BASIC RESEARCH NEEDS TO ASSURE A SECURE ENERGY FUTURE

A Report from the

Basic Energy Sciences Advisory Committee

Basic Research Needs To Assure A Secure Energy Future

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DEDICATION

This report is dedicated to the memory of Dr. Iran L. Thomas, Director, Division of Materials Sciences and Engineering, and Deputy Director for Basic Energy Sciences, Office of Science, United States Department of Energy. Iran passed away on February 28, 2003.

For many years, Iran was a major contributor to the design of the materials science program supported by the Office of Basic Energy Sciences. Throughout, he was always careful to emphasize that a primary responsibility of the program was to support first-class science. He was a strong advocate of the Basic Energy Sciences Advisory Committee, and he often commented on the valuable contributions that BESAC has made to the program.

His vision was a guiding force in the creation of the BESAC subpanel whose work is contained in this report. Without his contributions, and his leadership, it is doubtful that this report could have been produced. We are grateful that he had the opportunity to review the report before his death, and that he was so pleased with the result for which he had worked so hard.

Throughout his career, Iran's leadership and personal contributions helped to shape the basic materials research program in the United States. He will be sorely missed.

Iran Thomas, in his weekend working garb, is shown with the reports on the status and future of x-ray and neutron scattering research facilities. Iran's leadership fostered many of these reports through both BES and BESAC.

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REPORT OF THE BESAC SUBPANEL ON BASIC RESEARCH NEEDS TO ASSURE A SECURE ENERGY FUTURE

EXECUTIVE SUMMARY

Current projections estimate that the energy needs of the world will more than double by the year 2050. This is coupled with increasing demands for "clean" energy – sources of energy that do not add to the already high levels of carbon dioxide and other pollutants in the environment. These coupled challenges simply cannot be met by existing technologies. Major scientific breakthroughs will be required to provide reliable, economic solutions.

In October 2002, a workshop was held to assess the basic research directions that will assure a secure energy future. Over 100 scientists and engineers from academia (27%), industry (16%), and federal laboratories (39%) and agencies (18%) participated in the workshop. As a resource for the workshop participants, a factual document was compiled that summarized the state of energy sources and use at a national and international level. The discussion groups, or topical teams, at the workshop were organized by energy source and energy use. From the Department of Energy (DOE), both basic and applied mission representatives were included in each of the teams.

The results of the workshop are a compilation of 37 proposed research directions (PRDs). At a higher level, these fell into ten general research areas, all of which are multidisciplinary in nature:

- Materials Science to Transcend Energy Barriers
- Energy Biosciences
- Basic Research Towards the Hydrogen Economy
- Innovative Energy Storage
- Novel Membrane Assemblies
- Heterogeneous Catalysis
- Fundamental Approaches to Energy Conversion
- Basic Research for Energy Utilization Efficiency
- Actinide Chemistry and Nuclear Fuel Cycles
- Geosciences

Nanoscale science, engineering, and technology were identified as cross-cutting areas where research may provide solutions and insights to long-standing technical problems and scientific questions. The need for developing quantitative predictive models was also identified in many cases, and this requires better understanding of the underlying fundamental mechanisms of the relevant processes. Often this in turn requires characterization with very high physical, chemical, structural, and temporal precision: DOE's existing world-leading user facilities currently provide these capabilities, and these capabilities must be continuously enhanced and new ones developed. In addition, requirements for theory, modeling, and simulation will demand advanced computational tools, including high-end computer user facilities. All the participants agreed that the education of the next generation of research scientists is of crucial importance; and this should include making the importance of the energy security issue clear to everyone.

It is clear that assuring the security of the energy supply for the U.S. over the next few decades will present major problems. There are a number of reasons for this. The most important of these is the current reliance on fossil fuels for a high proportion of the energy, of which a significant fraction is imported. The Developing World countries will have greatly increased needs for energy, in part because of the expected population increase, and in part because of the increase in their presently very low standards of living. A second problem is related to concerns over the environmental effects of the use of fossil fuels. Third, the peaking of the production of fossil fuels is likely within the next several decades. For these reasons, it is very important that the U.S. undertakes a vigorous research and development program to address the issues identified in this report.

There are a number of actions that can help in the nearer term: increased efficiency in the conversion and use of energy; increased conservation; and aggressive environmental control requirements. However, while these may delay the major impact, they will not in the longer run provide the assured energy future that the U.S. requires. It is also clear that there is no single answer to this problem. There are several options that are available at the moment, and many – or indeed all – of them must be pursued.

Basic research will make an important contribution to the solution to this problem by providing the basis on which entities which include DOE's applied missions programs will develop new technological approaches; and by leading to the discovery of new concepts. The time between the basic research and its contribution to new or significantly improved technical solutions that can make major contributions to the future energy supply is often measured in decades. Major new discoveries are needed, and these will largely come from basic research programs.

It is clear from the analysis presented in this report that there are a number of opportunities. Essentially all of these are interdisciplinary in character. The Office of Basic Energy Sciences (BES) should review its current research portfolio to assess how it is contributing to the research directions proposed by this study.

The BES Advisory Committee (BESAC) expects, however, that a much larger effort will be needed than the current BES program. The magnitude of the energy challenge should not be underestimated. With major scientific discoveries and development of the underlying knowledge base, we must enable vast technological changes in the largest industry in the world (energy), and we must do it quickly. If we are successful, we will both assure energy security at home and promote peace and prosperity worldwide.

RECOMMENDATION: Considering the urgency of the energy problem, the magnitude of the needed scientific breakthroughs, and the historic rate of scientific discovery, current efforts will likely be too little, too late. Accordingly, BESAC believes that a new national energy research program is essential and must be initiated with the intensity and commitment of the Manhattan Project, and sustained until this problem is solved.

BESAC recommends that BES review its research activities and user facilities to make sure they are optimized for the energy challenge, and develop a strategy for a much more aggressive program in the future.

INTRODUCTION

The world is at a transition in the use of energy. Over the next 50 years, it is expected that energy use will double. The factual document included as Appendix B in this report includes a wealth of statistics and other information on the status of energy use, resources, research needs by energy sector, etc. A brief summary of some of these data follows.

There is a close link between energy usage and Gross Domestic Product (GDP), and thus standard of living. With some variation, this is generally true for all the nations in the world. The per capita energy use in the U.S. is very high. The primary energy resource consumption in 1999 was 102 EJ (97 Quads),* yielding an annual per capita energy use of 100,000 kWh (or 3.4×10^8 Btu).

Of these 102 EJ, 86% was generated from fossil fuels, with nearly one third of this being imported petroleum and natural gas. Nuclear power was about 8%; hydroelectric was 3%, and biomass and other sources was 4%. Electricity generation consumed 36 EJ of this total (35%) and transportation consumed 27 EJ (27%). Two other areas of energy consumption are Residential/Commercial, which consumes 19 EJ (19%), and Industrial which consumes 24 EJ (23%).

Also, about 60% of the 96 EJ used in energy production is rejected energy; that is, energy that is currently lost as heat or through other inefficiencies. The overall efficiency is thus about 40%. Considering energy sectors, the overall efficiency of the transportation sector is about 20%, the electricity sector is about 32%, the residential/commercial sector is about 75%; and the industrial sector is 83% ["U. S. Energy Flow – 1999," Gina V. Kalper, UCRL-ID-129990-99 (March 2001)].

From the point of view of energy security, there are two ways of looking at this information. First, of the 102 EJ of primary resource, 27 EJ were imported; essentially all of which was petroleum, natural gas, and related products. Second, 86 EJ are fossil fuels. While there is argument about the resource base for these, there is no argument that they are finite resources, and thus at some point will be exhausted; well before that, the cost of winning and transporting them will increase.

In the broader context, the energy demand in the rest of the world will increase markedly in the next few years for two reasons. First, the energy availability and use per capita in much of the world is very significantly less than in the U.S. In addition, the GDP and thus the standard of living are also much less. It can be expected that the standard of living will rise in other parts of the world; and particularly in the developing world where the standards of living are very low. Second, current models predict a large increase in world population over the next few decades, from its present level of 6 billion to 10 billion by the year 2050. Most of this expansion will take place in the developing countries. For example, in the specific case of electricity use, it is predicted that over this same time period the per capita demand will increase from its present level of 1,000 kWh per annum, to 3,000 kWh per annum. This is still far below the U.S. current demand for electricity, which is 13,600 kWh per annum; but when multiplied by the population increase it still represents an enormous growth in the required generation capacity. For the case of energy requirements for personal transportation, the current indications are that demand will also in-

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* An exajoule (EJ) is 10^{18} joules (J). The equivalent engineering unit is a Quad, 10^{15} Btu. 1 Btu = 1,055.06 J, so 1 Quad = 1.055 EJ. Also, 1 Kilowatt-hour (kWh) is 3,412 Btu; so 1 Quad is 2.93×10^{11} kWh. A large electricity generating station typically has a capacity of 1 Gigawatt; approximately 33 of these stations running continuously for a year will generate 1 Quad of energy as electricity.

crease greatly over the next few years in the developing world: China is a case where this is beginning to be apparent now.

Further energy-related questions that need to be addressed include environmental issues, notably those related to global warming and the availability of water. Environmental issues also vary with energy source and energy utilization technology.

There are several possible directions to go to address the problem of energy security for the U.S. in the relatively near term, the next 25 to 35 years. It is important to recognize that energy security is not the goal in itself: the goal is to maintain and improve standards of living. Thus, an increase in the GDP/energy ratio is important. This ratio has been increasing over the last several years, but the rate of increase needs to accelerate. This requires a number of steps. First, the efficiency of energy conversion must increase. Next, the efficiency of the end-use of energy must increase. Third, the overall cost of the processes involved in primary resource collection, transportation, and conversion must be reduced.

In the longer term, it is important to address the issue of the finite fossil fuel resources; this is likely to impact petroleum first, and longer-range research needs to address the issue of substitution of other primary sources.

It makes sense to use longer-term research to develop renewable energy sources. While the carbon-to-hydrogen ratio in primary fuels has been progressively decreasing for many years, the potential link between 'green-house gases' and global warming may require this to be greatly accelerated. From the U.S. point of view, energy security is favored by decreasing use of imported primary sources, and this would also argue for the development of renewable sources.

Historically, the approach to these issues has been largely evolutionary: the improvement in the efficiency of the generation of electricity by systems involving large coal-fired boilers by moving towards higher steam temperatures and pressures, for example; or the recent developments in large wind turbines. This research is necessary and important, and is being supported with the DOE by the applied research offices – in particular, Fossil Energy; Energy Efficiency and Renewable Energy; and Nuclear Energy, Science, and Technology.

One of the energy components of the DOE's mission that relates to the Office of Science is best described by the following element of the BES program description (SC-4) appearing in the DOE Annual Performance Plan for FY 2004:

"The mission of the Basic Energy Sciences (BES) program -- a multipurpose, scientific research effort -- is to foster and support fundamental research to expand the scientific foundations for new and improved energy technologies and for understanding and mitigating the environmental impacts of energy use."

The object of this report is therefore to propose basic research directions appropriate for the Office of Basic Energy Sciences (BES) that will deliver scientific knowledge and discoveries related to the applied energy missions. It follows that these research directions will be different and generally concerned with much longer-range objectives than those of the applied mission offices themselves.

PROPOSED RESEARCH DIRECTIONS

The workshop held in October 2002 assessed the basic research needs for energy technologies to assure a reliable, economic, and environmentally sound energy supply for the future. A subsequent activity to discuss Energy Biosciences in particular was held in January 2003. Over 100 people from academia, industry, the national laboratories, and federal agencies participated in these workshops and related activities. (The details on the charge, organization, program, schedule, membership/attendees, and related information can be found in Appendix C. The introductory presentations from the workshop are in Appendix D.)

The leaders of the workshop and the lead authors for the summaries of the discussion were:

- Marvin Singer (DOE Office of Fossil Energy), Fossil Energy;
- John Ahearne (Sigma Xi), Nuclear Fission Energy;
- George Crabtree (Argonne National Laboratory), Renewable and Solar Energy;
- Charles Baker (University of California San Diego), Fusion Energy;
- Lutgard C. DeJonghe (University of California Berkeley), Distributed Energy, Fuel Cells, and Hydrogen;
- Jan Herbst (General Motors R&D Center), Transportation Energy Consumption;
- Mildred Dresselhaus (Massachusetts Institute of Technology), Residential, Commercial and Industrial Energy Consumption;
- Rick Smalley (Rice University), Cross-Cutting Research and Education; and
- John Stringer (EPRI), Energy Biosciences Research.

The discussions at the workshop presented a sense of urgency for the need for basic research to assure the energy supply for the nation and the world. An underlying theme in the discussions was the need for low-carbon energy while adding 13 TW (13 TJ/s) of world-wide energy generation capability (a true grand challenge that was compared to the race for the moon in the 1960s), perhaps more critical in terms of security of the U.S.

There were many scientific and technological challenges across the energy spectrum. Currently there are no viable ways of meeting these challenges. Non-carbon energy sources have daunting difficulties that need innovative solutions for these to become a high percentage of the energy pool. Fossil fuels have equal challenges relative to environmental concerns, as well as the ability to use non-traditional reserves.

The workshop discussions produced a total of 37 proposed research directions, Table 1. The full text of the supporting statements is contained in Appendix A. The summary presentations given by each of the workshop leaders can be found in Appendix E.

These research directions can be aggregated into the following list of general recommendations for basic research directions. The balance of this section is devoted to a detailed discussion of each of these.

- Materials Science to Transcend Energy Barriers
- Energy Biosciences
- Basic Research Towards the Hydrogen Economy

Table 1. Proposed Research Directions (PRDs)

Fossil Energy

- Reaction Pathways of Inorganic Solid Materials: Synthesis, Reactivity, Stability
- Advanced Subsurface Imaging and Alteration of Fluid-Rock Interactions
- Development of an Atomistic Understanding of High-Temperature Hydrogen Conductors
- Fundamental Combustion Science Towards Predictive Modeling of Combustion Technologies

Nuclear Fission Energy

- Materials Degradation
- Advanced Actinide and Fission Product Separations and Extraction
- Fuels Research
- Fundamental Research in Heat Transfer and Fluid Flow

Renewable and Solar Energy

- To Displace Imported Petroleum by Increasing the Cost-Competitive Production of Fuels and Chemicals from Renewable Biomass by a Hundred Fold
- Develop Methods for Solar Energy Conversion that Result in a Ten-to-Fifty Fold Decrease in the Cost-to-Efficiency Ratio for the Production of Fuels and Electricity
- Develop the Knowledge Base to Enable Widespread Creation of Geothermal Reservoirs
- Conversion of Solar, Wind, or Geothermal Energy Into Stored Chemical Fuels
- Advanced Materials for Renewable Energy Applications

Fusion Energy

- Multiscale Modeling of Microstructural Stability of Irradiated Materials
- Deformation and Fracture Modeling
- Plasma-Surface Interactions
- Thermofluids and “Smart Liquids”
- Plasma Aerodynamics

Distributed Energy, Fuel Cells, and Hydrogen

- Advanced Hydrogen Synthesis
- High-Capacity Hydrogen Storage for Distributed Energy of the Future
- Novel Membrane Assemblies
- Designed Interfaces

Transportation Energy Consumption

- Integrated Quantitative Knowledge Base for Joining of Lightweight Structural Materials for Transportation Applications
- Vehicular Energy Storage
- Fundamental Challenges in Fuel Cell Stack Materials
- Integrated Heterogeneous Catalysis
- Thermoelectric Materials and Energy Conversion Cycles for Mobile Applications
- Complex Systems Science for Sustainable Transportation

Residential, Commercial, and Industrial Energy Consumption

- Sensors
- Solid State Lighting
- Innovative Materials for New Energy Technologies
- Multilayer Thin Film Materials and Deposition Processes

Cross-Cutting Research and Education

- Nanomaterials
- Preparing Tomorrow’s Workforce for the Energy Challenge and Heightening the Public’s Awareness

Energy Biosciences Research

- Energy Biotechnology: Metabolic Engineering of Plants and Microbes for Renewable Production of Fuels and Chemicals
- Genomic Tools for the Development of Designer Energy and Chemical Crops
- Nanoscale Hybrid Assemblies for the Photo-Induced Generation of Fuels and Chemicals

- Innovative Energy Storage
- Novel Membrane Assemblies
- Heterogeneous Catalysis
- Fundamental Approaches to Energy Conversion
- Basic Research for Energy Utilization Efficiency
- Actinide Chemistry and Nuclear Fuel Cycles
- Geosciences

Materials Science to Transcend Energy Barriers

Many of the current technological barriers related to energy hinge on improved materials. Thus, materials research is an area in which scientific advances could have a key impact on future energy security. Examples range from high-efficiency lighting to vastly improved solar cells to materials that last longer and function under more severe conditions. Nanomaterials offer the possibility of revolutionary advances while advanced characterization tools, coupled with modeling using parallel computers, may provide the fundamental understanding to improve materials properties for the challenges of the next decades.

The materials theme appeared in nearly half of the proposed research directions. Within these, there are a number of subthemes:

- Nanomaterials
- Materials Degradation
- Composite Materials
- Materials Fabrication Issues
- Advanced Materials and New Materials Opportunities

Nanomaterials. Possible roles for nanomaterials include new approaches to photovoltaics; thermoelectric materials with significantly improved figures of merit based on quantum dots, quantum wires and quantum well geometries; smart sensors of very small size with a wide range of capabilities, including wireless, self-powered, with on-board signal processing, networking, and communications capabilities. A specific need for basic research is the underlying science that will enable advanced robust wireless sensors with multifunctional detection capabilities in terms of variables, including chemistry, temperature, pressure, and other physical parameters, coupled with the ability to transmit the information and to be 'smart' in the sense of acting both as an active remediator and as a part of an interactive system.

Nanocomposites are also proposed as, for example, new battery concepts with significantly improved capacities and semiconductor/polymer nanocomposite photocells.

Another proposed research direction is inorganic, organic, and inorganic/organic hybrid porous materials with pores in the 1-30 nm range as biomimetic materials with the efficiency and specificity of natural systems in light-harvesting, charge separation, and chemical transformation. Nano-scale self-assembly is a related research area with potential revolutionary impact. Related to solar energy, research leading to storage of light energy in the form of high-energy chemicals was discussed as a possible solution. Also as part of this area, there were research directions related to multi-layer thin film assemblies, including creation of explicit mechanistic models that allow precise control and prediction of properties based on deposition conditions and film-growth chemistry. Research is also needed for the development of the next-generation of thin-film deposition techniques and in-situ characterization tools.

Materials Degradation. In systems that generate and use energy, there are pervasive problems with corrosion, high-temperature effects, and radiation-induced damage. These result in degradation of the materials properties, frequently leading to deformation and fracture. Further, there is a critical need to be able to make very confident predictions of lifetimes over very long times – from tens of years for components inside nuclear power reactors to as much as 10,000 years for radioactive waste containment systems. For corrosion processes, the complex chemistries coupled with the effects of radiation make this a very challenging problem. All of the proposed research directions related to degradation issues emphasize the need to develop fundamental understanding of the mechanisms and the increased importance of modeling in future research. These issues are not confined to metallic materials: ceramics, composite materials, polymers, and glasses are among materials that suffer degradation. The degradation issues for nanomaterials, and particularly nanocomposites, were not explicitly considered; but the high surface-area-to-volume ratios and the non-equilibrium nature of many of the composites is likely to lead to degradation in the future applications.

Composite Materials. A composite material behaves in ways that are different, sometimes very different, from materials that are essentially homogeneous. Composite materials for energy applications include not only the well-known polymer matrix-fiber reinforced materials, or metal matrix-oxide particle dispersion-strengthened materials, but also new and innovative materials and structures. Research on novel inorganic/organic hybrid porous materials for advanced light harvesting; advanced, small, dispersed smart sensors; thin-film multilayer concepts; and various nanocomposite materials is recommended. Characterization and modeling of the fundamental phenomena that control structure-property relationships will be of critical importance in realizing the potential benefits of this class of materials.

Materials Fabrication Issues. In the development of truly novel materials, the fabrication often requires specific research in its own right. Joining processes, for example, represent extreme conditions for the materials being joined, and there are generally both spatial and temporal gradients of temperature, composition, and structure. With the new strong lightweight alloys and composites that will be required for more economical fuel consumption, the issues related to assembling these components into a viable structure become very important. Joining of lightweight materials, while retaining their desirable properties, is one particularly challenging research direction. Non-destructive evaluation of joined materials is another. Once again, the path forward will depend on the ability to develop models and evaluation techniques capable of handling these extraordinarily complex problems.

Another proposed challenging research area is the fabrication of thin-film multilayers. This will require the creation of explicit mechanistic models that allow precise control and prediction of properties based on deposition conditions and film-growth chemistry. On the basis of these models, the next generation of thin-film deposition techniques, and the *in situ* characterization tools that will be required by the process control system can be developed.

While these were the specific items related to materials fabrication, it is obvious that many of the other systems described, particularly those based on nanostructures of various kinds, will require substantial research on the fabrication methods including self-assembly. These developments will require a considerable knowledge of the fundamentals of the processes and the evolution of models and characterization tools capable of leading to the design and realization of the necessary procedures.

Advanced Materials and New Materials Opportunities. There are opportunities for innovative materials research that fall outside of the above areas. Examples include materials for solid state lighting, advanced thermoelectric materials, advanced membranes, hybrid solar cells – porous wide bandgap semiconductors with a light-sensitive dye, organic semiconductors, new hydrogen storage materials, and new materials for fuel cell stacks. Development of more efficient and durable building materials – so called smart materials whose properties change with changing environmental conditions – is an interesting area for fundamental materials science.

Energy Biosciences

The use and understanding of biological processes has been a growing area of research. There are reasons to believe that there is a potential for biologically-inspired research to provide solutions to energy issues that we cannot presently imagine. This area was felt to be so exciting that the original workshop group suggested a follow-up workshop specifically to examine these research possibilities. Recommended research areas include biomimetic approaches to solar energy capture and generation of fuels and chemicals. Very exciting is the possibility of using emerging knowledge in functional genomics and molecular technologies to develop plants that are optimized to produce fuels and chemicals. This renewable biomass-generated fuel could eventually replace imported petroleum. The use of biomass could be enhanced if these plants could be made more tolerant of adverse environments, and optimized in terms of nutrient, water, and land use, so that they are not competing with food crops for available land, for example. Another promising research area is the development of biocatalysts to aid in the fractionation of the biomass. An interesting concept was to design-in properties of the plants that would have the effect of addressing the downstream processing of the biomass – a kind of driver for evolution that is totally different from that in a natural system. The development process would be faster with successful research on tools for directed genetic engineering of critical crop properties.

Basic Research Towards the Hydrogen Economy

The development of hydrogen as a substitute to current fossil fuels is a promising area for future energy generation. Consequently, methods of producing and using hydrogen received considerable attention in the workshop discussions. In connection with this, the importance of membranes, not only for separation of gaseous or liquid species, but as components in a fuel cell stack, was discussed extensively. Basic research opportunities recommended here, as in many of the other topic areas, lie not in duplicating applied research, but in fundamental science with the objective of developing appropriate understanding of underlying phenomena and the development of predictive models to guide research to new concepts.

The issue of the production of hydrogen is addressed, noting that some 9 million tons of hydrogen are produced per year in the U.S., primarily through the steam reforming of natural gas. In the future, other production technologies using sustainable feedstocks will be required that do not result in a net production of CO_2. Some of the most daunting research challenges are associated with hydrogen generation through the thermal splitting of water at high temperatures, with the source of the heat being solar collectors or high-temperature nuclear reactors. In thermochemical water splitting, a chemical step is introduced to reduce the temperature needed; however, the chemicals combined with high temperatures and gas production gave rise to very demanding materials problems. The photon energies in visible light are sufficient to split a water molecule, so that low-temperature water splitting using light is possible; the problem is to harvest the light in a way that allows the energy to be directed to a catalytic water splitting reaction. Basic research on fundamental mechanisms would underpin demonstration projects on advanced hydrogen production and help resolve the technological issues that will evolve during this development.

For fuel cell development, an atomistic understanding of high-temperature hydrogen conductors would allow the development of very highly selective membranes capable of operating at temperatures as high as 700^{o}C, using the integration of theory, modeling, and experimentation for new classes of oxide and amorphous metallic proton conductors. Understanding of the interaction of hydrogen with the atomic structure could be enabled with neutron characterization to study both the migration and the storage of hydrogen in various materials. Another approach to this same problem is to study nanocomposite membranes where the transport takes place along their internal interfaces.

The technological issues associated with hydrogen storage are well known. High-pressure storage of hydrogen presents risks that may not be acceptable; liquefaction is unacceptable because of the losses associated with the liquefaction itself, of the order of 30%. Recently, there have been some interesting studies of hydrogen storage using complex hydrides, such as the alanates, $Al(AlH_4)_3$, and others. Basic research efforts to explore the hydrogen storage properties of these materials are virtually nonexistent and is therefore a recommended research direction for the future. A particular issue is the high pressures that are needed to hydrogenate these materials; often the kinetics of the hydrogenation and the dehydrogenation are limiting steps.

Innovative Energy Storage

Energy storage – from traditional battery concepts to non-traditional methods, including hydrogen storage – has research challenges relating to long-term storage and distribution of energy. Use of transient renewable energy sources, such as solar photovoltaic and wind, would be greatly enhanced by improved energy storage. One research area recommended was the study of photoconversion of renewable substrates, such as water, CO_2, and N_2, to produce storable liquid or gaseous fuels. Other basic research directions include catalysis and research leading to inexpensive photoconversion systems. The use of phase transitions in materials as a means for energy storage was also discussed.

Novel Membrane Assemblies

Membranes appear in both new and traditional energy systems including hydrogen separation, fuel cells, environmental applications, etc. Improvements in membranes could lead to more efficient gas separation enabling lower-cost fossil-based hydrogen production processes. The materials problems associated with thermochemical water-splitting cycles for the generation of hydrogen could be reduced by advanced membranes that reduce the temperatures required. Fuel cell operation in the critical 200-600^{o}C range would be greatly beneficial, but it is specifically in this range that functionally useful membranes are yet to be discovered. Fuel cell stack materials, and particularly proton exchange membranes, require significant advances, and these can only be achieved with an improvement in basic understanding of how these membrane materials function. Membranes for fuel cell stacks and for chemical separations using nanotechnology and the development of highly specific membranes to enable economic recovery of elements from sea water, particularly uranium, are future technological needs. Basic research is recommended that will support the establishment of a fundamental understanding of the relationship between membrane structure and functionality.

Heterogeneous Catalysis

Catalysis is of large economic importance to the U.S. economy in a range of energy related areas, especially in the transportation and industrial sectors. Heterogeneous catalysis underlies a number of the concepts proposed for new directions in energy production and utilization. The development of new catalysts is hampered by the lack of detailed structure-function relationships that are essential to the development of a predictive capability for new process concepts and materials design. It is recommended that such research be pursued. In addition, further development of emerging and of wholly new local structural tools that can probe to length scales in the range 0.1-2 nm are required. Other critical research areas include the development of computational models of the governing catalytic reactions and approaches to integration of structural and spectroscopic data to yield self-consistent models of catalyst active sites, gas conversion and particulate oxidation.

Fundamental Approaches to Energy Conversion

Energy conversion, ranging from traditional combustion processes to fuel cells to the conversion of solar and other renewable energy supplies, are key to energy generation, transportation and many industrial processes. Fundamental combustion science to develop predictive modeling of combustion technologies is difficult due to turbulence of the chemically reacting systems. This is particularly true when one considers the very large scale of the combustors in energy generation systems and the complexities presented by the mixing and combustion propagation in internal combustion engines. Basic research to support advances in diagnostic tools, particularly laser-based, and high-performance computing capabilities is recommended as these present real opportunities to advance combustion science and to lead to the development of predictive models to allow improved design of combustors and real-time operation control algorithms. Only by developments of this kind can the environmental standards expected by the year 2012 be attained. Other fruitful proposed research areas are the related topics of heat transfer and fluid flow. These issues include heat transfer in solid-state devices, cooling systems, and heat exchangers. The key concerns are multiphase fluid flow and heat transfer. Recently the introduction of nanophase dispersions in fluids has been shown to produce potentially interesting effects in both fluid flow and heat transfer. However, characterization systems capable of generating data on the behavior of these systems with sufficient spatial and temporal resolution to allow the development of a fundamental understanding are only now becoming available, and this understanding will be essential to develop predictive models.

Improvements in the conversion efficiency of solar devices are critical to the expanded use of solar energy. The issues here include the rapid decay of the photogenerated carriers as they traverse the cells from the generation site to the conversion site. Proposed research areas include the development of interpenetrating network geometries. A related topic is the thermalization of the carriers at high energy levels. There may be potential advantages in utilizing nanostructured materials in circumventing some of the limitations.

Another recommended research area is innovative approaches to convert solar, wind, or geothermal energy into stored chemical fuels. The approaches suggested are: new catalysts to facilitate multi-electron transformations such as those required to produce hydrogen and oxygen from water, or reducing CO_2 to methanol, ethanol, or other carbon based-fuels. Direct solar photoconversion is also a possibility, with the development of photoactive organic, inorganic, or biological molecules or species, which can absorb a large fraction of the solar irradiance and drive the chemical reactions that produce the fuels of interest.

Fuel cells represent possible energy sources for transportation and for distributed power generation. Basic research to make fuel cells feasible for large-scale uses is recommended, including high selectivity membranes and low-cost, high-efficiency catalysts. In addition, utilization of hydrogen or carbon-containing fuels in electrochemical systems depends critically on the properties of interfaces that need to fulfill specific and often conflicting functions. The complexity of the problem requires novel approaches to interface design and modeling.

Extended use of thermoelectric energy conversion requires realization of a significantly improved figure of merit in thermoelectric materials; basic research on quantum well and other low dimensional systems offer this possibility. Possible uses of thermoelectric material systems include improvement in the use of otherwise waste energy in automotive systems.

Basic Research for Energy Utilization Efficiency

Fuel utilization and efficiency are not only important in energy consumption, but also in energy generation – and is an important issue in the use of nuclear fission energy. The research opportunities for improved energy efficiency in the residential and industrial areas are very interesting. Although the actual efficiency of end-use in the residential/commercial sector is quite high, about 75%, it is generally believed that the total amount of energy used in these applications can be significantly reduced. The most important system identified at the workshop was lighting. About 20% of electricity consumption is attributed to lighting. Incandescent and fluorescent bulbs currently provide the majority of that. Incandescent lighting is quite inefficient, with only 5-6% of the electricity consumption being converted to visible light. Fluorescent lighting is more efficient, at approximately 25%. Solid-state lighting, including light-emitting diodes (LEDs), has the potential to exceed these efficiencies. At the moment, white light emitting LEDs are close to twice as efficient as incandescent lights. Future research may result in perhaps an eight-fold improvement over the next 10-20 years. The fundamental physics of the solid-state light emitters is a recommended research area. In terms of new materials opportunities, proposed research directions include nitride-based wide bandgap semiconductors and polymer-based organic electronic materials that have the promise of significant lighting improvements.

Other proposed research areas related to energy generation include catalysis research for improvements in the utilization of fossil fuels. For biomass energy to be viable on a large scale, research is needed that would allow the utilization of marginal land, limited water supplies, and low fertilizer use.

Actinide Chemistry and Nuclear Fuel Cycles

There are a number of concepts currently being discussed for future generations of nuclear reactors in electricity generating systems. For some of these, present roadmaps for future nuclear fuel cycles suggest that fuel reprocessing will be important, and molten salt media may play an important part in improving the efficiency of the recycling process. Fundamental research is recommended that will establish the necessary understanding of the fuel cycle and the chemistry of the associated radionuclides in order to develop efficient processes and to insure the safety and public acceptance of these technologies.

In terms of long-term fuel availability for nuclear fission reactors, it is projected that extraction of uranium from seawater will become economic if the price of uranium increases by a factor of ten. If uranium from seawater is not included, there is sufficient uranium available for 65 years at current consumption rates. While there are additional known amounts of uranium in ore bodies, it will be difficult to recover those. Recycle of nuclear fuels will be critical as the availability of uranium diminishes.

Geoscience

Geosciences underpin discovery of new fossil resources, utilization of hard-to-access reserves and the storage of carbon dioxide in subsurface regions. Locating and extracting technically recoverable reserves of oil and natural gas, particularly in the U.S., is difficult and offers opportunities for high impact research. The two primary directions for recommended research are subsurface imaging and in-situ alteration of fluid/rock interactions. The latter topic is aimed at increasing the mobility of oil and gas phases, thereby increasing the amount of extracted resources. These advanced geoscience technologies will require the development of new fundamental understanding of geophysical, geohydrological, and geochemical processes. Specifically, fundamental research in wave propagation in complex media will provide the understanding needed to make advances in imaging. Rock is a very complex and heterogeneous medium, and the analysis of the propagation and scattering of acoustical waves is a very difficult problem. Furthermore, translating the scattered signals into an image of the geological configuration is also a very difficult computer problem, for which more basic study is recommended.

SUMMARY

This report has highlighted many of the possible fundamental research areas that will help our country avoid a future energy crisis. The report may not have adequately captured the atmosphere of concern that permeated the discussions at the workshop. The difficulties facing our nation and the world in meeting our energy needs over the next several decades are very challenging. It was generally felt that traditional solutions and approaches will not solve the total energy problem. Knowledge that does not exist must be obtained to address both the quantity of energy needed to increase the standard of living world-wide and the quality of energy generation needed to preserve the environment.

In terms of investments, it was clear that there is no single research area that will secure the future energy supply. A diverse range of economic energy sources will be required – and a broad range of fundamental research is needed to enable these. Many of the issues fall into the traditional materials and chemical sciences research areas, but with specific emphasis on understanding mechanisms, energy related phenomena, and pursuing novel directions in, for example, nanoscience and integrated modeling.

An important result from the discussions, which is hopefully apparent from the brief presentations above, is that the problems that must be dealt with are truly multidisciplinary. This means that they require the participation of investigators with different skill sets. Basic science skills have to be complemented by awareness of the overall nature of the problem in a national and world context, and with knowledge of the engineering, design, and control issues in any eventual solution. It is necessary to find ways in which this can be done while still preserving the ability to do first-class basic science. The traditional structure of research, with specific disciplinary groupings, will not be sufficient. This presents great challenges and opportunities for the funders of the research that must be done. For example, the applied research programs in the DOE need a greater awareness of the user facilities and an understanding of how to use them to solve their unique problems.

The discussions reinforced what all of the participants already knew: the issue of energy security is of major importance both for the U.S. and for the world. Furthermore, it is clear that major changes in the primary energy sources, in energy conversion, and in energy use, must be achieved within the next fifty years. This time scale is determined by two drivers: increasing world population and increasing expectations of that population. Much of the research and development currently being done are concerned with incremental improvements in what has been done in the immediate past; and it is necessary to take this path because improvements will be needed across the board. These advances extend the period before the radical changes have to be made; however, they will not solve the underlying, long-range problem.

The Subpanel recommends that a major program be funded to conduct a multidisciplinary research program to address the issues to ensure a secure energy future for the U.S. It is necessary to recognize that this program must be ensured of a long-term stability. It is also necessary that a management and funding structure appropriate for such an approach be developed. The Department of Energy's Office of Basic Energy Sciences is well positioned to support this initiative by enhancement of their already world-class scientific research programs and user facilities.