. Yet others include carbon capture and storage (CCS) as emission reduction option that is opposed by many including much of the broader public.

Only few countries besides those who rely on hydroelectricity as non-volatile RE have reached 50% RE content in their electrical grids and begin to run into the challenge of maintaining supply security while continuing de-fossilization. Fig. 1 gives an illustration that the German power system could not maintain stability without a European exchange. This is not a speciality of the German system but can also be observed in other European systems. In Fig. 3 the situation of Germany is compared to that existing in Denmark. This example was chosen as it has one of the highest fractions of RES in its electricity supply. The fuels for electricity generation besides wind and solar are largely biomass-based. The data are aggregated for the first 8 month of the year 2020. The interpretation of the data from Germany is intricate as such a large system has many influences affecting the trends. The example Denmark is much smaller and relates to a more homogeneous use case allowing for detecting some clear trends. In both graphs the effect of the corona pandemic with the drop in month April is detectable when comparing the trend data to the year 2019 (not shown here).

It is obvious that Germany has reached an enormous penetration of RE into its electricity system. Surprising is the high penetration for the small country of Denmark as is the fact that its use of wind (and solar) is less than expected. In both cases the system of imports and exports is used to maintain grid stability. The multiplicity of primary energy sources in both cases leads to instability patterns being compensated on short and medium timescales by a combination of import and export simultaneously. It is worth to notice that both countries have decided to act as net exporters of electricity. The motivation for this activity is expected to be very different in view of

Robert Schlögl

Robert Schlögl was born in 1954 in Munich. He is Director at the Fritz Haber Institute of the Max Planck Society in Berlin as well as Founding Director at the Max Planck Institute for Chemical Energy Conversion in Mülheim a.d. Ruhr.

Robert Schlögl's research focuses primarily on the investigation of heterogeneous catalysts, with the aim to combine scientific with technical applicability as well as on the development of nanochemically-optimized materials for energy storage. The application of knowledge-based heterogeneous catalysis for large-scale chemical energy conversion summarizes his current research focus.

In June 2020 he has been appointed to the National Hydrogen Council (Nationale Wasserstoffrat).

He is Vice-President of the National Academy Leopoldina as well as an Honorary Professor at Technical University Berlin, at Humboldt University Berlin, at University Duisburg-Essen, at Ruhr University Bochum as well as a Distinguished Affiliated Professor at TU Munich and an Honorary Professor of Boreskov Institute of Catalysis. He is member at acatech and BBAW and other numerous international organizations, received numerous national and international awards as well as is partner in numerous European and international joint projects.

He is author/co-author of more than 1200 publications, more than 550 presentations and invited talks as well as inventor of more than 20 patent families.

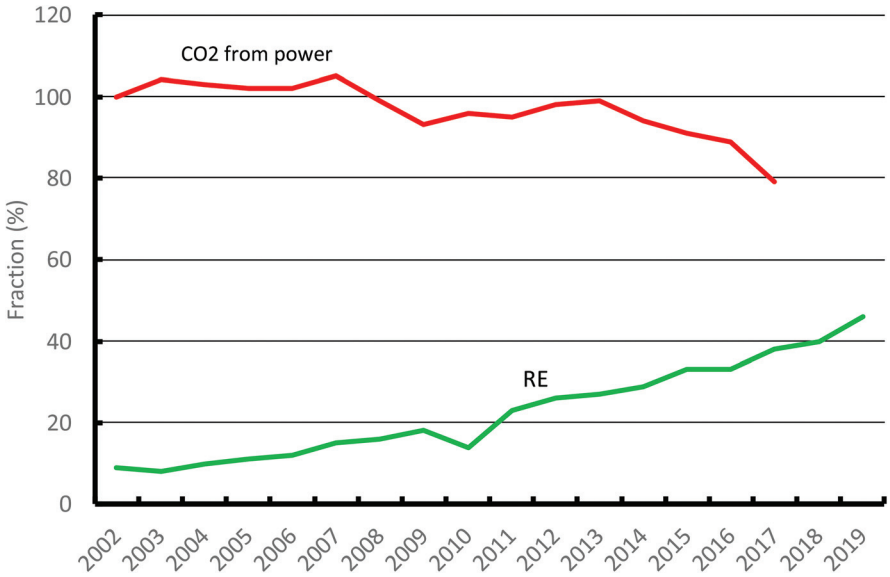

Fig. 2 Fractions of RE in the German power system (green) and change in power-related CO_2 emissions (red). The absolute CO_2 emission in 2002 was 372 Mt.

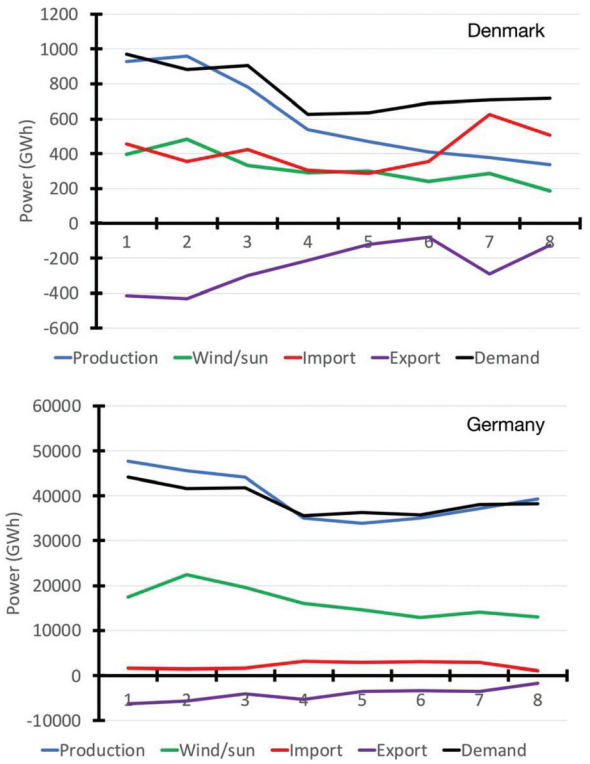

Fig. 3 Aggregated key data for the first 8 month of the year 2020 for the electricity systems of Denmark and Germany in the year 2020. Note the different ordinate scales. The green line for wind and solar indicates less than the total RE fraction in the systems, as all bio-based sources and the contributions from hydro-electricity are not shown here. The electricity export is indicated as negative values. (Data sources: https://ens.dk/en/our-services/statistics-data-key-figures-and-energy-maps/annual-and-monthly-statistics and https://energy-charts.info/charts/energy/chart.htm?l=de&c=DE.)

the availability of primary energy carriers in both countries. In short, the system of import/export options within Europe is absolutely critical to guarantee the stability of electrical supplies also with high fractions of volatile RE. No serious measures of energy storage besides smoothing short fluctuations buffered by electro-mechanical devices are needed as yet. This strategy relies on the cooperation of all countries interconnected and on the wide span of RE penetration into these grids (see *e.g.* France with high fraction of base load nuclear (Fig. 5) or Poland with high base load of coal). As the RE penetration gets larger in the high RE countries, the need for exchange gets rapidly much larger and eventually interferes with RE expansion in other countries. The only reliable countermeasure is chemical energy conversion in grid scales that is presently considered as not necessary as it is expensive and inefficient. The arguments here show that chemical technologies in energy storage will be needed in the longer run to allow eventually a deep defossilisation of the European energy systems and in this way to make the Green Deal. In addition, no country has started to use bulk amounts of RE in traditional non-electrical sectors of their energy systems that are together larger than the power sector. This "sector coupling" cannot happen without converting RE into chemical energy carriers.

Much of the discussion about energy transformation revolves around defossilizing the power sector by RE and a component for flexibilization being either gas power stations or nuclear fission or biomass combustion or a combination thereof. In such scenarios the storage of RE is of secondary relevance. Batteries are used as short-term buffers and pumped hydro installations as day-to-day storage options. The need for bulk amounts of RE for CEC conversion is negated on grounds of inefficiency and high specific cost of electricity gen-

erated from fuels made through CEC. This option is only advertised when high values of above 80% defossilization[3] of the power sector are considered.

There is quite a reluctance to accept that CEC or energy storage[4] is a relevant option besides carbon capture and storage (CCS). The origins of this conjecture are general efficiency arguments and the diffuse idea that sustainable energy systems should be largely electrical with a residue of below 30% molecular energy storage stemming predominantly from biomass and fossil sources. Efficiency is indeed a highly important factor when the dimension of energy systems is considered. It is however the efficiency of an element (technology) for the functioning of the whole system that counts most. Chemical energy conversion is indispensable for storage and transportation of RE across the whole system. It is thus the systemic efficiency across all services of energy that must be judged for an energy system and not only the process efficiency that is inevitably reduced when more conversion steps are necessary for reaching a certain function. The process efficiency is in competition to the path dependence of a technology: if a given task can be reached with low path dependence (no new infrastructure or large additional investments) a reduced process efficiency may be acceptable at least as transitory step in the multi-decade transformation of an energy system. These aspects reduce the relevance of the fact that round trip efficiencies of RE *via* chemical fuels for power generation or mobility are at the order of 20% of the initial RE.

It is argued that chemical energy storage and the relevance of chemical research into these issues are of minor relevance and contribute only niche solutions to the sustainable energy systems. The needs of the material-based industries[5] (steel, cement, glass, chemicals) are not considered in such views at all on grounds of their relatively small contribution to the size of the energy system. If there is a role for CEC, then electrochemical storage through the HCl electrolysis/synthesis are considered, for efficiency arguments[6] plain water splitting into hydrogen and oxygen is less favoured. This process, that powers the energy cycle of nature, will in the author's view have to play a decisive role in generating the hydrogen needed for technical energy systems. There are other options such as dehydrogenation of hydrocarbon molecules (ΔG_0 70 kJ mol^{-1} for methane) and biological synthesis pathways which may play some role in the future but cannot replace the energy-intense (ΔG_0 286 kJ mol^{-1}) water splitting through electrolysis or photo(electro)chemical activation.

A generic scheme of such an energy system is shown in Fig. 4. It is noted that Germany did start with its "*Energiewende*" in this concept and realizes only now that this may be inadequate with respect to the enormous additional installations of solar and wind devices required.

The elements "chemicals" and "unavoidable CO_2 emissions" (*e.g.* cement, lime) remain outside of the system.

Fig. 5 illustrates for Germany and France, two countries with similar sizes but different structures of their energy systems, how far the transformation was progressing over the last 15 years. Two of the large economies in Europe show a surprisingly parallel evolution of their energy consumption although their economic activities differ significantly. For France there was little change in RE penetration owing to its high fraction of nuclear fission energy. In Germany some reduction of primary energy consumption and a substantial growth of the RE supply mainly as electricity resulted in a significant transformation of the system without, however, reducing the total energy consumption. Some sizeable contributions to the renewable fraction like biomass and hydro-electricity cannot be scaled further. The burden on the solar and wind contributions thus will become larger for reaching the climate targets set in the Green Deal. In addition, as RE is increasing, the volatility challenge increases with the need to enter into the molecular storage regime that is much less energy-efficient than the direct use of RE with its low conversion losses. This factor substantially increases the demand for primary energy even further. It becomes clear that some significant additional element has to be brought into action if the target of carbon neutrality shall be reached within the next 3 decades.

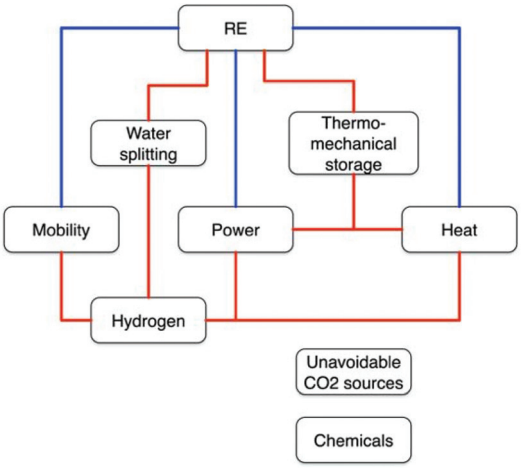

Fig. 4 A generic energy scheme with minimal energy storage. Blue lines indicate immediate use of RE, red lines use storage options for compensating volatility.

This additional element is the global exchange of RE. It is one critical task of CEC to convert free electrons in molecules[7] that are sufficiently similar to fossil oil and gas in order to provide the technological option for the continuation of using the infrastructure and application devices existing today. The main function of synthetic fuels and CEC is to make RE into a global commodity that can be exchanged in bulk amounts between areas of excess RE and highly demanding regions with limited local production capacity. Transport of RE in molecules rather than in free electrons is effective[8] and can use existing pipeline/shipping infrastructures that are operating today on fossil energy carriers.

Self-sufficiency within the reach of a transmission grid system is the basic concept of energy systems based upon RE only as indicated in Fig. 4. The electrification of energy applications through RE carries substantial advantages in efficiency

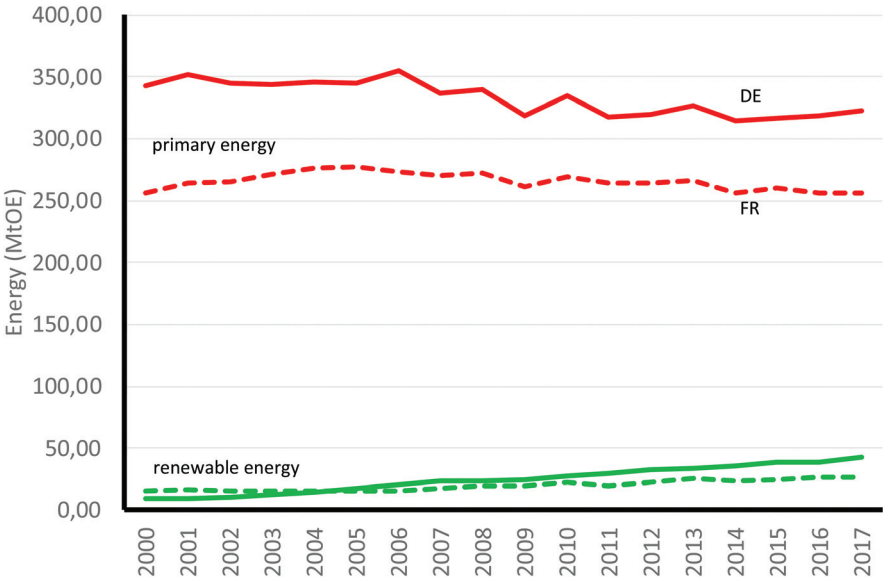

Fig. 5 Consumption of primary energy for two European countries (DE, FR) (red) and fractions of RE thereof (green). (Source EU energy statistics country data sheets edition 2019.)

as the conversion losses between primary energy fuels and end energy (today about 37% in Europe) disappear and reduce the size of the energy system by that number. In areas of the world where the energy system infrastructure is still growing or needs re-design, the "all-electrical" option is a distinct possibility. A pre-requisite is the availability of storage and flexibility options in these energy systems compensating the volatility of RE. Such compensation is possible with CEC (as water splitting to hydrogen and its re-conversion into electricity). See Fig. 4 for a generic layout of such a system.

If, however, part of the energy system is already in molecular carriers it is hard to understand why applications that operate facile with molecular carriers should be electrified enhancing the burden on the electrical system. The faster and less expensive path is to consider energy transformations using as much as possible the elements of the existing energy system and replace the fossil primary energy sources by sustainable ones. Then a global trade of molecular energy carriers made from RE is mandatory. Local RE is an additive and stabilizing factor in a given energy system but the majority of its needs will come from global trading. Energy storage disappears as a major issue in this view and merges into the challenge to convert large amounts (up to 80% of the global RE demand) into sustainable fuels. Fig. 6 illustrates such a generic mixed local-remote[9] energy system.

The RE is generated at spots on the planet where maximum capacity factors of combined wind and PV installations can be expected.[8] Capacity factors of 0.5 and above are possible in extreme locations where human life is difficult. The combined capacity factor for Germany is 0.17, within Europe values up to 0.35 have been observed. Please note that these values are not constant but vary with time and exact location as both climate and weather are determining factors. At the highly productive

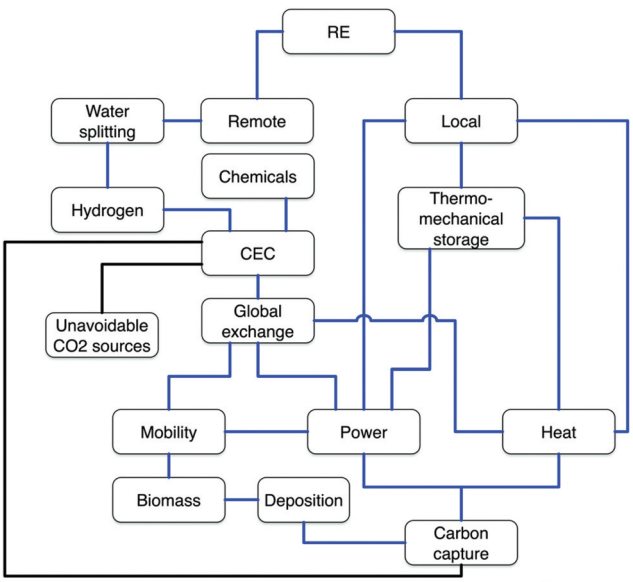

Fig. 6 A generic energy system with global exchange of RE. The black lines indicate how carbon for synthetic fuels is fed into the chemical energy conversion processes (CEC) without using fossil carbon sources. "Deposition" stands for formation and storage of solid carbon (or minerals) for long-term immobilization of carbon under full control. All essential elements of the system are now interconnected (compare to Fig. 4).

locations RE is converted first to hydrogen and then to a transport form of a synthetic fuel[10] allowing global trading. In this way fossil oil and gas are replaced by renewable oil and gas or as stated by "green oil and green gas".[8,11] Examples of such fuels are synthetic diesel, "C1 fuels", ammonia, synthetic

methane, LOHC or methanol.[12] Particular attention is needed for the mobility sector where synthetic fuels create "leaks" of significant dimensions in the circular use of carbon. They may be acceptable for some time in which fossil fuels are replaced by synthetic ones but must not be "removed" by double counting[13] of CO_2 utilization. Eventually they need closure with measures exemplified in Fig. 6. The data in Tables 2 and 3 support the delayed attention to this issue with respect to priorities in other energy sectors.

The local RE generation will be supported by CEC[14] as a flexibility measure in limited scales depending on the local capacity factor and on the extent of RE penetration into the energy system. Viewing the development from the target of maximal defossilization it may be expected that in Germany up to 20% of the RE production is used for chemical energy conversion, mainly for hydrogen production.[3] A good number for the dimension is 10 GW electrolysis capacity in Germany. It must be stated that this is by no means the demand in chemical energy fuels but rather indicates the contribution for local (national) generation. Energy storage is effectively also performed as mechanical and thermal storage[15] that will, however, not be considered here despite its clear technological and cost advantages, as they are always local and of limited volume compared to the potential of global RE exchange.

It occurs that the initiated energy transition with installing local RE systems[16] and gradually decommissioning fossil power plants is one part of the solution. The concept of remote RE and its CEC[7] followed by transport and utilization in densely populated areas is the critical second part of trajectories into sustainable systems. It is fair to say that energy storage into "green fuels"[17] represents an indispensable component for sustainable energy systems. It is not a final small addition as thought earlier but it is likely to carry a main fraction of the burden in defossilization. It is prerequisite that the primary converters of sunlight into RE (PV, CSP, wind) keep developing in scale[18] and reliability as in the past. The announcement of much more effective PV systems[19] in combination with converters enhancing the capacity factor coming into scalable application[12a,20] within this decade allows expecting that the conversion of RE into hydrogen will be able in suitably large dimensions at cost competitive for a global energy exchange.

Estimating the price of green gas is difficult as the technology in the form of a working supply chain does not exist yet in any scaled dimension. The critical regulatory framework determining to a large extent the final price of energy is also not existing yet. Hence the cost estimates are rather theoretical. The fact that the world and in a leading role Europe have decided to go ahead with the RE approach for defossilization makes discussion about this point less relevant: one is in search for the most cost-effective way to bring large amounts of chemically stored RE into a global trade and exchange situation. The extra cost for this is within the dimension of the difference between cost and price for the current energy carriers. The price of RE within the scalable scheme indicated in Fig. 6 for the energy user is to a large extent dependent on non-technical factors. Science and technology can reduce within limits the cost by optimizing the scalable technologies for the interconversion processes that require all interfacial chemical transformations driven by renewable heat or renewable electricity.

Dimension of energy storage

The dimension of the supply of green fuels can be estimated by the dimension of the existing fossil energy system minus the local generation corrected for possible efficiency effects by exchanging fossil with green fuels. This estimate is not simple as multiple scenarios may be followed. It is not the purpose of this work to discuss such scenarios as they contain multiple and difficult-to-validate assumptions. One critical value of such scenarios is to illustrate[3,21] how the various elements of an energy system can be combined in different quantities to arrive at similar defossilization for quite different investments. In this work the dimension of energy storage and transport in relation to a possible local RE supply in Germany shall be given. The sheer numbers for Europe imply that great care is needed not to underestimate the size of the undertaking, its time and capital requirements and audacity to start such an operation. The following figures are intended to highlight some trends.

The most general estimate is that green fuels replace fossil fuels with the equivalent final energy content. If one takes the energy equivalent of the global oil and global gas industry one gets an impression about dimensions. Relevant numbers for the world energy system of 2017 are taken from the BP world energy statistics and collected in Table 1.

The fraction of RE from biomass wind and sun is with roughly 3% still small when the target of complete elimination of fossil energy within 3 decades is considered. The situation in different parts of the world is quite different with respect to the dynamics of share of energy carriers and total consumption. In Asia the dynamics is enormous whereas in EU (28) the evolution is rather static. In Table 2 the breakdown of primary energy use is shown for Europe representing 13% of the global primary energy system.

In order to develop an impression of the dimensions of green energy storage the following quantitative framework shall be used. A circular economy of carbon is assumed to be based upon the couple of methanol[22] combustion and CO_2

Table 1 Global dimension of the use of energy carriers

Energy carrier	Value (TWh)
Total primary energy	156 702
- Oil	53 579
- Coal	43 240
- Gas	36 541
- Hydropower	10 700
- Nuclear	6943
- RES	5699

hydrogenation with electrolytic water splitting all based upon RE. Existing technologies[23] allow to produce MeOH with an energy investment of 10 MW h_e t^{-1}. The heating value of this MeOH is 5.5 MW h_{th} t^{-1}. In a modern power installation without waste heat use 2.2 MW h_e t^{-1} are recovered. An average efficiency loss of 80% for a cycle RE-CEC-RE is a plausible figure for dimensional estimates. From these numbers it follows that storage of 1 TWh electrical energy require 450 kt of MeOH for which one has to invest 4.5 TWh_e in RE. The units in Tables 1 and 2 multiplied by 0.5 give the number of megatons (or world scale plants) of methanol synthesis required to store the respective amounts of energy.

In the following a crude estimate will be given about the energy storage demand for Europe using the framework data from Table 2. The largest fraction of the system are conversion losses with 38% of the primary energy consumption. Hence the expectation to reduce the size of the energy system by electrification is well understandable. The volatility of RE requires, however, a massive effort[24] in energy storage if carbon neutrality is required and if no nuclear energy is added to the energy mix.[25] The estimation discriminates RE generated locally from remote RE requiring transportation as chemical energy carrier. Long term storage (more than 1 day) and backup power as well as the demand of the energy system for molecular energy carriers ("solar" or synthetic fuels") are assumed to be provided by converting remote RE into shippable energy carriers and transporting them to Europe. There it will be converted into hydrogen and used to cover the need of final energy that cannot be covered locally within Europe. The RE supply is not discriminated into storable (hydroelectric and biomass) and non-storable (solar, wind) forms in order not to further complicate the estimate. Table 3 presents a dimensional framework. This is not intended to replace any scenario of which many sophisticated versions exist. The sole purpose is to deliver an impression about the amounts of energy storage involved in a deep defossilization of the European energy system.

From line 2 it is seen that for power and mobility no net savings are assumed whereas the heat consumption is to drop substantially by building improvements. Smaller savings by efficiency gains are assumed to be compensated by moderately higher demands within the next 3 decades. The fractions of local RE from line 3 include all forms of RE and short-term storage idealized without losses. From lines 5 and 6 it is seen that electrification of mobility earns a massive reduction in energy demand. Line 6 adds up to 3465 TWh European final RE that is needed to support the assumptions about imports detailed below. This is about 3 times more RE than Europe produces today and should thus be an achievable number if all conversion potentials are used. Some countries have reached their potential whereas others have barely started to generate RE and the potential to exchange RE between countries is still rather limited.

A total of 5740 TWh RE as hydrogen has to be imported (line 7, Table 3) to balance the energy needs of Europe. In line 8 substantial efficiency losses are indicated for burning hydrogen in power stations and from converting CO_2 into synthetic fuels assumed as methanol. These losses are still idealized as no process energy and transport losses are included. From line 9 the gross hydrogen to arrive in Europe amounts to 7689 TWh. This number can be significantly reduced[15] if selected energy saving technologies (line 10) are implemented within whole Europe. Line 12 highlights the enormous savings with only 3752 TWh being required. The by far largest effect has the

Table 2 The dimensional framework of the EU (28) energy system in 2017

Energy use	Total (TWh)	Fraction thereof (TWh)	Fraction thereof (TWh)	Relative (%)
Total primary	19 992			100
Final energy	12 328			62
Heat		5394		27
Mobility		3640		18
- Road			3559	
Power		3294		16
- Fossil			1397	7
- RES			1006	5
- Nuclear			830	4

Table 3 Dimensional framework of a trajectory how Europe could defossilize its energy system (in TWh) based upon its present energy consumption. Red lines indicate local RE use, green lines show import figures. Lines 2, 5, 11 indicate assumptions about efficiency changes when using RE or when implementing technologies indicated in line 10

Nr.	Item	Power	Mobility	Heat
1	Final fossil energy as of now	2288	3559	5394
2	Declared intended savings	—	—	30% (3775)
3	Fraction of local RE supply assumed	60%	50%	30%
4	Fossil final energy to be replaced by RE	1976	1779	1133
5	Assumed efficiency gain from using RE	0%	80%	0%
6	Local RE needed from line 5	1976	356	1133
7	Final energy to be imported	1318	1780	2642
8	Efficiency loss from hydrogen to convert into final energy	60%	60%	0%
9	Hydrogen to be imported	2110	2937	2642
10	Possible improved conversion technologies in Europe	Fuel cell	Serial hybrid	Heat pump
11	Efficiency loss replacing line 8	40%	−80%	50%
12	Reduced amount of hydrogen import	1845	587	1320

electrification of all mobility with half of it as battery-electric and the other half of it as serial hybrid powertrains to be used mainly in heavy duty applications. The other large saving arises from the use of heat pumps for house heating purposes with the extra benefit of removing many small emission sources from otherwise gas heating installations.

This still large number does not contain any provision to remove fossil carbon from the material industry (chemicals, cement, lime, steel). These requirements are difficult to be estimated as none of the potential replacement technologies are existing at scale. It is safe to assume that this sector will require RE in the same dimension as all requirements given in Table 3. The frequent attitude to exclude these issues from the scenarios by assuming moving these industries outside of the unit of analysis is not useful in terms of the general intention to minimize the climate change on the planet.

This dimensional framework is crude and may be debatable in many points. It remains, however, that massive efforts are needed to deepen the domestic penetration of RE in Europe and in parallel engage in partnerships to utilize abundant RE reserves in remote areas of the world. It further occurs that efficiency gains projected in many sectorial scenarios are compensated by the losses arising from the need to generate molecular storage species. Nonetheless, there is a good chance that the whole energy system may become smaller without losing any of its functions by the efficiency gains from partial electrification. The projections are subject to the stability of the present fundamental economic and societal boundary conditions. They may change in the coming 3 decades by *e.g.* less available biomass due to increasing aridity and loss of biodiversity, changes in the global distribution of value chains due to changes in the globalization pattern or the need for more resilience with more regional value generation or climate change-induced waves of migration or changes in energy supply policies following local disasters. Such changes in the trend patters of culture and society cannot be built into projections of the evolution of energy systems and require flexible responses despite the enormous dimensions of infrastructures involved. In addition, the energy supply demands cannot be pre-planned and should be flexible enough to enable societal evolutions. Resilient energy supply strategies are needed offering maximal flexibility against eco-political threats and providing the energy forms needed for the societal evolution. These strategies are based upon a co-existence of electrical RE for direct use within a European grid structure, a storage strategy for short-term fluctuations and an import strategy for long term supply of RE stored in[26] hydrogen and its derivatives. In such a setting for sustainable energy supply presently used or considered, non-sustainable elements can be avoided such as fossil fuels, nuclear fission, CCS or extensive use of biomass and the loss of ecosystems stabilizing the biosphere by deforestation or excessive hydroelectric installations.

The broad portfolio of storage options discussed and required for the intended resilient sustainable energy system carries with it several negative effects. The sheer size of the infrastructures needed (like the electricity and the petrochemical industries combined) adds significantly to the land use for energy that is already large for the RE conversion devices (wind mills and solar panels). A rarely discussed aspect is safety of the infrastructure. The pure technical safety (accidents, spills, fires and explosions with chemical storage materials) is enhanced by digital threats. Future energy systems will rely on digital infrastructure to a much larger extent than it exists already today. The multiple couplings between energy sectors in real time and the volatility issues demand for a highly integrated measurement and control system. Technical failures and hacking attacks make such systems highly vulnerable with still few measures possible for effective protection and "hardening" of the systems. It can be expected that the resulting complexity may become a serious obstacle in constructing and operating future energy systems. Conventional electro-mechanical storage systems are not any better in this respect but carry other technical risks (battery fires, breaking dams) than chemical energy storage systems. These safety issues need constant care and open addressing in the essential dialogue with the public, being the users of the energy system. The example of nuclear power with its lost opportunities for safer energy supply sends a clear signal that safety aspects in energy systems are critical both in technical and in communication respects.

The way forward

The author is convinced that the transformation outlined in the previous sections can be achieved within economic and temporal limits acceptable by the societies involved. A few concepts enable such an undertaking comparable in its dimensions to the industrial revolution.

Internationalisation

CEC is by definition an international activity and must be planed and governed like this from its beginning. As international (minimum European) affair, rules for certification of energy carriers (how "green" is a carrier) are a first critical prerequisite for designing supply chains and find first users. The debate about the "colours of hydrogen" and their ramifications on legal definition of renewability is a warning example how action can be prevented by political uncertainty on the European level. Standardisation of technological parameters, operating of infrastructure and metering now in place for fossil energy carriers must be developed quickly and ahead of realization of first projects.

Regulatory framework

The intricate legislative body controlling individual energy sectors in each country needs a re-set and not additional corrections to enable CEC in order to provide a stable foundation of energy system design. The new framework must be reliable and transparent to all stakeholders (within Europe) for timescales relevant to infrastructure lifetimes (decades). It should follow a common rationale including a clear definition of the

roles of stakeholders in the energy system and must be universal in all sectors of the energy system. The states should abstain from technology-specific measures in favour for long-term universal measures. Initialization of the transformation may be triggered by incentives with clear temporal exits much shorter than they could serve as subsidies.

Roadmap

For states and stakeholder groups hierarchical roadmaps are to be developed describing the key actions, roll-out plans and interdependencies in time of all main steps of the energy transformation. The underlying systemic approach unites political acts with socio-economic actions[27] as well as technologies and their scaling under industrial leadership. The diversity of Europe renders a homogeneous action impossible. Based upon a fixed common understanding[28] of the concept in the roadmap, binding country-specific lists of action should be provided by member states similar as to the current practice of greenhouse gas reduction measures and should be homogenized in the Green Deal strategy. The roadmap must include procedures for auditing and milestones to be achieved by member states in order to arrive at a reliable network of interfaces between the different action lists. Fractions of relevant roadmaps[29] exist already today but their integration in an overall and widely accepted plan is missing.

This activity is the by far most critical action to initiate a coordinated energy transition. It is more important than liberating limited financial public resources. These can trigger action and should co-finance science and technology, including demonstrations in world-scale. The main body of resources must come from private investments requiring as foundation the stable existence of the roadmap and the two initial concepts.

The roadmap activity needs amongst multiple other issues some planning of the allocation of RE and imports as hydrogen and derivatives to major energy users, to enable designing infrastructures of suitable dimension and topology. Such planning further needs avoiding double allocation of local RE for immediate electrical use and for CEC applications for example by demanding a suitable market design.

Science

As soon as these actions are underway, a framework for scientific action enabling largely all disciplines of chemistry and engineering can be developed for the CEC part of the energy transition. In view of the pressing timeline for the transformation until 2050, a maximum of parallel action should be targeted that can be supported by clear and forward-looking actions of the political stakeholders and funding authorities. Their current focalization on financial aspects disconnected from concept development taking into account the natural timelines of science is insufficient as it hides critical disagreements in concept between stakeholders in politics, economy and between nations. Possibly, a segmented process ("hydrogen union" of the willing) may be needed to take the Green Deal into the action that its initiation promised. Scientific projects may acknowledge that much has already been done in the area. It is not needed to disregard the very substantial existing knowledge. Aggregation and evolution in methodology as in materials and devices is key to progress in a field of chemical science that is truly critical for the future on our planet.

Science for energy conversion may follow a dual strategy. One arm covers the world-scale initiation of a generation 1 (G1) CEC component of energy systems whereas the other arm should provide radically innovative approaches dealing with the minimization of the systemic inefficiencies of the G1 system. This will need deep insight into fundamental processes of interfacial and molecular catalysis as the common scientific foundation. Having available a toolbox[30] of design and synthesis methodologies, one could design from scratch chains of energy conversion with a maximal systemic efficiency. This may then involve other infrastructures and energy utilization appliances that can be realized after the G1 energy system has provided the climate protection as described in the Paris agreement. In this second arm the scientific creativity of basic science bare of constraints from techno-economic realizability is key to provide an ecosystem of options from which future concepts can begin to deal with the massive challenge of converting science into technology. In this period the life cycle assessments[6] and scalability questions become important; they may be based whenever possible upon data acquired in actual projects rather than on theoretical estimates.

It is important to understand that the G1 science and technologies are of utmost urgency to kick off the energy system transformation that will not come only from providing locally RE to the existing energy system. Rather, establishing a circular economy of carbon-based synthetic fuels[23,31] besides a suitable technology portfolio for global hydrogen exchange[32] are the actions needed now. A key issue is here the suitable integration of life cycle analysis in choosing the technology options[33] for example under conditions of "mixed" electrical energy supply containing fossil and RE components. Challenges[34] of system integration and operation control of dynamical energy supply structures,[35] engineering issues and the scaling of production of devices and systems required for CEC (electrolysers, CEC plants, small scale decentralized units) are the pressing issues. Digitalization of discovery processes[30,36] and their scale-up, material science and the molecular understanding of the underlying processes of chemical conversion[37] are cross-linking basic components of an integrated research and technology innovation roadmap representing an integral part of the transformation roadmap.

At present science is far away from such a coordinated and prioritized action. The essential plurality of communities involved may largely preclude substantial progress in coordination (as it may hamper creativity). An important step forward, however, could be done if in science the documentation of results and insights would occur in a clean and complete manner such that later the developing tools of artificial intelligence can re-use the information independent of its original context. The author strongly advertises a community-internal effort (see *e.g.* https://nomad-coe.eu) to develop a standard of minimum quality reporting for energy-related work. This would

not inhibit creativity by limitations imposed but multiply the usefulness of the ongoing rich scientific activities.

Conflicts of interest

There are no conflicts of interest to declare.

Acknowledgements

Open Access funding provided by the Max Planck Society.

References

1 K. Svobodova, J. R. Owen, J. Harris and S. Worden, *Appl. Energy*, 2020, **265**, 114778.
2 X. Deng and T. Lv, *J. Cleaner Prod.*, 2020, **246**, 118962.
3 A. Palzer and H. M. Henning, *Energy Technol.*, 2014, **2**, 13–28.
4 N. Mac Dowell, P. S. Fennell, N. Shah and G. C. Maitland, *Nat. Clim. Change*, 2017, **7**, 243–249.
5 K. De Ras, R. Van de Vijver, V. V. Galvita, G. B. Marin and K. M. Van Geem, *Curr. Opin. Chem. Eng.*, 2019, **26**, 81–87.
6 A. Valente, D. Iribarren and J. Dufour, *Int. J. Life Cycle Assess.*, 2017, **22**, 346–363.
7 R. G. Grim, Z. Huang, M. T. Guarnieri, J. R. Ferrell, L. Tao and J. A. Schaidle, *Energy Environ. Sci.*, 2020, **13**, 472–494.
8 M. Fasihi, D. Bogdanov and C. Breyer, in *10th International Renewable Energy Storage Conference, Ires 2016*, ed. P. Droege, 2016, vol. 99, pp. 243–268.
9 E. I. Koytsoumpa, C. Bergins, T. Buddenberg, S. Wu, O. Sigurbjornsson, K. C. Tran and E. Kakaras, *Trans. ASME: J. Energy Resour. Technol.*, 2016, **138**(4), 042002.
10 (*a*) R. Schlögl, *Angew. Chem., Int. Ed.*, 2019, **58**, 343–348; (*b*) R. Schlögl, *Top. Catal.*, 2016, **59**, 1461–1476; (*c*) R. Schlögl, *ChemSusChem*, 2010, **3**, 209–222.
11 M. Fasihi, D. Bogdanov and C. Breyer, *Sustainability*, 2017, **9**, 233.
12 (*a*) M. Reuss, T. Grube, M. Robinius, P. Preuster, P. Wasserscheid and D. Stolten, *Appl. Energy*, 2017, **200**, 290–302; (*b*) D. Teichmann, W. Arlt and P. Wasserscheid, *Int. J. Hydrogen Energy*, 2012, **37**, 18118–18132; (*c*) R. Schlögl, *Angew. Chem., Int. Ed.*, 2015, **54**, 4436–4439.
13 (*a*) N. Mahbub, A. O. Oyedun, H. Zhang, A. Kumar and W. R. Poganietz, *Int. J. Life Cycle Assess.*, 2019, **24**, 881–899; (*b*) R. M. Cuellar-Franca and A. Azapagic, *J. CO_2 Util.*, 2015, **9**, 82–102.
14 R. Schögl, *Top. Catal.*, 2016, **59**, 772–786.
15 F. Ausfelder, C. Beilmann, M. Bertau, S. Brauninger, A. Heinzel, R. Hoer, W. Koch, F. Mahlendorf, A. Metzelthin, M. Peuckert, L. Plass, K. Rauchle, M. Reuter, G. Schaub, S. Schiebahn, E. Schwab, F. Schüth, D. Stolten, G. Tessmer, K. Wagemann and K. F. Ziegahn, *Chem. Ing. Tech.*, 2015, **87**, 17–89.
16 C. Brunner, G. Deac, S. Braun and C. Zophel, *Renewable Energy*, 2020, **149**, 1314–1324.
17 G. A. Olah, A. Goeppert and G. K. S. Prakash, *J. Org. Chem.*, 2009, **74**, 487–498.
18 N. M. Haegel, R. Margolis, T. Buonassisi, D. Feldman, A. Froitzheim, R. Garabedian, M. Green, S. Glunz, H. M. Henning, B. Holder, I. Kaizuka, B. Kroposki, K. Matsubara, S. Niki, K. Sakurai, R. A. Schindler, W. Tumas, E. R. Weber, G. Wilson, M. Woodhouse and S. Kurtz, *Science*, 2017, **356**, 141–143.
19 A. Polman, M. Knight, E. C. Garnett, B. Ehrler and W. C. Sinke, *Science*, 2016, **352**, 6283.
20 (*a*) F. Dawood, M. Anda and G. M. Shafiullah, *Int. J. Hydrogen Energy*, 2020, **45**, 3847–3869; (*b*) N. A. Bahari, W. N. R. W. Isahak, M. S. Masdar and Z. Yaakob, *Int. J. Energy Res.*, 2019, **43**, 5128–5150.
21 (*a*) A. Palzer and H. M. Henning, *Renewable Sustainable Energy Rev.*, 2014, **30**, 1019–1034; (*b*) H. M. Henning and A. Palzer, *Renewable Sustainable Energy Rev.*, 2014, **30**, 1003–1018.
22 (*a*) G. A. Olah, *Angew. Chem., Int. Ed.*, 2005, **44**, 2636–2639; (*b*) F. Asinger, *Methanol, Chemie-und Energierohstoff*, Springer, Berlin, 1985.
23 E. I. Koytsoumpa, C. Bergins and E. Kakaras, *J. Supercrit. Fluids*, 2018, **132**, 3–16.
24 M. A. Basit, S. Dilshad, R. Badar and S. Rehman, *Int. J. Energy Res.*, 2020, **44**, 4132–4162.
25 F. J. de Sisternes, J. D. Jenkins and A. Botterud, *Appl. Energy*, 2016, **175**, 368–379.
26 X. Li, D. Teschner, V. Streibel, T. Lunkenbein, L. Masliuk, T. Fu, Y. Wang, T. Jones, F. Seitz, F. Girgsdies, F. Rosowski, R. Schlögl and A. Trunschke, *Chem. Sci.*, 2019, **10**, 2429–2443.
27 K. Riahi, A. Gruebler and N. Nakicenovic, *Technol. Forecast. Soc. Change*, 2007, **74**, 887–935.
28 J. Rockstrom, O. Gaffney, J. Rogelj, M. Meinshausen, N. Nakicenovic and H. J. Schellnhuber, *Science*, 2017, **355**, 1269–1271.
29 S. Perathoner, S. Gross, E. J. M. Hensen, H. Wessel, H. Chraye and G. Centi, *ChemCatChem*, 2017, **9**, 904–909.
30 R. Schlögl, *ChemCatChem*, 2017, **9**, 533–541.
31 A. Navarrete, G. Centi, A. Bogaerts, A. Martin, A. York and G. D. Stefanidis, *Energy Technol.*, 2017, **5**, 796–811.
32 Y. Ishimoto, A. Kurosawa, M. Sasakura and K. Sakata, *Int. J. Hydrogen Energy*, 2017, **42**, 13357–13367.
33 J. Artz, T. E. Muller, K. Thenert, J. Kleinekorte, R. Meys, A. Sternberg, A. Bardow and W. Leitner, *Chem. Rev.*, 2018, **118**, 434–504.
34 Z. W. Seh, J. Kibsgaard, C. F. Dickens, I. B. Chorkendorff, J. K. Nørskov and T. F. Jaramillo, *Science*, 2017, **355**, 6321.
35 G. Deerberg, M. Oles and R. Schlögl, *Chem. Ing. Tech.*, 2018, **90**, 1365–1368.
36 (*a*) A. R. Singh, B. A. Rohr, J. A. Gauthier and J. K. Nørskov, *Catal. Lett.*, 2019, **149**, 2347–2354; (*b*) J. K. Nørskov, T. Bligaard, J. Rossmeisl and C. H. Christensen, *Nat. Chem.*, 2009, **1**, 37–46; (*c*) A. Ziletti, D. Kumar, M. Scheffler and L. M. Ghiringhelli, *Nat. Commun.*, 2018, **9**, 2775.
37 G. Ertl, *Angew. Chem., Int. Ed.*, 2008, **47**, 3524–3535.