The Energy Frontier
(Curator Ferdi Schüth)

At a glance: Fundamental insight into the basic processes underlying energy transformation processes can strongly improve existing technologies and open up novel energy options.

While “energy” is a central and well defined concept in many scientific disciplines, in the mind of the public this term is mostly associated with the “immaterial substance” that powers the world, i.e. which lights our lamps or heats our houses. Many aspects of energy science are of a highly applied nature and thus do not belong to the original realm of the Max-Planck Society. However, on the underpinning of basic science, which is the main mission of Max-Planck Society, there could emerge completely new possibilities for supplying the world with energy. When Einstein, one of the first directors of the Kaiser-Wilhelm-Gesellschaft, the predecessor of the Max-Planck-Society, developed his famous formula $E = m c^2$, he could hardly have envisaged that this would lay the foundation for the biggest single one activity of the Max-Planck-Society nowadays, the development of nuclear fusion to a point where it can be used as a means of providing virtually unlimited amounts of energy to the world.
Fusion energy relies on the combination of hydrogen isotopes to form helium nuclei. In this process, vast amounts of energy are released which in principle could be harnessed to generate electricity. However, this harnessing process is extremely complex, since the fusion reaction only takes place in a plasma in which temperatures of several ten million to several hundred million Kelvin prevail. The confinement of such a plasma at sufficiently high density for sufficiently long time is a formidable challenge. Since no material can withstand the conditions in such plasmas, the confinement has to rely on magnetic fields. Presently two main development lines for magnetic confinement are being pursued, the so-called Tokamak- and the alternative Stellarator-concept, and for both lines the MPI for Plasmaphysics (IPP) plays a leading role. In a Tokamak, the plasma has a toroidal shape – more graphically, it can be described as a donut. This configuration forms the basis of the ITER project, a big international collaboration which has been created to build the first fusion experiment that produces more energy than needed for heating the plasma. ITER will thus be an important step on the way to the production of useable fusion energy. However, there are still challenging questions to be solved, concerning both basic physics problems and also the materials which are exposed to the plasma. Probably the biggest obstacle for the ITER concept, which also requires most fundamental work, is the discontinuous energy production. The very nature of the Tokamak principle implies pulsed plasma operation which may need storage systems to fulfill the requirement of continuous energy supply by a commercial power plant. If a tokamak can be run in continuous plasma operation hence is a matter of intensive fundamental research.
The alternative concept of magnetic inclusion, the Stellarator principle, may provide a radically different alternative. The operation principle does not – other than for the Tokamak - require a current in the confined plasma itself, and therefore in principle allows continuous operation. This advantage has to be paid for, though, by a very complex shape of the plasma which requires very complicated magnetic coils. Based on decades of basic research and the tremendous increase in computing power, a Stellarator design optimised with respect to several physics constraints such as low transport and high stability, the so-called Wendelstein 7-X experiment – is under construction at the IPP in Greifswald. Experiments are foreseen to start in 2014, and it is expected that exciting new directions in reactor design could be opened by this large scale experiment.
It is hoped that a design for a demonstration fusion power plant will be fixed in 2030, with the technology choice being dependent on the success in the different development lines. First commercial power plants may start operation in 2050.

However, not all energy-related research is targeting at such long time scales and not all the research in this field reaches this size scale – with a large Max-Planck-Institute focussed on a single and singular problem. Nevertheless, basic science is a major driving force also in other fields of energy research. Electron transfer is at the heart of most processes relevant for our energy supply, ranging from the elementary steps of photosynthesis over charge separation and charge diffusion in solar cells to energy transfer in batteries. Thus, understanding the fundamentals of electron transfer processes and electron transfer systems is of paramount important in many energy related problems. For instance, elucidation of the structural details of the centers responsible for electron transfer in the photosystem of plants may provide the blueprint for mimicking the processes occurring in plants during photosynthesis by simpler, artificial systems[1,2], which could eventually lead to the realization of an old dream, the splitting of water into hydrogen and oxygen by solar radiation with the help of a catalytic system.

Whether this dream can be realized and hydrogen would become accessible by this pathway, or whether other production routes would be more interesting, a hydrogen infrastructure could be an important element of future energy systems. In such a system the availability of suitable methods for hydrogen storage is a key requirement. While high pressure storage or liquid hydrogen are the favored methods now, hydrogen storage in form of chemical compounds would in many respects be favourable, if sufficiently high storage densities at moderate conditions could be achieved. Intensive efforts are being invested in the discovery of such storage compounds.[3]

However, at present it is not clear which molecule would form the basis for chemical energy storage in future energy systems. Research has to explore the available options, synthetic pathways for the production of such storage molecules, and further conversion routes starting with them. In addition, the systemic implications related to the choice of specific storage options, including socio-economic research, have to be considered. While hydrogen is the most frequently discussed storage molecule, other options should be explored as well. Methane, the main component of natural gas, seems to be attractive in this respect. There is well developed catalytic chemistry around methane, and, in addition to the direct use of natural gas, access to methane is possible via the anaerobic conversion of biomass. This is one of the most efficient pathways for the conversion of biomass to a fuel. However, biogas production units contain many different microorganisms, and not all aspects of the metabolic pathways are clear[4]. For instance, the methanogenic organisms, the archaea, have most of the genes required for the direct conversion of glucose to methane. Yet, their synthetic pathway starts with hydrogen and carbon dioxide. The hydrogen is supplied by completely different microorganisms. Understanding – and tailoring - these processes in more detail would be very interesting for the targeted improvement of the productivity of biogas fermenters, not even speaking about the possibilities for genetically modified strands of organisms. As a side remark, methanogenic organisms are also of high relevance in the context of global warming, since methane is a much more potent greenhouse gas than carbon dioxide. Coming back to biogas production plants, while biomass rich in sugars and oils are very efficiently converted to biogas, this is much more difficult for lignocellulose biomass, for instance wood or straw. For this, microorganisms are required which depolymerise the biopolymers forming the lignocellulose.

Such depolymerisation processes are not only of high interest in the complex ecology of biogas plants, but also more generally in chemistry as an important entry point in future biorefineries. Catalysis – as treated in depth in a different chapter – is a key technology for chemical conversion of biomass to fuels and chemicals[5]. Polymeric biomass needs to be broken down and the units produced then need to be converted by controlled chemical reactions to target molecules which could supplement our oil-based value chains in the chemical industry and finally possibly even replace part of the oil-based product slate.

However, fundamental work is required, since conventional chemical transformations rely on the introduction of chemical functionality in hydrocarbon molecules. Biomolecules, on the other hand, are highly functionalized, and controlled defunctionalisation reactions are needed which suggests a paradigm shift in at least part of catalysis science.
Whether biomass is used following pure biological pathways, such as in biogas production, or whether chemical transformations are employed, the overall yield per area could be improved, if plants would produce biomass faster. While breeding has been used in the past to optimize the yield of fruit and seeds – they, after all, form the basis of our food supply – if energy plants are desired, other properties need to be optimized. Thus, a fundamental understanding of the genetic and metabolic requirements for high biomass production is required for improving yield, both by conventional breeding techniques and genetic engineering.
Using biomass for the production of fuels and chemicals is an indirect pathway for harnessing the power of the sun. Photovoltaics produces one of the most versatile forms of energy – electricity – directly. Fundamental semiconductor physics has paved the way for the solar panels as we know them today, based on silicon. While the success of silicon-based photovoltaics is tremendous, polymeric materials as the basis for solar cells promise more cost efficient solutions with a much higher degree of flexibility, with the ultimate dream of paint-on or spray-on solar cells. However, before this goal can be reached, the efficiency of the materials has to be improved and the life-time needs to be extended. This will require fundamental work in the synthesis of novel molecules to be used in organic solar cells and methods for assembling controlled nanostructures which are most probably required for efficient systems. In addition to the electronically functional components of photovoltaic cells, there are sometimes underestimated factors which might nevertheless be decisive. The transparent electrodes rely nowadays on indium-tin-oxide (the so called “ITO”). However, indium is very expensive and its availability is limited. Alternative materials are therefore urgently required. Graphene, single layers of carbon atoms which correspond to one layer from the graphite structure, could become a cheap basis for conducting transparent coatings. Since graphene has been discovered less than 10 years ago, its controlled synthesis is still in its infancy. However, novel bottom up strategies promise great progress in the next years and graphenes obtained by such methods may become one of the key electronic materials of the future.[6]
Novel technologies to guarantee our energy supply are certainly urgently needed. Equally important are methods for efficient electric energy storage. Most renewable energies are supplied in a highly discontinuous fashion, and while the grid can buffer to some extent this uneven energy supply, different kinds of electrochemical storage systems could become key elements in future energy systems. Moreover, the strong move towards electromobility will require either breakthroughs in fuel cell technology and hydrogen storage or highly efficient batteries. Fuel cells for mobile applications will greatly benefit from improved electrodes, which could, for instance, rely on controlled nanostructures, novel high-temperature proton conducting membranes, or improved system designs. Advanced lithium ion batteries or more advanced systems, such as metal-air batteries, will depend on novel materials for electrodes, electrolytes, separators and novel cell designs. Different types of carbon based composite materials promise exciting developments in this field, if the stability of such composite systems can be maintained over sufficiently many cycles. Generally, not only just the materials need to be improved, even greater progress is expected, if novel concepts can be implemented, such as the creation and use of hierarchically organized systems in which, for instance, electronic and ionic conductivity are improved by the superposition of a transport system on the nanoscale. In addition, understanding the fundamental features of and the processes occurring in nanoscale systems is equally important.[7]
Fundamental materials science does not only play an important role in the development of active components of solar cells or batteries. Immediate effects on our energy system can also

be expected by the use of lightweight structural materials, which can substantially improve energy efficiency in a number of different ways. High performance polymers and novel alloy steels which provide excellent mechanical properties at reduced weight can immediately lead to savings in fuel consumption of the cars produced by such lightweight materials. High temperature ceramics, such as for instance Si-B-N-C materials, produced via suitable precursor routes, could help to increase the operation temperature of motors or turbines.[8] Since such systems are Carnot-machines, increasing the operation temperature immediately leads to improved energetic efficiency. Another interesting field where basic materials science has shown its strength is the search for novel thermoelectric materials, which generate electric energy directly from temperature differences. While little progress had been made over decades, in recent years novel structure types and novel nanostructuring concepts promise new opportunities.[9]

Energy questions are often discussed solely on a technological level, involving exclusively views from the natural sciences and engineering. Input from the social sciences and the humanities is rarely sought. It is now increasingly acknowledged that this is often not appropriate, as the decade-long discussions concerning nuclear energy have demonstrated. Many important questions of energy science have to be asked by sociology, law, economics and related sciences. Novel energy systems need innovations, and thus the fundamental questions, how innovations are generated and diffuse into society are crucial when the step from scientific discovery to technological implementation should be made. Also fundamental studies in decision making are important in our energy systems. In choosing energy technologies, there are typically complex choices to be made while some information is typically missing. The fundamental principles governing such decisions are important in many fields, but especially also in selecting components of our energy systems. Since our energy infrastructure is becoming more and more integrated within Europe and also the world, questions of international law are gaining increasing importance. It needs, for instance, to be studied how rules and contracts can be formulated which are long term stable in changing socio-political environments.

Perspectives: Energy science in the future can only be strong and successful over long periods of time, if it can rest on a strong basis of fundamental research into the basic processes governing energy transformations, basic materials science, and the socio-economic framework conditions in which our societies implement energy systems.

Electron transfer is crucial in most energy transformation processes, and a fundamental understanding of multi-electron transfer processes will provide stimulus for fields such as artifical photosynthesis, fuel cell science and photocatalytic water splitting. Materials science, increasingly supported by theoretical models, calculations, and predictions, will be used to study the effects of nanoscaling of materials on electronic properties which are important, for instance, for photovoltaics, thermoelectrics and batteries, or on structural requirements for high temperature and lightweight materials. Catalytic processes govern the key transformations of our current energy infrastructure and biomass transformation pathways, i.e. progress in catalysis has immediate consequences on our energy systems. Understanding the factors controlling plant growth and metabolism of microorganisms can help the breeding or genetic modification of organisms with improved energy performance, and which are targeted at the production of desired compounds. Social sciences and the humanities will provide answers on how our energy consumption patterns can be influenced to meet the supply structure, and vice versa, technology has to optimize energy supply to satisfy demand. The fields traditionally active in energy science, the natural sciences and engineering, will be more closely integrated with social sciences and the humanities in the future to tackle questions of our energy systems. This close interaction between different branches of science is important in many fields of science and technology. In the energy field, it is not just beneficial, on the long run it will be mandatory in order to solve one of the biggest challenges of this century.

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