

# Future Energy Supplies

– the contribution of chemistry –



## Subject matter

Our future energy supplies and the adaptation of our energy system to future challenges will not be possible without breakthroughs in chemistry. For the urgently needed increase of efficiency in utilisation of energy, chemistry is the key discipline. In this position paper “Future Energy Supplies – the Contribution of Chemistry” the German chemistry organizations demonstrate the key position of the chemical sciences in achieving a sustainable energy supply. Essential potentials for development and the need for scientific research in the upcoming decades are being described and assessed.



## 8. List of authors

Prof. Dr. Barbara Albert, TU Darmstadt

Prof. Dr.-Ing. Friedrich-Wilhelm Bach, University of Hanover

Dr. Dana Demtröder, DECHEMA e.V., Frankfurt

Dr. Jürgen Engelhard, RWE Power AG, Cologne

Prof. Dr.-Ing. Stefan Ernst, Technical University of Kaiserslautern

Prof. Dr. Claus Feldmann, University of Karlsruhe

Dr. Andreas Förster, DBG – Deutsche Bunsen-Gesellschaft für Physikalische Chemie e.V., Frankfurt

Prof. Dr. Angelika Heinzl, University of Duisburg-Essen, Duisburg

Dr. Renate Hoer, GDCh – Gesellschaft Deutscher Chemiker e.V., Frankfurt

Prof. Dr.-Ing. Werner Hufenbach, Technische Universität Dresden

Prof. Dr. Dieter Jahn, BASF Aktiengesellschaft, Ludwigshafen

Prof. Dr. Klaus-Michael Jüttner, DECHEMA e.V., Frankfurt

Prof. Dr. Holger Kleinke, University of Waterloo, Waterloo/CDN

Prof. Dr. Wolfram Koch, GDCh - Gesellschaft Deutscher Chemiker e. V., Frankfurt

Dr.-Ing. Mathias Noe, Research Centre Karlsruhe

Dr.-Ing. Ludolf Plass, Lurgi AG, Frankfurt

Dr. Hermann Pütter, Neustadt

Prof. Dr.-Ing. Norbert Rübiger, University of Bremen, Bremen

Dr. Martin Reuter, VCI Verband der Chemischen Industrie e. V., Frankfurt

Dr.-Ing. J. Schmalfeld, DGKM – Deutsche Wissenschaftliche Gesellschaft für Erdöl, Erdgas und Kohle e.V., Hamburg

Prof. Dr. Ferdi Schüth, Max Planck Institute for Coal Research, Mülheim

Dr. Peter J. Seifried, Shell Deutschland Oil GmbH, Hamburg

Dr. Gisa Teßmer, DGMK – Deutsche Wissenschaftliche Gesellschaft für Erdöl, Erdgas und Kohle e.V., Hamburg

Dr. Kurt Wagemann, DECHEMA e.V., Frankfurt

Prof. Dr.-Ing. Jens Weitkamp, University of Stuttgart, Stuttgart

Prof. Dr.-Ing. Joachim Werther, TU Hamburg-Harburg, Hamburg

Created and supported by the Coordinating Group for Chemical Energy Research\* of the following organisations:

**DECHEMA** – Gesellschaft für Chemische Technik und Biotechnologie e.V.  
(Society for Chemical Engineering and Biotechnology)  
Theodor-Heuss-Allee 25, 60486 Frankfurt am Main, [www.dechema.de](http://www.dechema.de)

**GDCh** – Gesellschaft Deutscher Chemiker e.V.  
(German Chemical Society)  
Varrentrappstraße 40-42, 60486 Frankfurt am Main, [www.gdch.de](http://www.gdch.de)

**DBG** – Deutsche Bunsen-Gesellschaft für Physikalische Chemie e.V.  
(German Bunsen Society for Physical Chemistry)  
Theodor-Heuss-Allee 25, 60486 Frankfurt am Main, [www.bunsen.de](http://www.bunsen.de)

**DGMK** – Deutsche Wissenschaftliche Gesellschaft für Erdöl, Erdgas und Kohle e.V.  
(German Society for Petroleum and Coal Science and Technology)  
Überseering 40, 22297 Hamburg, [www.dgmk.de](http://www.dgmk.de)

**VDI-GVC** – Gesellschaft Verfahrenstechnik und Chemieingenieurwesen  
(VDI Society for Chemical and Process Engineering)  
Graf-Recke-Straße 84, 40239 Düsseldorf, [www.vdi.de/gvc](http://www.vdi.de/gvc)

**VCI** – Verband der Chemischen Industrie e.V.  
(The German Chemical Industry Association)  
Mainzer Landstraße 55, 60329 Frankfurt am Main, [www.vci.de](http://www.vci.de)

March 2007

\* Chairman: Prof. Dr. Ferdi Schüth, Max-Planck-Institut für Kohlenforschung (Max Planck Institute for Coal Research), Mülheim, tel: 0208/306 2373, e-mail: [schueth@mpi-muelheim.mpg.de](mailto:schueth@mpi-muelheim.mpg.de)

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## 1. Introduction

The development of new energy sources and the partial changeover of our energy supply infrastructure from one reliant primarily on fossil sources to a new mix is one of the greatest challenges of the 21st century – if not the greatest. The solution to the many complex problems requires a well-coordinated strategy which ranges from short-term measures to a fundamental investigation of alternative energy sources and an adapted energy infrastructure. Due to its high significance for the future of our society, this field holds a prominent place in the high-tech strategy of the German Federal government.

The importance of chemistry in the process of supplying our society with energy was already emphasized in the joint position paper of the chemistry related learned societies and the VCI in the summer of 2006 (“Energy Research: Innovative contributions of chemistry for future energy supplies and reduction of energy consumption”). Furthermore, numerous aspects are addressed in the national implementation plan of the European Technology Platform Sustainable Chemistry (SusChem). The present paper provides a more detailed depiction of the key position which chemistry holds in the respective areas of the energy sector in order to enable an assessment of the potential for development and the need for scientific research in the upcoming decades.

### The role of chemistry in our energy system

An analysis of the past development of our energy system demonstrates that chemistry is of increasing importance in the generation and transformation of energy and has become a key technology in this field. This trend will continue to grow. We would like to use the following example to explain this: the oil which was produced in the early part of the oil period was – in the best cases – simply distilled, and then directly burned. Today, refineries are more than facilities for the distillation of crude oil – the various components of oil are transformed through numerous chemical processes so that the energy content of crude oil is optimally utilised for the desired purposes. When the raw materials base for the provision of fuels changes as crude oil supplies dwindle, the significance of chemical transformation processes will increase considerably, since the chemical characteristics of the raw materials which will be available will be much farther from those of the target products than when crude oil was used as a base.

However, the significance of chemistry goes farther. New technologies in the field of energy production constantly require decisive advances in chemistry:

- Fuel cell catalysts are currently still too expensive and inefficient, and even new electrolytes such as thermostable polymer membranes for fuel cells would significantly simplify the large-scale technical use of such systems.
- Future generations of solar cells require new molecular systems which can be produced more efficiently and cost-effectively and would thereby enable a shorter energy amortisation period in the transformation of sunlight into electricity.
- Advances in battery technology depend crucially on improvements in the chemistry of the electrodes and electrolytes.
- New types of thermoelectric materials could initiate a revolution in the generation of electrical energy through the direct utilisation of waste heat. With cost-effective systems, the existing residual heat in any exhaust line could be transformed into electrical energy, and the efficiency of such systems could additionally be increased through linkage with solar cells.
- All techniques for the separation of CO<sub>2</sub> from exhaust out of power plants or other industrial processes are expected to be based on chemical processes.

This list is not complete by far – nearly every advanced energy system requires key innovations in chemistry, as the main part of this presentation will demonstrate.

Finally, the switch of chemical production itself to less energy-intensive and more efficient processes is also a major future task; and cost reasons will necessitate at least a partial shift from the use of crude oil as a raw material base to other (including renewable) feedstocks.

### Available options and opportunities

The final path that will be followed for our energy supply is essentially a societal and political decision. However, there are a number of clearly defined scientific-technological and economic conditions which must be taken into account, such as the current and expected costs, the usable potential of new energy sources and the environmental compatibility in practice. And it is important to remember that resources can only be utilised once: if the entire available agricultural areas were to be utilised for the production of energy plants, the land would no longer be available for the production of feedstock for the chemical industry or for food production.

Plans for a future energy system and for directing investments into research activities must be based on a realistic assessment of the potential utilities of the various options. The development of various energy sources is dependent on key innovations in chemistry: among the sustainable energy options, the potential of solar energy in the form of radiation is currently utilised at a very low level in Germany. However, with the exception of heating purposes, this option is not even close to being done at competitive costs. There is still a long way to go here. For biomass, a total potential contribution of approx. 10 % of our current energy consumption is estimated but only approximately one third of this is presently a reality. A considerable proportion of this could be produced in the form of liquid fuels. Here, it is necessary to keep in mind that biomass is one of the few available energy sources within Germany which are relatively easily transformed into liquid fuels. This is important because bottlenecks are most likely to be feared for liquid fuels and this is where dependence on imports is highest. Among the fossil energy carriers, coal has the longest projected range (155 years worldwide) and it is the only significant fossil source within Germany aside from far lesser quantities of crude oil and natural gas. Coal can be utilised for the production of electrical energy, but can also be transformed into liquid fuels. In the utilisation of synergy effects with other energy sources and carriers in combinations, the usually high emissions of CO<sub>2</sub> from the use of coal could be reduced. Other energy sources, such as wind energy, require energy storage technologies in order to buffer the spasmodic production of energy output and ensure an optimal utilisation of potential.

### Conclusions

Clear advances in the development of these potential options and an improved utilisation of conventional forms of energy supply will require intensive research efforts, particularly in chemistry, the science which cuts across the entire energy sector. Our future energy supply is expected to become more dependent on chemistry, and the adaptation of our energy system to future challenges will not be possible without breakthroughs in chemistry. Even though intensive work on meeting the challenges of chemistry is already taking place in various companies as well as universities and research institutions, currently, the key role which chemistry plays in solving the energy problem frequently remains unrecognized. Since the task is long-term, future generations of scientists will also have to work on these problems. It is therefore important to embed suitable content more deeply in education and training curricula.

In addition, the expert public must be made aware of these needs. To some degree, this is already being done with this paper and accompanying measures. However, the mechanisms which act in our research system also necessitate stimulation of research activities through financial incentives. Due to the long time scales which are characteristic for transforming the energy supply system of a society, it is important to make the decisive directional changes now. The following measures appear to be sensible and necessary:

1. Explicit support and funding measures with the goal of strengthening chemical energy research should be implemented to direct a significant proportion of chemical research into this field. Such measures should range from long-term programmes in more knowledge-oriented research to short and mid-range programmes with the goal of immediate practical implementation.
2. At the present time, funding policies in this field often do not seem to be optimally coordinated. Even though support by various instruments and sponsors appears to be sensible due to the large variety of individual questions, coordination would be helpful. The present one-sidedness of funding programmes must be overcome in order to enable the development of complex systems and encourage synergistic effects

between energy carriers and energy sources. This is a current imperative, since there are currently various programmes which (partly) provide support for chemical energy research, yet these somewhat isolated programmes lack coherent research-guiding messages. Indeed, they are usually not explicitly aimed at energy related questions.

3. Coordination with the European Technology Platform “SusChem” and the corresponding national implementation plan is also important. Among others, SusChem names the Smart Energy Home as a flagship project, which is centrally positioned in the field of chemical energy research.

## 2. Preliminary remarks

The following text explains the significant lines of development in the energy sector in greater detail and places them in the context of innovations which will be required from chemistry. Not all available energy sources are addressed, since the contributions chemistry can make are likely to be relatively small in some cases. For instance, nuclear energy is not included in this discussion. This does not imply a lack of appreciation for the importance of this technology but rather that nuclear energy can be regarded largely as a physical technology, even though chemical steps (e.g., in the context of the nuclear fuel chain) have considerable significance and numerous fundamental material problems – that is, chemical problems – must still be solved in the development of fusion technology. Wind energy, geothermal energy and water energy are also not included in the discussion, since the energy in these cases is harnessed primarily through the use of physical principles. However, chemistry can make important contributions here as well – for instance, in storing energy derived from wind power, the production of which is necessarily uneven. Chemical storage technologies may well be very relevant here.

Some general comments appear to be helpful in the following discussion to permit a better assessment of the statements made. Our energy system is currently based on a series of energy sources the status and possible developments of which are addressed in Chapter 3. However, we have only two significant energy carriers, namely electrical current on the one hand and hydrocarbons in the form of natural gas, gasoline and diesel fuel or heating oil on the other hand. These energy carriers do not function equivalently, even though they can be transformed into each other to some degree, though always with the loss of some usable energy. However, aside from their function as energy carriers, hydrocarbons play another important role: they are our main means of storing energy. Electrical energy must be generated to the same levels as consumption, apart from buffers in the form of storage power stations. At this time, energy can be stored for the long term solely as hydrocarbons, a form in which the stored energy can be mobilised again relatively quickly. This additional function of the hydrocarbons must be taken into account in a discussion about a future energy system. If the baseline operating rules are to be changed from oil to another energy source, new energy storage technologies must be developed simultaneously. This is a particularly pertinent issue to remember, since many renewable energy sources (wind, solar energy) occur with major fluctuations in production rate and it is therefore necessary to maintain buffers in order to balance the varying production and changes in demand. This aspect of our energy system is discussed in Chapter 4.

Another general point must also be taken into account: for fundamental physical reasons, the transformation from one energy form into another is always accompanied by losses. Therefore, transformation processes should be avoided as far as possible, and energy sources should be utilised in a manner which requires the fewest possible steps to reach the desired purpose. For instance, biomass can be transformed into heat energy and electrical energy with relatively high efficiency in combined heat and power units. If, however, the same biomass is initially gasified, then turned into diesel fuel through the Fischer-Tropsch process, and this diesel fuel is then utilised to drive the motor in a vehicle, only a relatively small part of the energy which is contained in the biomass is actually used for the intended purpose – to power the vehicle. In other words, the same biomass can deliver completely different amounts of end energy depending on the way in which it is put to use.

Therefore, an attempt should be made to use each energy source as efficiently as possible in accordance with its specific characteristics and properties.

Finally, it is necessary to point out that one of the greatest “energy sources” lies in saving energy. Instead of satisfying energy requirements through the development of new sources, the same result can be achieved by reducing the demand. Hence the range of existing and future energy resources can be extended. This will also require significant contributions from chemistry, such as the development of new superinsulators, or materials for light emitting diodes for lighting purposes, or light construction materials which significantly reduce the fuel consumption of vehicles. These aspects are largely considered in chapters 5 and 6.

## 3. Energy provision

### 3.1. Provision of fuels

#### 3.1.1 Fuels from crude oil, natural gas, coal and biomass

» **Development line:** Conventional fuels on the basis of hydrocarbons – namely fuel for spark ignition engines (gasoline), jet fuel (kerosene) and diesel fuel – will, for the foreseeable future, continue to provide the basis for transport mobility within our society. Quality requirements for these fuels will continue to increase – primarily with the goals of largely protecting the environment, ensuring compatibility with more efficient motors and achieving lower fuel consumption. It is necessary to ensure that these high-grade fuels can be produced in the future not only from petroleum, but also from natural gas, coal and/or biomass as raw materials at reasonable costs.

» **State of the art:** Today, gasoline, kerosene and diesel fuel are almost entirely produced from crude oil by means of distillation and subsequent catalytic upgrading processes. Only small quantities of first-generation biofuels – namely bioethanol, ethyl-tertiary-butyl ether (ETBE) and biodiesel – are produced from renewable raw materials. Some countries are currently developing technologies for producing synthetic diesel fuel and kerosene from natural gas via synthesis gas and wax as intermediates. Synthesis gas is also produced from coal or from residues of crude oil distillation through gasification.

» **Deficits and development goal:** There are important goals for development in numerous places along the value chain from raw fossil materials or biomass to future fuels. Even in the processing of the conventional high-grade crude oils which are utilised today, there are still shortcomings in the upgrading processes. For instance, there is no known efficient method for transforming polycyclic aromatics in diesel fuel or kerosene into high-quality open-chain hydrocarbons through hydrogenative ring opening processes. It also seems that the conventional hydrotreating processes for the removal of sulphur and nitrogen from fuels have presently reached their limits in terms of pollutant reduction. There is also a clear need to improve cracking processes for converting distillation residues, with their elevated contents of pollutants, into high-quality fuels and chemical raw materials. Such processes will gain significant importance when the heavy crude oils, oil sands and oil shales which are present on the planet in very large quantities increasingly take the place of conventional crude oils as raw materials.

The technology for the transformation of natural gas and other hydrocarbon gases into liquid fuels („Gas-to-Liquids“, GTL) comprises the generation of synthesis gas ( $\text{CO} + \text{H}_2$ ) through catalytic steam reforming or partial oxidation, the Fischer-Tropsch synthesis into wax-like long-chain n-alkanes and mild hydrocracking of these substances into very high-quality diesel fuel and kerosene, unfortunately still at relatively high costs. Since the greater part of the total costs is incurred in the first step, it is imperative to provide more cost-efficient ways of generating synthesis gas from natural gas. In the long term, research must aim at directly converting methane into higher hydrocarbons through completely new carbon-carbon bond forming processes. Coal can be transformed into liquid fuels in two ways, viz., through gasification with water vapour and oxygen into synthesis gas followed by the technology described for natural gas, as well as through direct liquefaction using hydrogen under high pressure. Both technologies were applied on an industrial scale in Germany in the past; however, today's perspectives require a substantial modernization of the earlier processes.

With the aim of making clearly better use of renewable raw materials than what has been done before, processes for the generation of second-generation biofuels must now be developed. This is summarized into the following routes:

- 1) Gasification of the biomass into synthesis gas, followed by its transformation into synthetic biofuels by means of the technology described above for natural gas („Biomass-to-Liquids“, BTL);
- 2) enzymatic production of bioethanol not only from sugar components of the plants but also from cellulose, hemicellulose etc.;
- 3) enzymatic generation of other compounds which are better suited as fuels than is bioethanol, e.g. biobutanol. Furthermore, synergy effects in processes during the combined use of biomass with coal and organic raw materials must be considered.

» **Technical-scientific challenge:** For the last half century, crude oil has proven to be the optimal raw material for the production of liquid fuels. Methane, the main component of natural gas, lacks C-C bonds, and it is thus far not possible to generate them in a single chemical step, since methane is thermodynamically quite stable and kinetically slow to enter into reactions. Coal is low in hydrogen (and its transformation into qualitatively high hydrogen-rich fuels therefore results in comparatively high CO<sub>2</sub> emissions). It is often high in noxious heteroatom content (sulphur, nitrogen and others) and difficult to handle as a solid material. The availability of renewable raw materials for the fuel sector is limited (the substitution potential is estimated at a maximum of 20 to 25 % of the national supply), and some routes (such as rape oil into biodiesel) produce large quantities of by-products (glycerol).

» **Solution approaches:** A key technology which offers primarily the potential for overcoming existing obstacles is found in catalysis. Both heterogeneous catalysis and biocatalysis are particularly suitable for consideration. Some possible development lines are outlined as examples here:

Today, all fuels within Germany are largely desulphurised (down to 10 wt.-%ppm) by means of hydrotreating. The trend towards fuels which are even lower in sulphur (and nitrogen) will continue. This requires innovative processes – the beginnings of biocatalytic, oxidative and reactive adsorption processes are currently identifiable. In the production of diesel fuels and kerosene from natural gas, the search for catalytic and process technological measures which enable more cost-effective production of synthesis gas must be continued. There is also potential for the further improvement of catalysts and reactor technology for Fischer-Tropsch synthesis. In view of the very large coal deposits on the planet, the technologies for chemical upgrading of coal should, in the long term, be developed with the inclusion of all options in modern catalysis, process technology and synergy effects. In terms of renewable resources, the main attention for research and development must naturally be focused on the second-generation biofuels with an emphasis on gasification of biomass and genetic optimisation of plants and biocatalysts. Where large amounts of by-products are produced, e.g. glycerol in the generation of biodiesel through transesterification of rape oil, their catalytic upgrading into chemical products could make an important contribution to improving the economy.

» **Potential for improvements:** Technical advances in the field of production of high-grade liquid fuels from fossil and renewable raw materials will take place overall as a result of international research and development efforts and cooperative ventures. However, the targeted funding of such research and development activities also offers excellent chances of success, particularly in Germany. Reasons for this include the high current levels of catalysis in research and industrial application as well as an already leading role in the production and utilisation of biofuels.

### 3.1.2 Bioenergy

» **Development line:** The term “bioenergy” covers the utilisation of biomass with a future oriented significance, since a clear worldwide reduction of dependency on fossil energy carriers, and of CO<sub>2</sub> emissions which are related to this, must take place. Aside from the energy utilisation of biogas, bioethanol and ETBE (ethyl-tertiary-butyl ether), the low-molecular substances (methanol, ethanol etc.) furthermore have the potential of being usable as platform chemicals for the creation of new “chemical family trees”.

» **State of the art:** The production processes which are currently being utilised are largely based on anaerobic technology for the biological fermentation of renewable raw materials and product generation (biogas, bioethanol). Thermal processing immediately after the production process takes place solely with biogas in block heating power plants, within which exhaust heat utilisation takes on a special significance in increasing the effectiveness of the overall process. Regarding energy substance utilisation of bioproducts with small molecules (bioethanol, methanol etc.), product separation and concentration must take place from the fermented substrate. The demands which are placed on the purity level of the product frequently require interim steps with high cost in terms of energy and materials. For instance, in the case of bioethanol, this involves distillation, rectification and dehydration through the use of zeolite. A purification chain can also end with a large-scale chemical transformation, as in the case of ETBE production. At the present time, the costs for raw materials, facility construction and operation, product processing and – to some degree – chemical transformation, are all too high. Last but not least, there are also insufficient energy options for the disposal and utilisation of fermentation residue.

» **Deficits and development goals:** Within Germany, the large societal demand for bioenergetic products is met only by the very limited resource availability of “renewable raw materials”. Currently, approx. 10 % of the present primary energy requirements can be met by renewable raw materials. Special attention should be directed towards the development of innovative processes for the production of biotechnological products which clearly possess greater resource efficiency and an expanded variety of raw materials. Furthermore, the entire value creation chain should remain in the eye of research and development. In this sense, the development or invention of new methods for renewable raw materials, concrete product applications, raw material alternatives and if applicable, utilisation of fermentation residue, must be coordinated at the earliest possible stage. This applies particularly to biogas production – thus far, biogas yield is the only subject which is at the centre of interest in this field. So far, little attention has been directed at an expanded consideration of products (secondary metabolites which are produced parallel to biogas in fermentation), altered process control strategies as well as optimal utilisation of fermentation products (utilisation of nitrogen). An analogous statement also applies to the production of bioethanol, within which improved resource efficiency with an altered selection of raw materials and fermentation techniques, product separation and dehydration with low expense and energy consumption, should clearly be given higher priority. Resulting from this, the economic/ecological competitiveness of the ability to utilise regenerative energy sources as well as renewable raw materials could be noticeably boosted.

» **Technical-scientific challenge:** To date, no technical systems which would be suitable for the above named optimization of the tasks are being utilised. The technical and scientific challenge lies in the development of new suitable processes which 1) enable increased yields per hectare of renewable raw materials and/or 2) show an innovative process control strategy for fermentation with optimized product yield and resource efficiency. It is also necessary to give more thought to possible uses for valuable substances at the end of the process chains, which have not been considered so far. Below are two concrete examples to illustrate this point:

- In biogas production with facilities where electrical output is greater than 200 KW, there is a positive nitrogen balance which is not being utilised at the present time. The stripping process for volatile nitrogen components which was previously favoured has been shown to be unusable due to high consumption of chemicals and the precipitation processes.
- In the production of bioethanol, apart from fermentation, the technical processes for dehydration have been shown to be a key technology. The zeolites which are currently used in this process, with preceding rectification, require excessively high energy consumption and investment costs.

» **Solution approaches:** At this time, various approaches are being pursued to improve cost-intensive cleaning and separation processes. Here, a key factor could lie in the production of specifically functionalized solid material surfaces. In the form of adsorption agents and membrane materials, these could easily find entry into technical system developments, such as multiple-stage or hybrid membrane processes. However, in addition, concrete consideration must be given to advancements in ethanol dehydration in the direction of more favourable energy consumption and investment costs. This also applies to the separation of the ammonium components in the fermentation residue in biogas production. Here, the ammonia-enriched water offers itself as the product of expanded value creation. It is suitable for use as an industrial solvent and as a usable component for removing nitrogen from exhaust in power plants. This could bring about definitive improvements in the gains situation and ecobalance assessment of biogas facilities. In the case of the solid residue, phosphorus compounds are potentially of interest as valuable substances; consequently, their separation and collection by means of extraction processes should receive closer consideration. Due to the very limited resources in terms of renewable raw materials, the use of organic residue from foods processing must be taken into account in the optimization of the fermentation technique, since this could bring about a clear increase in the biogas share of total bioenergy quantities. However, these raw materials cannot be used by the facility operators without economic disadvantages due to the regulations of the German EEG (renewable energies act). Expansion of raw material utilisation and fermenter techniques with adaptable space-time yields in the case of high solid matter content seems promising. In addition, it is also important to take a look at the use of “green gene technology” for developing better energy plants.

» **Potential for improvements:** Due to the limited quantity of available renewable raw materials, the innovations discussed above are urgently needed to make the sufficient substitution of fossil energy carriers possible. Furthermore, an expanded product portfolio would definitely reduce dependence on subsidies. Regarding

these economic and ecological aspects, it is also necessary to look at the export market in environment technology, since global competitiveness would then be decisively improved within this major growth market.

### 3.1.3 Production of hydrogen

» **Development line:** Hydrogen is being considered as a promising energy carrier in future energy systems. Since hydrogen is not an energy source, it must first be produced from an available energy source. This requires the provision of efficient conversion processes.

» **State of the art:** Hydrogen is largely produced from hydrocarbons, mainly from natural gas, through steam reforming or partial oxidation. The majority of currently produced hydrogen is directly used for ammonia or methanol synthesis or in refinery processes. Only a small share is traded as hydrogen. Hydrogen generation from hydrocarbons is largely optimized from energy viewpoints.

» **Deficits and development goal:** In view of the foreseeable shortage of fossil energy sources, particularly hydrocarbons, a transition to hydrogen as an energy carrier would require new access routes to hydrogen; basically, known processes for hydrogen production would have to be optimized which so far have not been utilised for cost reasons. The goal of development lies in the provision of regeneratively produced hydrogen at costs which are comparable to future costs for fossil energy carriers.

» **Technical-scientific challenge:** Currently, electrolysis of water is the best developed technology. Electrolysis itself is already operating at high energy efficiency (> 60 %). However, the generation of the required electrical energy (power plants, photovoltaic cells, wind etc.) typically tends to remain inefficient. Hydrogen generation without a detour via electrical energy through thermochemical processes has potential for higher energy efficiency. On the other hand, most of the discussed processes involve unanswered questions about long-term stability and scalability. Catalytic water splitting, which is the most attractive route at first glance, remains far from satisfying space-time yields both when using solid catalysts and with the utilisation of biochemical or biomimetic systems.

» **Solution approaches:** In the sector of electrolysis cells, alternative catalysts could lead to higher efficiency both for the anode process and for the development of high-temperature electrolysis cells. However, the low efficiency of electricity generation remains a problem. Interesting thermochemical processes have been developed in connection with high-temperature reactors and solar tower power plants. Here, it is important to improve the existing systems and identify further chemical routes which are suitable for hydrogen production via thermally driven redox cycles. Investigations of catalytic water splitting processes are still in their initial stages. Promising approaches utilise new solids for the direct use of radiation energy in water splitting processes, or imitate the function of plant photosystems at a molecular level, or attempt – in some cases by using gene technologically altered organisms – to obtain satisfactory hydrogen production rates in bioreactors.

» **Potential for improvements:** The improvement potential is largely found in the change to another, CO<sub>2</sub>-neutral basis for hydrogen production. Current production is based on fossil energy sources which are finite, even though coal resources still have a relatively long lifetime. The solution approaches which were outlined above will render hydrogen production from renewable energy sources considerably more efficient. In fields such as catalytic water splitting processes on solid materials, it should be possible to increase efficiency to a higher scale. It is likely that this would usually be sufficient to make hydrogen production from fossil energy sources competitive.

### 3.1.4 Non-conventional fuels

» **Development line:** Alternatives to currently used fuels, which are largely based on mixtures of hydrocarbons, are methanol (with a research octane number of 100) as well as dimethyl carbonate, DMC (research octane number ca. 110) as a replacement for Otto fuels and dimethyl ether, DME (cetane number from 55 to 60), as replacement for diesel fuel.

» **State of the art:** The large-scale production of methanol from synthesis gas is a state-of-the-art technology. The ability to transform this into a product mixture which corresponds to the quality of premium gasoline

is similarly state of the art. Likewise, it is state of the art to obtain DME through the catalytic dehydration of methanol. Furthermore, processes which enable the production of methanol and its dehydration into DME in a single step have been developed. Beside the classic route via phosgene, there are several new approaches for the production of dimethyl carbonate on a phosgene-free basis. Currently, the route via oxidative carbonylation of methanol on copper chloride as catalyst seems to be the most well developed. Concepts which are based on the transformation of methanol with carbon dioxide have also been investigated.

» **Deficits and/or development goal:** Primary development goals include the following:

- 1) the production of methanol through selective direct oxidation of methane (viz. without synthesis gas as an intermediate product);
- 2) the production of methanol using CO<sub>2</sub> as a source of carbon (requiring hydrogen from – wherever possible – renewable sources);
- 3) direct production of DME from CO and H<sub>2</sub> or from CO<sub>2</sub> and H<sub>2</sub>;
- 4) the production of DMC based on methanol and carbon dioxide with high yields (conversion limited by the thermodynamic equilibrium).

» **Technical-scientific challenges:** Challenges are seen particularly in the fields of catalysis and reaction engineering: in particular, catalysts which selectively transform methane into methanol/DME are required. Likewise, the (catalytic) conversion of CO<sub>2</sub> with H<sub>2</sub> into DME is a challenge if “exhaust gases” are to be included in the production of fuels. This is also true for the production of DMC from methanol and carbon dioxide. In this respect, the major challenges involve the development of more active catalysts as well as options for separating product water from the reaction mixture (e.g. via membranes, to shift the thermodynamic equilibrium).

## 3.2. Provision of electrical energy

### 3.2.1 Generating energy from sunlight

» **Development line:** From today's perspective, renewable energies must encompass significant proportions of the planet's overall energy requirements, which will double by 2050. The potential of wind, water, biomass and geothermal energy together is not sufficient to meet this challenge. By contrast, the radiation energy from the sun which arrives on the planet exceeds these energy requirements several times over. The goal of all developments in the solar cell sector must therefore lie in obtaining a sufficiently cost-effective, efficient and long-lived technology to make energy from the sun better usable.

» **State of the art:** Solar cells of crystalline silicon are currently dominating the market. Sun energy cannot be utilised in a cost-effective manner with today's solar cell technologies. It is expected that the thin-layer solar cells, the development of which is not yet market-ready (α-Si, μc-Si, CdTe, Cu(In,Ga)Se<sub>2</sub>), will provide the next generations of solar cells. To be competitive, drastic cost reductions in existing technologies are required, and new cell concepts based on new materials will also be needed.

» **Deficits and development goal:** The transformation efficiency of solar cells is limited by the energy threshold (band gap) of the respectively utilised semiconductor. In order to capture the greatest possible range of sun spectrum frequencies, semiconductors with a small band gap are used. This has the disadvantage that the energy of photons which exceeds the bandwidth is partly lost as heat. Therefore, the goal must be to obtain a more efficient transformation of light into electrical energy through suitable cell and module architectures.

» **Technical-scientific challenges:** Cell architectures which transform light at various energy levels into smaller linked steps probably form the concept which has the best chances of realization. Such a process is already used today in the high-performance cells for space travel. Now, simpler realization routes for such multi-band gap cells are required (at more competitive costs). Corresponding cell concepts can only be realized on the basis of new materials.

» **Solution approaches:** Both inorganic and organic solar cells can be used for the implementation of multi-band gap solar cells. Inorganic multi-band gap concepts are possible with the aid of interband states in a material. Through a simple structure of stacked layer structures, organic cells can be structured into so-called



tandem cells, which are switched in series. Herein, the synthetic variety of organic semiconductors permits the optimal coordination of the absorption characteristics of the respective layers.

» **Potential for improvements:** If solar modules with a price-performance ratio just below 1 €/Wp (Watt peak) were to be successfully produced, the generated electricity then becomes competitive at today's consumer prices. It may be possible to reach this goal with presently developed thin-layer technologies.

Clearly moving below this mark to approx. 0.20 €/Wp would mean that solar energy has to be able to hold its own alongside the current primary energy costs. This can only be done with new technologies. A simple calculation shows that the goal is worthwhile: With an efficiency level of 25%, 0.3 % of the planet's land area is required to cover a total energy requirement of 28 TW in 2050 through solar energy – provided that corresponding storage methods and distribution routes for the generated energy are available by that time.

### 3.2.2 Fuel cell technology

» **Development line:** The efficiency of energy transformers can make a decisive contribution to saving fossil energy carrier resources and therefore helping to protect the climate. Fuel cell systems are already efficient, even in small-scale performance ranges. The aim would be therefore to develop cost-effective fuel cell systems with a long service life as building blocks of a future energy supply structure.

» **State of the art:** Various fuel cell types are known: The development lines are based on various material combinations which, in turn, require various operating temperatures. The spectrum ranges from room temperature to 1000°C. The application spectrum of the fuel cells differs correspondingly. They can be used to serve as driving power in electrotraction, mobile or portable electricity generators, or for the stationary generation of electricity and heat. Combined-heat and power supply (CHP) is the measure which could already be implemented today without major difficulty or a new infrastructure, and could make a significant contribution to increased efficiency if fuel cells were available at competitive costs. The applicable energy carriers for fuel cell technology range from using pure hydrogen for powering automobiles, through the utilisation of methanol and other liquid energy carriers for applications in the small-scale performance range, to natural gas and biogas for the stationary sector. Large-scale hydrogen production from fossil energy carriers is state-of-the-art. Decentralised units in the small-scale performance range are often in demand for fuel cell systems, at least as a transitional technology, until renewable electricity is available for electrolytic hydrogen production.

» **Development goals:** The utilised materials are generally ones where new chemistry is potentially important. Materials, catalysts and particularly the electrodes and electrolytes of the fuel cell itself are important work fields. In terms of the materials, cost reduction and processing methods which are suitable for mass production are important. Catalysts are required both in the electrodes of the fuel cell itself and for the provision of hydrogen – precious metals are frequently involved. Further reduction of the required amounts of precious metals and better catalytic properties are goals in development. The service life of electrolytes and electrodes under operating conditions is also in need of improvement.

» **Technical-scientific challenges:** High power densities up to several Amperes per cm<sup>2</sup> coupled with safe separation of fuel and air and a service life which is equal to the state-of-the-art technologies, are basic requirements for the new materials – while simultaneously reducing material costs. The nature of the membrane itself and the optimized production of membrane electrode units (MEE) are core issues the fuel cells. Perfluorinated membranes for the membrane fuel cell show high chemical stability, at least to approx. 80°C; however they are expensive and require precise water management. The molten carbonate fuel cell operates at 650°C with molten salt as its electrolyte – here, questions about corrosion and the solubility of the cathode material in the electrolyte dominate the material aspects. Yttrium-doped zirconium oxide is a good oxygen ion conductor for solid oxide fuel cells operating at temperatures of 900 – 1000°C, which represents a difficult challenge for all other materials. Improvements – including those which are very application-specific – are important prerequisites for the market introduction of fuel cell technology.

» **Solution approach:** For membrane fuel cells, intensive research into new electrolytes is already taking place. Better conductivity and service life is presently attained through modification of fluorinated polymers. A working temperature higher than 100°C requires entirely new approaches. Inorganic-organic hybrid mem-

branes are being developed, wherein the inorganic component is hydrophilic and temperature-stable, so that the attributes of the resulting hybrid membrane may be better in respect to both these properties. When the inorganic materials exhibit proton conduction, good conductivity attributes are to be expected. In a second route, functionalized silicon-organic membranes are being developed on the basis of zeolites and hetero-polysiloxane substances. A stable carrier material is functionalized, or it is even possible to fill a porous substrate. The greatest challenge surely continues to lie in obtaining high conductivity coupled with anhydrous proton conduction. This is the starting point for the third development line involving intrinsically conducting polymers.

For the molten carbonate fuel cell, research primarily involves modifications of the known materials to reduce the corrosion. More detailed long-term tests are being conducted to optimize material properties.

On the other hand, there is also a need to search for new electrolytes with sufficient ion conductivity at lower temperatures for solid oxide fuel cells. Oxidic systems, e.g. those using cerium, gadolinium or scandium, are candidates. However, it is simultaneously necessary to pay attention to the processing ability, with a thermal expansion coefficient which matches the electrode materials, as well as good material availability, so that a complex set of tasks remain to be resolved. The particle size of the starting materials, the coating processes for MEE production and the sintering process determine the quality of the solid oxide fuel cell. Major advances have already been achieved in terms of service life and performance density.

» **Potential for improvements:** Determining the overall potential for improvement which can be obtained through the use of fuel cells is a complex set of tasks. Here are three examples: According to a simulation example, the use of stationary fuel cells in the energy supply of a single-family home could save approx. 18 % in CO<sub>2</sub> emissions and 23 % in energy costs by comparison to conventional heating technology, thereby realising a reduction of electricity usage from the network which amounts to 81 %. For larger stationary fuel cell facilities, merely the fact that CHP is realized brings about a decisive advantage compared with conventional energy supplies. A 20 – 50 % reduction in energy consumption, and thereby CO<sub>2</sub> emissions, was determined. For fuel cell vehicles with hydrogen fuel, vehicle efficiency levels of more than 37 %, corresponding to 3.8 l diesel equivalent, are obtained over 100 km (compared to 26 % with combustion motors), so that a CO<sub>2</sub> reduction is possible even with hydrogen from natural gas. CO<sub>2</sub> emissions are reduced by nearly 100 % through the use of regeneratively produced hydrogen.

### 3.2.3 Thermoelectric devices

» **Development line:** Thermoelectric energy conversion transforms heat into electrical energy. If it were more efficient, this type of electricity generation would find widespread use. Electricity can be generated from waste heat, for instance in combustion processes (motor vehicles, airplanes, ships, garbage incineration) and power plants.

» **State of the art:** Nevertheless, thermoelectric electricity generation is still finding only limited use. However, it has been held in high esteem for some decades especially in space travel and in the telecommunications industry. Furthermore, field tests in the USA involving thermoelectric modules that generated electricity from the exhaust heat of diesel trucks (to run the accessories) have proven the practicality of this approach for the reduction of gas consumption of automobiles.

» **Deficits and development goal:** The presently utilised materials operate with a conversion efficiency below 10 %. Here, innovative materials with higher efficiencies must be developed by materials chemists. Interdisciplinary collaborations are needed to optimize the physical properties.

» **Technical-scientific challenges:** Thermoelectric materials must possess low conductivity combined with high electrical conductivity. This is the greatest challenge, since materials with high electrical conductivity also usually exhibit high thermal conductivity. This is due to the fact that the charge carriers causing the high electrical conductivity similarly exhibit high thermal conductivity.

» **Solution approaches:** Various research groups are following different approaches. On one hand, attempts are being made to reduce the thermal conductivity of known materials such as Bi<sub>2</sub>Te<sub>3</sub>/Sb<sub>2</sub>Te<sub>3</sub> and PbTe by means of nanotechnology without reducing the electrical conductivity. On the other hand, new materials are

being synthesized, their properties explored, and then good candidates are being optimized with respect to their thermoelectric performance. The latter approach largely utilises the PGEC concept (PGEC = phonon glass, electron crystal), which is based on the fundamental idea of developing materials whose heat conductivity behaves as in a glass, and whose electrical conductivity is similar to that of well-ordered crystal. Promising materials include  $\text{CsBi}_4\text{Te}_6$  as well as several compounds of the clathrate family, the skutterudite type and the  $\text{Ir}_3\text{Ge}_7$  type. First field tests have already demonstrated the technical viability of some of these new materials.

» **Potential for improvements:** Within the past ten years, the thermoelectric figure-of-merit, calculated from specific material properties (and the temperature), has been more than doubled, from approx. 1 to significantly above 2 (higher values correspond to greater efficiency). An end to this increase is not envisaged, and theoretically, there is no limit. Experts expect materials with a figure-of-merit of 3 – 4 in the near future; this would then enable large-scale utilisation of thermoelectric energy production from waste heat and solar heat.

### 3.2.4 Continued development of power plant technologies

» **Development line:** Coal-fired power plants will continue to provide the backbone of the electrical energy supply for a long time. The continued development of power plant technology should lie primarily in the reduction of  $\text{CO}_2$  emissions through increased power plant efficiency. A route which is being discussed today involves power plant concepts in which the  $\text{CO}_2$  emissions are avoided through the separation and storage of the  $\text{CO}_2$  in subterranean storage facilities.

» **State of the art:** Today,  $\text{CO}_2$  emissions from coal fired power plants account for approx. 30 % of all  $\text{CO}_2$  which is emitted within Germany. Throughout the world, the black coal power plants which are in operation only reach average efficiency levels of approx. 30 %, whilst new facilities reach efficiency levels of more than 45 %. On average, the facilities require 480 g of coal to generate 1 kWh of electricity and emit approx. 1100 g  $\text{CO}_2$ , whilst modern power plants only emit approx. 750 g  $\text{CO}_2$ /kWh.

» **Deficits and development goal:** Fundamentally, reduction of  $\text{CO}_2$  emissions from burning coal in power plants can be obtained through two routes, namely by increasing the efficiency as described above, or by separating the  $\text{CO}_2$  in the power plant and subsequently placing it in subterranean storage units.

» **Technical-scientific challenges:** Fundamentally, upgrading the efficiency of the power plant requires elevation of live steam pressure and temperature. Controlling these working steam conditions requires the development of new materials which are usable to the live steam temperatures of 700°C, which is the present target.

Regarding  $\text{CO}_2$  separation, the great challenge lies in the development of processes which can be operated economically and with high availability levels in the large operating units that are customary in power plant technology. Focal points for development include the demonstration of suitable coal gasification processes, the development of oxygen combustion and the development and testing of large hydrogen turbines. Further important development goals include new washing fluids for separation of the  $\text{CO}_2$  from the combustion gas as well as a reduction in energy consumption during the regeneration of the washing solutions. The development of processes for  $\text{CO}_2$  separation which are well suited to being retrofitted into existing power plants would also be of importance.

» **Solution approaches:** Regarding the material developments which are necessary to elevate the efficiency levels, various materials are already being tested in a realistic power plant environment in cooperative ventures between power plant operators and power plant builders. An interesting solution approach to upgrading power plant efficiency in the case of brown coal is the pre-drying of the moist raw brown coal with steam in a fluidized bed dryer. Similarly to the case involving the elevation of the working steam parameters, this development promises an efficiency increase in power plant efficiency by up to 4 percentage points.

Regarding  $\text{CO}_2$  separation, three process routes are currently regarded as promising. The so-called pre-combustion technology is based on the IGCC (integrated gasification combined cycle) process in which the coal is first transformed into a synthesis gas in a gasification step.

A subsequent conversion with the addition of water vapour produces a combustion gas which largely consists of  $\text{CO}_2$  and  $\text{H}_2$ . The  $\text{CO}_2$  is separated before the actual power plant process by means of a synthesis gas washing process. The energy of the gas, which is high in  $\text{H}_2$ , is transformed into electricity in a combined gas and steam turbine process. The second process route is the oxyfuel process, in which the nitrogen is separated from the combustion air by means of a preceding air separation facility and then only the remaining oxygen is brought to combustion. The flue gas which leaves the steam generator then consists of approx. 70 % carbon dioxide. The remainder largely consists of water vapour which can be condensed out by cooling the flue. The third process route consists of separating the  $\text{CO}_2$  out of the flue gas of a conventional power plant process, and currently various processes are being discussed and considered as options for this gas scrubbing process.

» **Potential for improvements:** All processes which lead to "CO<sub>2</sub>-free" power plants have one thing in common: the removal of  $\text{CO}_2$  is linked to a 5 – 14 percent loss of power plant efficiency – highest in post-combustion processes. The spread of the parameters already indicates the large potential for future developments. Merely replacing the black coal power plants which are in operation worldwide and have an average efficiency level of 30 % by modern facilities with an efficiency level of 46 % would result in as much as a 35 % reduction of  $\text{CO}_2$  emissions from black coal fuelled electricity generation. The continued development of power plant technology in the direction of increased efficiency therefore provides a lever for reaching both nationally and globally significant reductions of  $\text{CO}_2$  emissions. However, the integrated  $\text{CO}_2$  separation which can only be implemented on a large scale after a longer development and demonstration phase reduces the efficiency levels again, which – if it must be accepted due to intensifying climate change regulatory problems – leads to increased fuel consumption and therefore elevated use of fossil raw material resources.

## 3.3. Provision of heat energy

### 3.3.1 Materials for collectors

» **Development line:** The exploitation of solar and geothermal energy requires collectors which can absorb and store solar energy or geothermal heat. Energy efficiency levels up to 75 % are currently attainable.

» **State of the art:** Customary types of thermal collectors range from flat devices to vacuum tube collectors and parabolic trough collectors. Vacuum tube collectors include "getter" metals such as barium to provide a longer lifetime. The most important components of collectors are specific absorber materials, heat insulating layers (polyurethane foam, mineral wool), reflectors and heat carriers. The latter usually comprise mixtures of water with propylene or ethylene glycol. The absorbers must be black, thin and possess good heat conductivity. They consist of sheet metals (copper, aluminium) with highly selective coating materials or of glass tubes which are optimized for maximum absorption and minimal emission. Coatings consist either of "black" chromium (fine needles) or of „black“ nickel – both of which are electro plated. They reach absorption coefficients (sunlight 0.4-0.8  $\mu\text{m}$ ) of up to 96 % and emission coefficients of 8 % to 12 %. Alternatively, absorbers comprise layers of aluminium nitride, metal carbide or blue titanium oxide nitride which are applied by high-vacuum deposition or sputtering processes. These coatings reach excellent emission coefficients around 5 % and can therefore perform noticeably better, particularly at high operating temperatures. In these cases, absorption parameters of approx. 94 % for sunlight and emission parameters of less than 6 % are reached for the infrared radiation which is re-emitted due to the absorber's own temperature (wavelength approx. 7.5  $\mu\text{m}$ ). Glass with particularly high transmission levels is used to cover the collectors. It is specialized low-iron, hardened borosilicate glass or anti-reflective glass. Increasingly, trough-shaped, so-called compound parabolic concentrator (CPC) reflectors are employed. They collect radiation within a specific angle range and focus it onto the absorber. Outside this range, some of the incoming radiation is reflected back out of the collector. Additionally, there are white diffuse reflectors which are made from very pure aluminium.

» **Deficits and development goal:** Electro plating with absorber materials such as chromium or nickel is ecologically and toxicologically problematic. The novel materials for the absorber coating – carbide, nitride and oxide nitride – are relatively costly in terms of synthesis, application and processing. Further absorber materials must be sought and developed. The goal is improved economy with the same efficiency.

» **Technical and scientific challenges:** The operational efficiency of the solar or geothermic installations is still lower than stated above, since the mounting of the collectors depends on the structural situation and is thus often suboptimal. A collector design which is less dependent on angles would significantly favour the economy of the process. Vacuum tube collectors already represent an improvement in this respect – however, there is still room for improving their long-term leak tightness.

» **Solution approaches:** An interdisciplinary approach of material synthesis and deposition of thin layers will lead to optimised absorber substances. Their conditioning and application must be modified in order to obtain greater tolerances regarding the angle of incoming solar radiation.

## 4. Energy storage

### 4.1. Materials storage

» **Development line:** For the foreseeable future, large quantities of energy can only be stored in the form of energy-rich compounds, which must generally be produced through chemical reactions. For reasons of secure supplies and to balance seasonal variations in demand, such storage methods will also be urgently required in the future, and will affect a large part of the total transformed energy.

» **State of the art:** The material storage of energy is currently based mainly on fossil energy sources. This includes stored supplies of coal, oil (and its derived products) or gas. In a future energy system which is no longer or not exclusively based on such substances, alternative storage media are required.

» **Deficits and development goal:** Research in this field must take place in close coordination with the development of future fuels. In a future energy system, gasoline and diesel fuel produced from coal, solar energy or biomass via the routes named under 3.1 are likely to continue to play the main roles. These substances would then also serve as significant material storage methods in themselves, since their energy density exceeds that of most other substances. In this case, no special new challenges would result for material storage. Methanol, ethanol, biodiesel and other possible liquid fuels could also be used similarly, using again customary technology.

On the other hand, hydrogen, which is subject to intensive discussion as an energy carrier and fuel, has major new requirements for its storage. Physical processes are linked to a series of disadvantages (low storage density, energy losses) which make other solutions appear sensible in the long term. Here, chemical storage methods for hydrogen might represent interesting alternatives, with the goals for such developments including higher storage capacities, low energy losses, acceptable costs and the highest possible safety standards.

» **Technical-scientific challenges:** However, to date, none of the chemical storage methods is thus far practicable in technical applications. Sorptive systems do not reach the required storage capacity except at low temperatures and simultaneously high pressure. Hybrid storage systems also have insufficient capacity within the relevant temperature range, and the kinetics of these systems is too slow. The energy balance seems to be unfavourable across the entire process chain for a variety of other systems, especially those which require off-board regeneration.

» **Solution approaches:** Numerous development lines are currently being followed to solve these problems. Complex light metal hydrides are still largely unresearched, numerous possible compounds are not yet described, and neither the structure nor the thermodynamics are known for many known hybrids. Technically usable systems could be found in this field. The linkage of several reactions to shift the thermodynamics of the overall system into a more favourable range is also of interest. Concerning sorptive storage methods, “metal organic frameworks” (MOFs) appear to provide storage capacities which clearly exceed those of carbon. Both in the field of MOFs and in the field of hydrides, the utilisation of theoretical methods for the exploration of the possible parameter fields is promising. Hydrogen storage in covalent compounds such as methanol or ammonia also seems possible. Here, however, it would be necessary to find efficient methods for the synthesis and release of hydrogen. Furthermore, the direct use of such molecules as energy carriers / storage media must always be considered as an alternative.

Finally, there are potential material storage systems based on energy-rich solids. For instance, silicon and carbon are being discussed as possible energy stores. However, the considerably simpler handling of liquid energy carriers / stores makes it seem unlikely that solid energy stores will play a significant role.

» **Potential for improvements:** The system decision for a new energy carrier / storage medium should be considered very carefully, since the consequences are enormous. In particular, it seems important to verify the production of the current energy carriers/stores from renewable energy sources and compare this approach with the transition to new energy carrier/storage media, both in terms of economic aspects and with regard to the overall energy balance. Since the nature of the energy carrier/storage medium concerns a large part of energy consumption, even slight differences in the overall efficiency of the systems could have major effects on the entire world energy requirements.

## 4.2. Storage medium

» **Development line:** In a highly technological society, electrical energy holds a special place, since it is almost universally usable in any location and can be changed into other energy forms such as light, heat and mechanical energy. The bidirectional storage and supply of electricity without a detour through other energy forms is preferable but difficult to achieve. Electrochemical storage media such as rechargeable batteries (accumulators) and electrolytic double layer capacitors (supercaps) are particularly suited to this purpose. In comparison to other electricity storage media, in which electrical energy is statically or dynamically stored as heat or mechanical energy, electrochemical systems are superior with respect to performance, energy density and efficiency. Another advantage lies in their favourable operating conditions which permit the mobile or stationary use of batteries at normal pressure and relatively low temperatures. A disadvantage is that batteries only provide direct current and the voltage of individual cells is relatively low (1-3 V). Furthermore, safety and environmental aspects have not yet reached optimal levels in some systems.

### 4.2.1 Batteries

» **State of the art:** So far, only relatively few accumulator systems have become technologically ready for markets and are commercially available. A dominant position is held by the lead acid battery, whose technical development and optimization for various applications is most advanced. It has a broad spectrum of applications which range from starter batteries via emergency current supplies or railroad, airport and mining applications, through to onboard electronics in airplanes and boats as well as backup systems in the telecommunication sector. The nickel cadmium, nickel metal hydride and lithium-ion batteries with their simpler technical handling are better suited to small mobile devices. They are indispensable for the operation of high-tech electronic devices such as mobile phones, digital cameras, or laptop computers.

» **Development goals:** Further applications will open up for the mobile use of batteries in the future. In the consumer area, accumulator operation of electrical tools, such as screwdrivers and drills (cordless tools) and other small devices such as lawnmowers, continues to expand. This requires high-performance batteries with improved energy and power density. However, electrical accumulators might also gain increased importance in the future as electrical power sources for road vehicles alongside fuel cells. Hybrid cars are especially of topical interest – such as Toyota's Prius, whose propulsion concept is based on a combination of a combustion engine and a battery. At the present time, such systems make nearly exclusive use of nickel metal hydride batteries. In the medium term, however, the trend is likely to be towards high-performance lithium-ion batteries, which have better chances as a standard technology for technical and economic reasons. The market of lithium high-energy batteries for mobile devices is mainly served by manufacturers from the Asian region. However, various German companies, together with established research institutions, are already engaged in lithium technology along the value added chain (materials suppliers – component producers – cell producers – battery assemblers – system integrators) in order to gain a technological advantage and market leadership using large-scale lithium batteries.

Furthermore, there is a need for electricity storage devices to cover peak loads of power networks as well as to act as buffer systems for discontinuously operating sun or wind power plants far from networks. These applications require accumulators with high storage capacities and these are not so far available. Research and development of modern accumulator systems, such as redox-flow batteries, could also be significantly expanded in this direction.

» **Technical-scientific challenges:** Since the fundamentals of electrochemical electricity storage devices are well known, advances in the field of accumulators can basically be obtained solely through optimization of the material characteristics and the components. The goal must be improved performance properties and characteristics, such as energy and power density as well as cycle stability and service life.

» **Solution approaches:** In the field of lithium ion batteries, advances in the direction of higher performance through new electrode materials and electrolytes are possible. Anodes and cathodes with higher charging and discharging capacities must be developed (lithium intercalation). Higher energy densities can also be obtained through higher cell voltages, e.g. through cathodes made from mixed oxides of the type  $\text{LiMPO}_4$  with (M = Co, Ni, Mn). Here, special attention should be focused on the reactivity of the electrode in contact with the electro-

lyte (SEI = solid electrolyte interface). New mesoporous structures could be found by nanostructuring carbon as an alternative to conventional graphite. Greater safety and stability of the lithium systems should be possible through the substitution of organic liquid electrolytes by polymer electrolytes, more stable electrolyte salts and electrolyte additives as well as by employing new overload protection mechanisms.

### 4.2.2 Supercaps

» **State of the art:** The principle of electrical energy storage in supercondensers, also known as supercaps or ultracaps, is of a purely physical one and is based on the recharging of the electrolyte double layer (Helmholtz layer) which is formed at the phase boundary of an electron conductor in contact with an electrolyte. No chemical substance transformation takes place here. The first patents for the use of such double layer condensers were registered as early as 1957. In comparison to conventional capacitors, supercaps have a much greater storage capacity. Parameters of 100 Farad/g based on active charcoal as the active electrode material with approx. 1000  $\text{m}^2/\text{g}$  specific surface are typical. This makes it possible to reach energy densities of 5–10 Wh/kg. Compared with batteries, supercaps can release this energy much more rapidly during discharge and provide high electrical power of more than 20 kW/kg in the short term. However, the specific energy is much lower than with batteries.

» **Development goals:** Applying double layer capacitors together with batteries or fuel cells is aimed towards increased performance and service life of the electrical components. Supercaps might also be usable as replacements for batteries. They gained a lot of attention in the 1990s in connection with the development of hybrid cars. Here, they fulfil the function of short-term energy storage which, in addition to the fuel cell or battery, covers peak power loads and can additionally recuperate brake energy. Today, companies such as Maxwell Technologies, EPCOS, Panasonic, NEC, NESS and others are investing in this technology.

» **Technical-scientific challenges:** In order to achieve a significant market share, the specific energy data and the performance data of supercaps must be improved further.

» **Solution approaches:** One way to increase the energy and performance density is by increasing the nominal voltage from approx. 2.5 V to 3 V with an equal cycle stability of approx. 500 000 charging/discharging cycles. As with batteries, research into new electrode materials and electrolytes, such as ionic liquids, is of central significance here. Optimization of the design with reduced volume and weight is another option. Customized pore systems and functional characteristics of the three-dimensional electrode structures could lead to improvements through nanotechnological applications. All in all, better use should be made of synergies in the future developments of double layer capacitors and lithium ion batteries.

### 4.2.3 Stationary electricity storage media

» **Development line:** The increased significance of regenerative electricity generation, particularly wind energy and – in the future – photovoltaics, takes the existing power networks to the limits of their current capabilities. The increasing discrepancy between electricity supply and demand can only be covered by expanding storage capacities. Due to the large spatial distances between wind farms and pump storage plants, investments into electrical power grid expansions are required. The costs for this and the limited hydroelectrical storage capacities necessitates a search for further solutions.

» **State of the art:** Electrochemical storage devices offer one of the most important options. Earlier attempts to store electricity in the MW range with the aid of lead batteries had limited success. The stationary sodium-sulphur battery with ceramic electrolytes as separators is currently winning the market in Japan. As "classic" batteries, these two systems have a modular structure: Each individual cell contains the entire redox-active mass. Inevitably, this results in high system costs. Redox flow batteries overcome this modular limitation. These separate the electrochemical cell from the storage of the redox systems, similarly to what takes place in fuel cells. So far, redox flow batteries have only been developed to the pilot stage. Canadian, English and Japanese companies were or are leading in this field.

» **Deficits and development goal:** Even though many of the named technologies were developed in Germany or were owned by German companies, these development lines have not been followed through.

A large share of the know-how is no longer readily accessible. The situation can only be rectified using new innovative approaches. However, for success early on, new research and development activities need to address as a coherent whole separate areas such as ionic liquids, new solid electrolytes, separators, electron conductors and electrode materials.

» **Technical-scientific challenges:** Redox flow batteries in the multi-MW range are chemical large-scale structures with a performance class of chloralkali electrolysis plants. Selection and evaluation of possible redox systems must take place in the same manner, and using similar criteria to those that would be applied when assessing a safe, cost-effective large-scale chemical process.

» **Solution approaches:** The necessity of a cost-effective solution requires a new system approach and the early inclusion of all interested parties (energy producers, network operators, politics, engineering sciences, and research of basic principles). Here we can observe how chemistry fulfils an integrating function in an exemplary manner.

» **Potential for improvements:** The structure and the cost targets of the future European energy networks define the potential for the new developments which must be taken up. The expansion of the electrical power grids and alternatives for storing electricity (keyword: hydrogen economy) will compete with these new batteries, but will also profit from them.

## 5. Efficient energy utilisation

### 5.1. Luminescent materials and light emitting diodes

» **Development line:** Currently, drivers for research and development of luminescent materials and/or light emitting substances include:

- 1) New technical applications which require the utilisation of new materials.

Included here are flat screens, dielectrical barrier discharge lamps, electroluminescent screens and lamps, optical storage media, and modern tomographic devices.

- 2) Discoveries of novel materials which initiate new applications.

Here, particular attention must be given to the so-called quantum dots as well as two-photon luminescent materials from which transparent luminescent components, optical imaging and diagnostics in medicine, three-dimensional image structuring in displays, new laser applications, as well as highly efficient, energy saving screens and lamps can in principle be developed.

Organic light emitting diodes, abbreviated as OLEDs, are thin-filmed, light-emitting components derived from organic semiconducting materials with structures similar to that of an inorganic light emitting diode (LED). OLEDs can be used to fabricate flat light sources, which is why this technology is utilised primarily for new lighting methods (lighting tiles) and screen applications (such as mobile telephones, PC or laptop screens, televisions and displays in the automobile sector). Due to the workability of these materials, the use of OLEDs as flexible displays and/or as E-paper is possible and likely.

» **State of the art:** The large number of known light emitting substances have been developed and optimized for activation by means of UV light, X-rays or electron beams. However, the use of these materials (e.g. under the conditions of a Xe gas discharge such as a plasma display panel, or as a dielectrically obstructed discharge or as a light emitting diode) is often only possible with significant limitations.

» **Deficits and development goal:** Bearing in mind numerous general requirements (such as energy efficiency, service life, production costs, emission spectrum, light extraction, material stability, biocompatibility), new light emitting substances for the named new applications still need to be discovered, and known materials with potential for delivering some of these requirements must be suitably modified and optimized. For OLEDs however, insufficient stability in particular remains a major problem.

» **Technical-scientific challenges:** Challenges lie mainly in the production of thin, stable, flexible and cost-effective layers for application as screens and light sources, in the energy efficiency of the systems, as well as in the usability / biocompatibility of light emitting substances for medical diagnostics and therapy. The interdisciplinary interplay of the participating fields of expertise as well as the 'material' and the 'component/device' is of decisive significance for each particular case.

» **Solution approaches:** Some solution approaches, which can be named here, are nitride materials on the one hand (e.g.,  $\text{LaSi}_3\text{N}_5:\text{Eu}$ ) as light emitting substances in light emitting diodes, or fluoride salts (e.g.  $\text{LiGdF}_4:\text{Eu}$ ) as a two-photon light emitting substance on the other hand. Both material classes received almost no attention as efficient light emitting substance materials until a few years ago. Quantum dots (such as ZnS or CdSe) as well as nano-scale light emitting substances in general represent a promising solution approach with regard to thin, flexible, cost-effective screens and light sources. Furthermore, the latter are of great interest in medical diagnostics and therapy. However, chemical syntheses of nitride light emitting substances for LED applications is – so far – costly and only possible in small substance quantities. Further problems lie in their emission behaviour and the chemical-physical stability. Among the nano-scaled light emitting substances, quantum dots show high-energy efficiency and light yield. However, intrinsically, they often possess significant levels of toxicity coupled with comparatively low chemical-physical stability.

In OLEDs, model-supported coordination of the individual components (emitter, matrix, hole conductor, hole blocker, electron conductor and electron blocker) shows promising approaches for the future. The discovery of new material classes is broadening the choice of material base. However, in addition to the materials, the fabricated structure of the OLED devices is also decisive for performance. For instance, important influential parameters include the choice of carrier materials, order and thickness of layers, use of doping substances and purity of the utilised materials. To improve the quality of light emission, materials with adapted refraction indexes are also being examined.

» **Potential for improvements:** Currently, approx. 10 % of generated electrical energy is used for lighting purposes. Some of it is very inefficiently transformed into light by means of incandescent bulbs. Light emitting substance lamps have an energy efficiency of approx. 30 %. If one assumes an improvement in efficiency factor of 2, which is almost certainly conservative, the calculated potential savings equal 5 % at least.

## 5.2. Superconductors

» **Development line:** Superconductors allow nearly loss-free transport of electricity and reduction of the size of structural components in energy technology due to the high current density. The discovery of high-temperature superconductors and the possibility of producing layers of yttrium-barium-copper oxide (YBCO) on metallic carriers (coated conductor – CC) makes it possible to extend the application of the systems from niche areas into many fields of energy technology.

» **State of the art:** Global activities concentrate on the development of CCs, which are already being produced in lengths up to >200m using various techniques. Operating prototypes in energy technology, such as a 600m high-voltage cable (Albany/NY), 4 MW motor (Siemens) or residual current limiters, are successful in practical tests, but these are still based on a relatively expensive silver-containing BSCCO (bismuth-strontium-calcium-copper oxide) conductor of the first generation, since the corresponding material lengths and qualities of the YBCO CC are still absent.

» **Deficits and development goal:** The development of CCs is currently concentrating on upscaling to greater lengths of 300 – 500 m and in improving both transport flows and field dependencies through the designed introduction of nano-scale flow anchoring centres into the superconducting materials. Shortfalls in currently utilised vacuum deposition processes include limited production speeds, expensive facilities and high manufacturing costs. However, a clear positive factor is their reproducibility. For economic reasons, another development goal is to obtain the high reproducibility and current-carrying abilities of vacuum deposited layers using chemical manufacturing processes as well.

» **Technical-scientific challenges:** The most important current challenge is the production of all deposited layers (superconductors and buffer protection layers) by chemical means from cost-effective preceding stages with a simultaneously simplified conductor structure in order to lower the costs of the conductor to a value which is economically attractive. Special difficulties are presented by the required cubic structure of the layers, an optimized microstructure in the superconductor, and the avoidance of unwanted chemical reactions in the layer structure. Further novel processes which generate the nano-scale flow anchoring centres with a specific orientation, both homogeneously and simply, must be pursued. In addition, the production processes must comply with modern environmental regulatory requirements.

» **Solution approaches:** To solve these problems, numerous development lines are currently being followed using chemically based technologies, such as MOCVD (metal-organic chemical vapour deposition) and MOD (metal-organic deposition) on textured substrate bands using dip coating as the manufacturing process. The layer textures are adjusted through growing on cube textured substrate bands. Nano-scaled inclusions are additively produced by foreign particles or as initiated defects in phase formation. Important aspects include the attainment of high deposition rates through new, adapted starting chemicals and a homogeneous, highly textured microstructure of the layers.

» **Potential for improvements:** Chemical deposition processes are currently regarded as being capable of achieving an economic breakthrough even in the mid-term. The electric current carrying properties and magnetic field tolerances of the best known short-term prototypes examined to date open up expectations of major improvements in the performance and structural size of electrotechnical components. The electric current

carrying capacity of the CCs is beginning to exceed that of the high-temperature superconductors of the first generation by a factor of more than 3, and they are therefore likely to take the place of these materials in the future.

## 5.3. Lightweight materials

» **Development line:** Fast running and/or accelerated machines and components in process technology and biotechnology must aim in the future to be lighter, safer, thriftier and simultaneously ecologically compatible – and all of this has to be attained whilst maintaining a high level of competitiveness and with the creation of the greatest possible value creation. The potential conflicts between these properties coupled with trends for weight-optimizing multi-material design a large variety of materials, each with accompanying advantages and disadvantages, make it easy to anticipate the complexities of these tasks.

The purpose of using modern lightweight materials in the motor vehicle industry lies in the reduction of fuel consumption by reducing the masses which have to be moved. Compared to the other alternatives, such as reducing rolling and air resistance as well as improving the level of effectiveness in the drive train, the manufacture of new lightweight structures is the most promising route to be pursued.

» **State of the art:** Modern lightweight structures currently utilise a multitude of different metallic, polymer and ceramic materials in order to correspond to different product requirement profiles in terms of mechanical, thermal and medial loads. Due to the widely adjustable spectrum of available plastics, their use is increasingly observed in many current products. To increase their thermomechanical parameters, plastics are reinforced with fibre and particle materials, although another option for improving component materials attributes lies in the use of polymer blends and copolymers.

Furthermore, in addition to the classic lightweight materials (e.g., titanium, aluminium and magnesium) lightweight structures using modern steel-based materials have also gained great significance. In the automobile industry, new steel materials dominate chassis construction; the combination of high strength combined with simultaneous good processing attributes places these in the foreground here as the materials of choice.

» **Deficits and development goal:** In the development of lightweight components within machine and facility construction as well as in the areas of process technology and biotechnology, high value is placed on recording the complex strain conditions the materials may be subjected to. In addition, implementation of appropriate design concepts in accordance with the properties of the materials and their structure, and including any applicable manufacturing restrictions, is required. At the present time, constructive and material separation of the carrying function from corrosion and wear protection (among others) is commonly required. This arises from the fact that the available range of materials is only able to fulfil the thermomechanical, medial and tribological requirements within limits. For instance, additional wear and corrosion protection layers are applied to the weight-bearing structures.

Therefore, the goal for developments in material technology and design lies in new lightweight structures with high functional integration, in which (e.g. through the use of new lightweight materials) both thermomechanical and functional requirements are fulfilled simultaneously.

» **Technical-scientific challenges:** Currently, it is especially the specific operating temperature limits of plastics and fibre compound materials with a polymer matrix which limit their large-scale utilisation. However, it is true that modern high-performance polymers are expanding these limitations.

However, the greater costs of production and processing still mean that these improved performance materials usually remain too costly for industrial applications.

» **Solution approaches:** To solve the conflicts of goals involved in developing cost-effective improvements in materials performance, lasting and close cooperation between material developers, designers and technologists is required along the entire value creation chain. Aside from the development of new plastics and polymer-based fibre composites with application-oriented properties, the further development of near-net-shaped processes is of leading importance for cost-effective component manufacturing.

Through the use of special copolymerisates, new lightweight materials can be prepared for a large variety of industrial applications. This makes it possible to adjust both the required thermomechanical parameters and functional characteristics, including for example acoustic, tribological or electrical parameters.

Novel possibilities for new lightweight structures are also offered by including new textile reinforcements in plastics, which are tailored to meet the required operating loads. The variable, direction-dependent structural properties of components which are made from textile composites are created in a simultaneous process of material construction and component design, which – unlike conventional materials – necessitates a particularly close linkage of all process stages. This makes it necessary to work out fundamental knowledge about all steps of the value creation chain, starting with the filament via hybrid yarn, semi-finished products and textile performs, through to consolidated components and parts, in a function-integrating multi-material design with reproducible quality and short cycle times.

For metallic materials, current research is focused on the following fields: in steel materials, new production methods for the production of high-alloy steels are being studied, and new processes and coatings for fabrication at elevated temperatures are being examined. In titanium, current efforts are being concentrated on the improvement and modification of production processes in order to counteract the very high material prices. There are also many different research projects involving aluminium at this time. However, it would be especially worthwhile if the identification of novel alloys which could be fabricated through welding for use in the air travel industry were to transpire. In magnesium, aside from improved corrosion resistance and heat resistance, the development of easily fabricated, cost-effective sheet metals for automobile chassis construction particularly stands out at the present time.

» **Potential for improvements:** The continued development of lightweight materials has significant potential for energy savings in the future. In automobile construction, for instance, the reduction of 5 % of the chassis weight could produce approximately 3 % savings in fuel consumption.

#### 5.4. Nanoporous foams

» **Development line:** Rising energy costs represent a major challenge for our industrial society, in which approximately one third of consumed energy is used for heating and cooling of private housing and working environments. In order to make more efficient use of this energy consumption whilst simultaneously maintaining living comfort, it is necessary to develop new materials and/or new systems with significantly improved thermal insulation properties. Furthermore, such materials are urgently required to help reduce CO<sub>2</sub> emissions in line with sustainability requirements and regulations.

» **State of the art:** At this time, building thermal insulation primarily utilises mineral wool, expanded polystyrene (EPS, XPS), polyurethane (PU) and a large variety of composite systems. Both in new construction and in refurbishment, composite systems containing vacuum insulation panels or latent heat stores are already being used in small quantities to obtain improved energy efficiency.

» **Deficits and development goal:** Even though vacuum insulation panels (VIP) with very good thermal insulation properties are available today, this technology has not so far been able to make its mark significantly within the field of construction. This is primarily due to the fact that the existing VIP technology is, in many ways, not sufficiently robust, as well as being too cost-intensive. Consequently, the required development goal is to develop a material or system which is approximately at the level of the VIP in terms of its insulation properties and – in terms of its mechanical robustness as well as life time – is at least as good as the present conventional systems, such as mineral wool or PU. The added costs entailed from using such a system must be assessed every few years against the clear environmental benefits arising from a lower energy consumption.

» **Technical-scientific challenges:** Even though it is known that a foam material with a cell or pore size in the range of the average free path length of the cell gas molecules is extremely efficient in reducing heat transfer, there is currently no class of materials which possesses the required overall profile in terms of desired material properties. The production of nanoporous foams through conventional foaming processes has been unsuccessful so far, despite major efforts, and is physically almost impossible. The production of nanoporous polymer

foams through a wet chemical process (e.g. from a gel) is technically possible, though very demanding in terms of the structuring and drying behaviour (compared to earlier attempts in the production of silica aerogels).

» **Solution approaches:** In particular, the polymerization of organic monomers in a structure-oriented (templated) process can be utilised to produce materials with low density and small pores. In order to avoid cost-intensive steps such as the supercritical drying process of the reaction medium, corresponding chemical modifications must be made to the structure of the foam.

» **Potential for improvements:** To obtain a very high efficient thermal insulation effect, the primary requirement in addition to nanoporosity consists of very low foam density. Thus far, a density which is comparable to that of conventional foams has not been successfully produced, and probably represents the greatest technological challenge. Low foam density is of decisive importance not only for the performance of the material, but also for the economy, since only relatively thin film foams can be produced economically. Other questions with major significance include processability, handling, service life etc. – these all depend strongly on the choice of the polymer system.

## 6. Energy efficiency of chemical production processes

Technical processes in the chemical industry are frequently linked to high-energy input requirements. In the chemical industry, the average proportion of energy costs compared to total operating costs equals about 10 %, but it ranges from 2 % in the pharmaceutical industry to 40 % in basic chemicals industry. It can be seen that basic chemicals industry, along with metal production and the processing of stone and earth materials, is among the greatest energy consumers. Energy-efficient manufacturing of products therefore represents a major challenge for the chemical industry.

The potential for energy savings ranges from the energy optimization of entire locations and facilities (transport, packaging, lighting, heating etc.) to the improvement of individual devices, processes and reactions. Regarding the energy efficiency of facilities, German chemistry already takes a leading position in international competition. German construction of chemical facilities offers systems with the highest standards in the areas of environment, safety and health. In order to maintain and/or expand this leading position, advances are particularly required in the development of innovative product lines and in corresponding production processes/technologies.

### Three points are of fundamental importance:

- Each product has a specific minimum energy consumption or gain, given through the energy difference between the reactant and the product, which cannot be exceeded or undercut even with perfect processes.
- An activation energy must be overcome in most chemical reactions in order for the reaction to proceed.
- Product processing is often very energy-intensive due to associated costly separation processes.

The following technologies can make significant contributions towards further increases in the efficiency of chemical processes:

### CATALYSIS

Catalysis, which plays some role in the production of at least 80 % of all products manufactured in the chemical industry, continues to be a key technology within chemistry. Catalytic reactions can lower the activation energy, thereby increasing the selectivity of a required reaction and, if desired, catalysts can also enable the reaction to take place at lower temperatures. The continued development of catalysts is therefore of decisive importance for improving the energy efficiency of chemical processes.

### MICROREACTOR TECHNOLOGY

In microreactor technology, reducing the dimensions of chemical reactors down to the millimetre or even micrometre range results in an intensification of the efficiency of heat and substance exchange processes. Amongst other things, this brings about greater selectivity and higher yields in chemical reactions, and thereby, higher energy efficiency of processes.

### NEW REACTION MEDIA, SUCH AS IONIC LIQUIDS

Ionic liquids are highly polar salts which are usually liquid at room temperature. They can be utilised in reactions both as solvents and as reactants, and consequently they can frequently open up more selective reaction routes in processes. Intelligent solvent systems can be designed to form two phases after the reaction is complete, which means that product separation can be carried out with much better efficiency.

### NON-CLASSICAL FORMS OF ENERGY INPUT

A method for reaching the highest energy efficiency in processes can be to improve the selectivity and specificity of energy input using less conventional energy sources (e.g. electrons, microwaves, plasma, light, ultrasound). Amongst other things, this enables access to new products with new functionalities which may be difficult to obtain through conventional processes. However, this technology is only worthwhile when the effect of using these energy sources leads to an acceleration of the reaction rate or an increased product yield the benefits of which outweigh the higher intrinsic costs that may accompany utilising these energy sources.

### PROCESSING OF PRODUCTS

It is also a worthwhile goal to further develop technologies which enable increased product yield in a process so that the target product is present in the highest possible concentration even before processing takes place. Amongst other things, this goal can be attained through catalytic processes, the use of the microreaction technology, and reactions in ionic liquids.

Furthermore, the development of innovative separation processes is of high significance for lowering energy costs. This includes, for instance, chromatographic processes, which can now be used on a large scale. A practical example is the use of ionic liquids as solvent in extractive distillation, which makes it possible to obtain energy savings of up to 60 % as compared to customary processes.

### PROCESS INTEGRATION

Process integration is concerned with the reduction of the number of process steps through the combination of several process steps into a single process. This concept may involve either the linkage of heat and substance transport or the combination of reaction and separation in one device and these lead to significant reductions in operating costs and energy input for the overall process.

All described technologies represent innovative concepts in process intensification; that is, they make contributions to economically and ecologically improved efficiency of chemical processes, as well as to the generation of new products and product qualities. To increase the energy efficiency of production processes, a holistic process perspective is necessary, which includes everything from the chemical reaction to the formulation of the product and the further development of accompanying innovative technologies.



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