

CHAPTER 4

RESEARCH & POLICY

Reaching the goals of increased energy security and reduced carbon emissions poses significant challenges for science and technology, but it also creates substantial opportunities for innovative research and development (R&D). In this chapter we highlight some of the key opportunities and identify public policies that are needed to enable the endeavors, maximize the probability of their success and facilitate their introduction into the marketplace.

Introduction

It has become common practice to divide innovation activities into two principal categories: upstream basic and applied research and downstream product development, design and testing. Such a simplistic division belies the complexity of the enterprise, which is far from linear in nature. Nonetheless, the demarcation provides a reasonable way of distinguishing between public and private activities as they are often practiced. Most frequently, the private sector finances and conducts the downstream activities, although in a few cases the federal government funds and actively supports them. Weapons systems and space and aeronautics are two such examples. In both of those cases, however, the federal government is the prime customer for the product.

Five decades ago, private industry also shouldered much of the burden of basic and applied research. It funded the activities privately and, most frequently, carried them out in large central laboratories, such as AT&T's Bell Laboratories, IBM's Thomas J. Watson Laboratories and General Electric's Mohawk Valley Research Center. But today, U.S. technology companies have largely abandoned basic research, and where they perform research at all, they commonly restrict it to applied projects that have very short time horizons, typically no more than three to five years. The reasons for the industrial research transformation are quite well known and we will not dwell on them.

Today, the federal government serves as the principal source of financing for basic research, terminology we assume the reader is quite familiar with and "long-term applied research," a phrase that may require some clarification. In general, applied research does not lead to a change in the understanding of fundamental science. Nonetheless, in some cases the applied research objective may take many years to achieve. Two illustrations, one past and one current, should suffice to illuminate the point.

The first is the development of optical fibers for communication, which began several decades ago with fibers that had "attenuation lengths" of less than one meter, woefully inadequate for their envisioned application. Many years and many research dollars later, scientists figured out how to keep the light from losing intensity over distances of many kilometers, and the fiber communication revolution began.

Today, the challenge of developing a dramatically improved battery represents a prime technological focus for the vehicle of the future, as we emphasized in the chapter on transportation. Many experts believe that applying nanotechnology to lithium-ion batteries—which rely on single electron transfer—holds some of the greatest promise for success. But the scientific problems are difficult and complex and will likely take

years of work to resolve. The task provides a signature example of long-term applied research in the current context.

For completeness, we note by contrast that the development of a multi-electron battery system would fall in the realm of targeted basic research, since it will probably require substantial improvement in our understanding of some fundamental questions in physical chemistry and materials science.

Beyond supporting basic and long-term applied research, the federal government also supports significant shorter-term applied research, but with the exception of defense and space, the work it supports almost always takes place at the pre-competitive stage. Universities and national laboratories act as the primary venues for most federally funded research, although government-industry partnerships, such as FreedomCAR, play a role as well.

Although no one deliberately set out to design the current structure of the U.S. innovation system, the last two decades have shown it to be generally robust, effective and, for the most part, quite efficient. It has been emulated by a number of other nations around the world.

In the case of energy efficiency, the Department of Energy (DOE) serves as the primary source of federal funding for basic research through its Office of Science and for applied research through its Office of Energy Efficiency and Renewable Energy (EERE). In this chapter, we consider the financial and programmatic strengths of these DOE programs and comment briefly on opportunities that the department might have to strengthen its energy efficiency research portfolio. We note that the National Science Foundation, the National Institute of Standards and Technology and several other federal agencies play a secondary role in energy efficiency research, but we do not address them in this report.

Finding 1:

The DOE Office of Science has a broad energy-related mission. Through enacted authorization legislation in 2005 and again in 2007, Congress and the administration have asserted that the DOE Office of Science requires significant funding increases to carry out its basic research mission. However, Congress and the administration failed to agree on appropriating the necessary funds.

Discussion:

The Office of Science generally has received very high performance marks for its research programs. Yet in fiscal year 2008, the total congressional appropriation (including emergency supplemental funding) of \$4.03 billion fell almost 18 percent below the level authorized by the 2005 Energy Policy Act (Public Law 109-58) and the 2007 America COMPETES Act (Public Law 110-69) and 11 percent below the presidential request. In the previous two fiscal years, the congressional appropriations similarly fell far short of the authorized levels. The continued funding deficits make it impossible for the Office of Science to achieve the policy goals established in Public Laws 109-58 and 110-69.

The Office of Science organizes basic research funding related to the energy needs of the nation through five major program areas: Advanced Scientific Computing Research (ASCR), Basic Energy Sciences (BES), Biological and Environmental Research (BER), Fusion Energy Sciences and Nuclear Physics. Although ASCR and BER have responsibility for some activities that can affect future energy-efficiency technologies, BES unquestionably has the largest share. In addition to supporting individual-investigator and team research programs at universities and government laboratories, BES is responsible for operating national user facilities, such as neutron and X-ray light sources, which provide the platforms needed for many facets of the long-term energy-efficiency research

opportunities. For FY 2008, Congress appropriated \$1.27 billion for BES, 18 percent below the presidential request; the shortfall resulted in the cancellation of 200 planned energy research projects at universities and reductions in the operation of many of the user facilities at national laboratories.

In its FY 2009 budget request, the White House proposed establishing a new program of Energy Frontier Research Centers funded through the Office of Science at \$100 million per year. The centers, which would be located at universities, national laboratories and other eligible institutions, would promote “innovative basic research [in targeted areas relevant to energy] to accelerate scientific breakthroughs needed to create energy technologies for the 21st century” and would address a number of areas critical to energy-efficiency technologies. Those areas would include catalysis; electrical energy storage; solid-state lighting; hydrogen production, storage and use; and materials under extreme environments. Although the Frontier Centers program is clearly strategic in its selection of research areas, DOE officials say it would not be excessively prescriptive, but instead would seek “to engage the Nation’s intellectual and creative talent to tackle the scientific grand challenges associated with determining how nature works.”

Recommendation 1:

Congress should appropriate and the White House should approve funds for the DOE Office of Science consistent with the spending profiles specified in the 2005 Energy Policy Act and the 2007 America COMPETES Act. Congress should exercise its oversight responsibility to ensure that basic research related to energy efficiency receives adequate attention in the selection of Energy Frontiers Research Centers.

Finding 2:

Within DOE, indeed within the federal government as a whole, long-term applied research, whether it is general or strategic in nature, often is the orphan child of science and technology programming.

Discussion:

During the 1990s, much of EERE’s programming focused on either short-term applied research or demonstration projects. Although many of these activities were meritorious, the program’s focus on short time horizons prevented it from addressing compelling long-term applied research opportunities of the kind we describe in this report. Today, long-term applied research has begun to enter EERE’s portfolio, a promising sign for further development. However, the support for long-term applied research is still too small compared to the need, and increasing that support under constrained budget conditions carries the danger that other important research may be squeezed out. The hydrogen program provides an example in which accommodating a long-term presidential initiative prevented EERE from adequately supporting other long- and short-term applied research.

Recommendation 2:

To meet the out-year technology goals we have proposed for energy efficiency, DOE must take steps to fold long-term applied research into its scientific programming in a more serious way than it currently does. The department has several options. It can charge the Office of Science with the responsibility and provide the necessary budget, but if it does so, it must protect the culture and budgets of its current basic research programs. It can designate EERE with the responsibility and augment its budget for that purpose, but if it does so, it must be careful not to allow the short-term activities to continue to diminish long-term opportunities. The department can also create a new structure to support long-term applied research or adapt ARPA-E (Advanced Research Projects Agency–Energy) that was established by the America COMPETES Act.

Finding 3:

Historically, coordination between basic and applied research programs within DOE has been far from ideal.

Discussion:

The Office of Science, which has the responsibility within DOE for supporting basic research, has generally done an excellent job, given its budgetary constraints. It designs, constructs and operates at its national laboratories user facilities that provide the technological resources for research conducted by university and industrial scientists and engineers. It also directly supports university and national laboratory research groups across a variety of fields. The Office of Science generally has received high ratings from the Executive Branch's Office of Management and Budget, congressional oversight committees and external review panels.

In recent years, the Office of Management and Budget has also given EERE excellent ratings, and congressional criticism of EERE has focused principally on the reluctance of the White House to request more robust funding for the office and on the relative emphasis of the programs within its purview.

But in the 2005 Energy Policy Act, Congress expressed its concern about poor coordination between the science and technology programs. First, in Sec. 1006 (Improved Coordination and Management of Civilian Science and Technology Programs), the act created a new Under Secretary for Science, who would also serve as the Science and Technology Advisor to the Secretary of Energy. Second, in Sec. 994 (Strategic Research Portfolio Analysis and Coordination Plan) the act required the Secretary to develop a "plan to improve coordination and collaboration in research, development, demonstration, and commercial application activities across Department organizational boundaries." It is too soon to evaluate whether DOE has fully dealt with coordination problems EPACT 2005 identified.

Recommendation 3:

DOE should fully comply with the 2005 Energy Policy Act mandate to improve the coordination between its basic and applied research activities. Congressional oversight committees should ensure that DOE fulfills its obligation.

Finding 4:

The ARPA-E program mission is to bring to market the fruits of high-risk, high-payoff research in the energy sector. ARPA-E is modeled after the Department of Defense's highly successful DARPA program, but its customers are not in the agency that created it, and its mandate is unclear.

Discussion:

ARPA-E is regarded by some as a cross between a venture capital firm and a program to transfer energy technology to industry from DOE's laboratories and universities. Others regard it as a way to re-create the Bell Laboratories of old. It has not yet received funding, although the America COMPETES Act of 2007 authorized it at an annual level of \$300 million. ARPA-E's goals and methodology have to be quite different because ARPA-E's and DARPA's customers differ in kind.

DARPA's customer is DOD, and the relationship between the two is such that DARPA knows what the defense agency needs and wants. Therefore, DARPA can select projects that DOD will likely adopt. For example, ARPANET (the predecessor of the internet), large-scale integration (placing thousands of transistors on a chip) and missile submarines, all DARPA projects, were not outcomes of undirected R&D. They filled a DOD need.

Other venture funds have been created by government agencies. The CIA and U.S. Army created, respectively, the In-Q-Tel and OnPoint funds. NASA started down the same road with its Red Planet Capital fund, but decided not to proceed. As in the case of DARPA, these funds have as their customer the agency that created them.

For ARPA-E the ultimate customer is the private sector, and anything that is developed has to fill a need in a competitive way. It is not just the “thing,” but the cost of the thing compared to other things that is important.

The key question for DOE to determine about ARPA-E is its purpose. Its modus operandi and the nature of its portfolio depend on clarification of its rationale. If ARPA-E is to function as a venture capital firm, it needs the perspective of one. If its investments are in partnership with the private sector, as some DOE R&D programs have been, it needs to have that perspective. If it invests on its own, it needs a particularly hard-nosed group of outside advisors. If ARPA-E functions as a bridge to bringing technologies out of its labs to the private sector, it needs outside advisors who can bring the competitive private sector’s perspective to bear.

Recommendation 4:

ARPA-E, if funded, needs to have its purposes better defined. Its time horizon must be clarified, and the coupling to its ultimate customer, the private sector, needs better focus. This report takes no position on whether ARPA-E should be funded.

Finding 5:

Many long-term basic and applied research challenges and opportunities exist in the area of energy efficiency, and many of them are of a crosscutting nature.

Discussion:

In the previous chapters we described some of the long-term research challenges facing the transportation and buildings sectors, but we placed great emphasis on many of the “on-the-shelf” efficiency gains that can be implemented in the near and intermediate terms using existing knowledge and technology. Here we highlight longer-term prospects, especially those that have crosscutting energy-efficiency applicability. The opportunities we highlight often illustrate the close connections between the basic and applied nature of the research and underscore the need for close coordination of basic and applied research programs.

Recommendation 5:

Many areas of long-term basic and applied research in energy efficiency offer unusual opportunities. A sample list follows, and a more complete description of each appears in the endnotes of this chapter. In the case of transportation, we note that the opportunities we highlight often illustrate the close connections between basic and applied research and underscore the need for close coordination of the two activities. In the case of buildings, we note a serious lack of long-range applied R&D due to the fragmented nature of the industry and EERE’s focus on near-term research and demonstration programs. Therefore, the buildings opportunities we highlight focus on critical longer-term applied research.

Sample List

Fuel Cells: Dramatic improvements in these areas are well within reach, if materials science breakthroughs that have occurred through basic research within the last five years serve as any guide [Crabtree and Dresselhaus, 2008].

Batteries and Electrical Energy Storage: Novel materials can greatly improve battery performance. For example, silicon nanowires can store ten times the energy density of the conventional graphite anode, while still maintaining a delicate surface structure as lithium ions are inserted and extracted [Chan et al. 2008]. In the longer term, developing batteries that transfer two or more charges at a time would dramatically improve energy storage but represents the greatest challenge and the greatest research opportunity.

Solid-State Lighting: Producing white light requires combining colors, and the available phosphors and the available bandgaps currently provided by semiconducting materials limit the nature and quality of the resulting white spectrum. Materials research in doping and defect control of semiconductors and in the development of new efficient phosphors offers fertile ground for science and technology investment [Humphreys, 2008].

Catalysts: The natural biological world provides the most dramatic example of their impact on the efficiency of energy conversion [Kraut, Carroll and Herschlag, 2003]. Catalysts, which have taken millions or billions of years to evolve, control virtually every biological energy process. Human-engineered catalysts, by comparison, are astonishingly simple, typically providing only a fraction of the speed and selectivity of their biological counterparts. Catalysts can play a central role in raising energy efficiency [Gates et al., 2008]. At a relatively primitive stage of development for now, they offer an extraordinary opportunity for research to drive them toward the capabilities already demonstrated by biological catalysts.

Thermoelectric Devices: On the way to its end use, more than 55 percent of the primary energy we generate is lost to waste heat [PCAST, 2006]. Thermoelectric devices offer a simple route to capturing waste heat, converting it directly to electricity at its source [DiSalvo, 1999; Dresselhaus et al. 2007]. Thermoelectric devices that either use electricity to produce cooling directly or use waste heat to generate electricity directly have obvious applications in the auto industry. The conversion efficiency has been low, but advances in nanocomposite materials research have demonstrated a thermoelectric conversion efficiency of more than 20 percent in the laboratory, not very different from the internal combustion engine.

Lightweight Materials: Replacing steel with aluminum can reduce a vehicle's weight by 40 to 60 percent. Magnesium as a replacement has a 60 to 75 percent benefit, and graphite fiber reinforced polymer composites, a 50 to 60 percent benefit [Carpenter et al. 2008]. The barrier to such replacements is simply the price tag. New opportunities lie in composites and nanostructured materials with tailored properties [Tjong and Ma, 2000; Wang et al. 2002], and development of new, affordable materials can have huge benefits.

Advanced Windows: Future window systems have the potential to reduce the amount of energy used for heating in the winter and cooling in the summer. Active façades could modulate daylighting and ventilation in response to detailed monitoring of interior conditions, and advanced daylight distribution systems that project daylight deeper into the interior could displace more than half of electric lighting used in commercial buildings.

Advanced Ventilation: Increased air conditioning demand has been the major driver of the growth in building energy usage. Natural ventilation has the potential to reduce the seasonal cooling energy requirements by 50 percent or more in many U.S. climates. A better understanding of the fundamental fluid mechanical behavior could improve design and control of ventilation and enhance indoor air quality.

Ultrathin Insulators: Very thin insulators can provide a practical means of retrofitting existing buildings for improved energy efficiency. Nanoscience and nanotechnology research offer opportunities for achieving such a goal.

Thermodynamic Cycles: Major efficiency losses in heat pumps are caused by inefficiencies in the heat transfer process. Nanomaterials and nanofluids offer the possibility of decreasing thermal losses in conductivity and convection.

Behavioral Research: A wide array of factors clearly influence how people reach their decisions involving energy usage. Behavioral research into the way energy decisions are made, implemented and accepted, including economic, cultural and psychological factors that affect priority setting, would contribute significantly to designing incentives for increased energy efficiency, facilitating the performance of markets and arriving at regulatory practices where they are needed.

CHAPTER 4 ENDNOTES

There are enormous opportunities for achieving greater energy efficiency by replacing inefficient conversion processes with efficient ones. For example, in the transportation sector, gasoline engines that are only 20 percent efficient might be replaced with fuel cells that are up to 60 percent efficient coupled to electric motors that are more than 90 percent efficient. In the case of lighting, incandescent bulbs that are only 5 percent efficient can be replaced with fluorescent bulbs having an efficiency of 20 percent today, and, when we learn to control the bandgap and color of semiconductor lighting, with light-emitting diodes having efficiencies of 50 percent or more.

Replacing an inefficient conversion process with an efficient one may pose long-term challenges if major barriers stand in the way. Often, the barriers remain resistant to incremental technological advances. In some cases they can only be surmounted through transformational basic research discoveries that reveal new phenomena or new behavior. In other cases, even if the basic phenomena are understood, long-term applied research may be needed to overcome the barriers.

Two examples of the latter that have relevance for transportation are nanostructured membranes, which can separate small molecules such as carbon dioxide and water based on their molecular conformation, and battery electrodes, which can maintain their optimized nanoscale “morphology” through millions of ionic charge–discharge cycles. In both cases we have a good understanding of the basic phenomena, but in neither case is our knowledge sufficient to allow us to apply the scientific principles to specific purposes, such as intelligent tuning of engine operation matched to changing driving conditions.

We highlight key examples of long-term research that is needed to advance the critical technologies for the transportation and building sectors.

1. Fuel Cells

Fuel cells offer the promise of efficient energy use in applications from electricity production for distribution on the grid to transportation in cars and light trucks. The viability of fuel cells is shown by a recent test of fuel cell vehicles that achieved 52 to 58 percent efficiency running at 25 percent power [Wipke et al., 2007]. While such efficiencies demonstrate viability, they must be extended to higher power levels to make fuel cells for transportation competitive with internal combustion engines in the commercial market.

The basic fuel cell design is well established by now, much as the basic design of the internal combustion engine was established a century ago. Decreasing the cost of fuel cell production and increasing fuel cell performance and durability represent today’s major technological challenges. Electrode materials, catalysts, and electrolytic membranes offer the most promising research opportunities for meeting those challenges. We believe that dramatic improvements in these areas are well within reach, if materials science breakthroughs that have occurred through basic research within the last five years serve as any guide [Crabtree and Dresselhaus, 2008].

One example of a pertinent advancement pertains to the use of platinum as a catalyst in motor vehicle applications. The catalytic converter in the exhaust system of cars and trucks is well known to motorists. But platinum catalysts are also essential components in fuel cells used by hydrogen vehicles. Until now, platinum’s natural scarcity, high demand and consequential high price have posed major barriers to its widespread application as a facilitator of oxygen reduction in fuel cell cathodes. But a recent basic research discovery has shown that adding nickel to the second and third layers beneath the exposed pure platinum surface enhances the catalytic activity ten times over, thereby significantly reducing the amount of platinum needed in a fuel cell cathode and the consequential cost of the fuel cell [Stamenkovic, 2007].

2. Batteries and Electrical Energy Storage

Electrical energy storage in batteries, supercapacitors and other media is central to achieving energy efficiency in electricity production and transportation. The diurnal cycle of electricity demand requires that utility companies vary the production of electricity by as much as 100 per cent within any single 24 hour period.

For base load operation, utility companies employ sophisticated combined-cycle plants designed for continuous operation. But to meet peak demand, the companies typically use simple single-cycle gas turbines that minimize capital costs and operate well below the efficiency of the more sophisticated plants. Because they operate only a few hours a week, some utility companies still use old, coal-fired “peaker” plants that, by and large, emit significantly greater quantities of carbon dioxide than the base load plants. However, if effective electricity storage existed at the utility scale level, it could bridge the diurnal demand cycle and eliminate or significantly reduce the need for inefficient peaker plants.

Large-scale electrical storage is also required if solar and wind power are to become major contributors to our nation’s electricity production. These renewable resources operate on intermittent production cycles, and if they are in widespread use, they will have to be matched to demand with a response time of several minutes or at most a few hours. Unless a large-scale energy storage medium accompanies a large-scale solar or wind generating plant, it will be extremely difficult for the power grid to accommodate the intermittent nature of those plants.

As we noted in the chapter on transportation, inefficient fossil-fueled cars can be replaced with efficient all-electric vehicles only when high energy-density batteries become widely available at a reasonable cost. Such batteries do not exist today, and their absence constitutes the primary obstacle to extensive penetration of electric vehicles in the transportation sector. If electric vehicles become prevalent, in principle they could help level the diurnal cycle, since they would mostly be recharged at night. In a sense they would serve as a natural, large-scale, distributed storage medium for electricity.

The technological challenges for electrical energy storage, like those for fuel cells, lie in electrochemical materials and processes. For example, in the case of the current generation of lithium-ion batteries, the lithium-ion density at the cathode and anode serve as limitations on the energy density of the battery. And as lithium ions are inserted and extracted at the electrode surfaces during charging and discharging, the electrodes degrade and the cycle lifetime of the battery suffers.

Novel materials provide a wide horizon and rich promise for improving batteries. Consider the case of the lithium-ion battery anode, for example. There silicon nanowires can store ten times the energy density of the conventional graphite anode, while still maintaining a delicate surface structure as lithium ions are inserted and extracted [Chan *et al.*, 2008]. But achieving similarly dramatic improvements in the performance of the lithium-ion battery system as a whole will require equivalent materials advances in the other components. It will also require integration of new technologies that will allow the components to work effectively in partnership. If there is one overwhelming bottleneck for optimizing the energy density of lithium-ion batteries today, it lies in the cathode material. Silicon nanowires might be able to provide a tenfold improvement over the theoretical limit for materials presently being used [Tarascon and Armand, 2001].

In the longer term, developing batteries that transfer two or more charges in the electrochemical reactions at the electrode surfaces represents the greatest challenge and the greatest research opportunity. Success depends on finding a new class of electrode materials with valence greater than one, such as the alkali earths or transition metals. The potential increase in energy density grows with the number of electrons transferred in the basic electrochemical reaction, so that fourfold or greater improvements beyond the best lithium-ion battery technology are conceivable.

Supercapacitors offer an alternative and a complement to batteries for storing electrical energy. In contrast to batteries, which are most efficient when charging or discharging occurs at a slow, constant rate, supercapacitors can store and release electricity very rapidly. In electric cars, batteries are well suited to steady highway driving, but supercapacitors are more compatible to starting, stopping and high-speed acceleration.

Despite rapid progress in the development of supercapacitors in recent years, their stored energy density remains smaller than that provided by batteries. The challenge for supercapacitor research currently lies in the development of high-density charge storage at metal-electrolyte interfaces. Nanostructured interfaces that can store multiple charges at a single site are needed. Recent results indicate that the capacitance of porous interfaces increases 200-300 hundred percent as the pore size decreases below 1 nm. Further research in understanding and controlling this remarkable nanoscale phenomenon is clearly needed, and it is likely to be very fruitful.

3. Solid-State Lighting

Lighting consumes 22 percent of the electricity we use, and it provides a basic human need that is common to many human activities. The incandescent bulb, the staple of the lighting industry since the time of Thomas Edison, remains a major source of light in industrialized countries, particularly in the residential sector. But as we have already noted, incandescent lamps typically convert only 5 percent of their energy into visible light.

The Federal Energy Independence and Security Act of 2007 requires that by 2012–2014 common light bulbs use 70 to 80 percent of the energy used by present-day incandescent lamps. And by 2020, the act requires that new bulbs use no more than 65 percent of the energy of present-day incandescent lamps. Meeting the new standards will require using different technologies.

Today's high-efficiency fluorescent lamps, for example, convert 20 percent of their energy into light and offer a reasonable approach to meeting the 2012–2014 standard. But it seems virtually impossible that fluorescent lamps will improve sufficiently for them to play a dominant role in 2020. Solid-state lighting offers a far more promising approach.

Commercially available solid-state light-emitting semiconductors already rival high-efficiency fluorescent bulbs in reducing energy consumption, and in the future they promise to offer conversion efficiencies of 50 percent or more [Phillips *et al.*, 2007]. Solid-state lighting not only provides a path to reduced energy utilization, as required by the 2007 federal law, but the dramatically higher efficiency of light-emitting semiconductors makes them natural partners with solar cells and batteries that can free lighting from the electricity grid in many applications.

Solid-state lighting has already penetrated the commercial market for specialty uses, such as traffic lights, road signs and architectural lighting. But most of these applications involve colored light. Where white light is needed, semiconductors face significant challenges, both in cost and technology. Producing white light requires combining colors, and the available phosphors and the available bandgaps currently provided by semiconducting materials limit the nature and quality of the resulting white spectrum. Materials research in doping and defect control of semiconductors and in the development of new efficient phosphors offers fertile ground for science and technology investment [Humphreys, 2008].

4. Catalysts

Catalysts exert enormous influence over the speed and selected outcomes of chemical reactions. The biological world provides the most dramatic example of their impact on the efficiency of energy conversion [Kraut, Carroll and Herschlag, 2003]. Catalysts that have taken millions or billions of years to evolve control virtually every biological energy process. They regulate the metabolic pathways of

reproduction and growth with minimal energy input, using energy ultimately derived from the Sun.

Biological catalysts are enzymes of elaborate structure and functionality, orchestrating every step of the reaction process, from the placement and orientation of reactants to the seamless hand-off of products from one catalytic environment to the next. Human-engineered catalysts, by comparison, are astonishingly simple, typically providing only a fraction of the speed and selectivity of their biological counterparts. At a relatively primitive stage of development for now, they offer an extraordinary opportunity for research to drive them toward the capabilities already demonstrated by biological catalysts.

Catalysts can play a central role in raising energy efficiency [Gates *et al.*, 2008]. In the transportation sector, for example, hybrid and plug-in hybrid cars would benefit from more selective, faster and more stable electro-catalysts that significantly increase the chemical-to-electrical conversion efficiency in batteries. In the case of hydrogen vehicles, fuel cells currently depend on platinum catalysts to convert chemical energy into electricity. Replacing platinum—which is scarce and expensive—with another material remains a critical technology barrier and a major research challenge.

Although this report treats end-use efficiency, we pause to note that catalysis technology can have significant import for energy production and distribution. For example, as easy-to-reach resources of conventional oil continue to dwindle, the nearly untapped supply of heavy carbon-rich shale-oil or tar sands are likely to assume increasing importance. But extracting and refining these heavy liquid fuels efficiently remains a technological challenge. Developing new catalysts to promote the refining of shale oil and tar sands ultimately will determine whether they can provide petroleum products at reasonable financial and energy costs.

One of the major inefficiencies in our present use of energy is its once-through character. We extract the energy contained in fossil fuels by first converting the fuels into carbon dioxide and water and then exhausting the products into the environment. If we could use the Sun's energy and any excess heat from inefficient energy processes to replace the chemical energy removed by combustion, we could convert the waste products into hydrocarbons and hydrogen for re-use. Developing catalysts that could promote the specific reconstituting reactions poses a major research challenge and opportunity.

Rapid advances in nanoscience and nanotechnology during the past 5 years have created the potential for converting catalysis from an empirical art into a fundamental science capable of targeting specific reactions and producing materials that promote them. Such a transformational objective is clearly within sight, and it warrants significant increases in the support of fundamental research on nanoscale materials and mechanisms of catalysis.

5. Thermoelectric Devices

Our present patterns of energy use are remarkably inefficient. On the way to its end use, more than 55 percent of the primary energy we generate is lost to waste heat [PCAST 2006]. Harnessing that heat for productive energy use provides a major opportunity for improving energy efficiency. Thermoelectric devices offer a simple route to capturing waste heat and converting it directly to electricity at its source [DiSalvo, 1999; Dresselhaus, *et al.*, 2007].

The thermoelectric conversion process is fairly easy to understand. Electrons moving from hot to cold regions of a semiconductor create an electric current proportional to the thermal gradient—the temperature difference between the two regions divided by the distance between them. Neither moving parts nor chemical reactions are required to generate the electric current, and the thermoelectric conversion takes place within a homogeneous material. The efficiency of a thermoelectric device is characterized by a figure of merit that depends on the temperature at which the device is operating, its electrical conductivity, its thermal conductivity and a parameter known as the Seebeck coefficient,

or thermoelectric power.

Only a decade ago, the figure of merit of the best thermoelectric devices was about unity, relegating them to niche markets and the research laboratory. But in recent years, rapid advances in nanocomposite materials research have raised the figure of merit to 2.5, corresponding to a thermoelectric conversion efficiency of more than 20 percent, not very different from the internal combustion engine.

Thermoelectric devices that either use electricity to produce cooling directly or use waste heat to generate electricity directly have obvious applications in the auto industry. Some of the devices are already penetrating the auto air-conditioning market with electrically driven, seat-mounted coolers producing passenger comfort on hot days and using much less energy than full compartment air conditioning. Their use for this purpose is expected to increase dramatically during the next five years.

Thermoelectric converters that exploit the waste heat produced by an internal combustion engine can power the increasing number of auxiliary electrical devices used in cars and trucks, such as windows, locks, windshield wipers, lights, GPS navigation systems, video displays and audio for cell phones and digital music sources. If a thermoelectric device could completely replace a vehicle's alternator, it would save 2 to 10 percent of the primary chemical energy of the vehicle's fuel.

In hybrid vehicles, thermoelectric devices could have an added advantage. Whenever the internal combustion engine is running, thermoelectric devices could capture a sizeable fraction of the engine's waste heat, convert it into electricity and store the resulting energy in the vehicle's battery. Regenerative braking, which hybrid vehicles currently employ, functions in a similar fashion, capturing up to half of the vehicle's kinetic energy, converting it into electricity and storing the resulting energy in the battery, rather than turning it into heat as is done with conventional braking.

To achieve a high figure of merit, the current generation of thermoelectric materials uses multilayer geometries that scatter "phonons" and thereby lower the thermal conductivity of the device, but they do not scatter the electrons that carry the converted thermal energy as a current [Harman *et al.*, 2002]. High-performance multilayer materials are presently made only from deposited films that are not sufficiently robust or available in sufficiently large quantities for the necessary applications.

For thermoelectric devices to be deployed broadly, either bulk materials must be found that possess the same properties as the multilayer materials and can be produced in larger quantities and at lower cost, or other approaches must be found to raise the figure of merit. Nanoscale compositional doping as a means of introducing peaks in the "density of states" of the material is one possible approach [Dresselhaus *et al.*, 2007].

We believe that investing in research to advance the application of nanoscale phenomena in bulk materials for thermoelectric devices has high potential to recover much of the energy we now lose to waste heat.

6. Lightweight Materials

Lightweight materials present a major opportunity for reducing the amount of energy used in transportation, as we have already pointed out. By most estimates, lowering the weight of a vehicle by 40 percent will increase its energy efficiency by 25 percent. Such weight reductions are well within the technical reach of materials now known in the laboratory or used in specialty applications. For example, replacing steel with aluminum can reduce a vehicle's weight by 40 to 60 percent. Magnesium is even better, offering a 60 to 75 percent reduction, and graphite fiber reinforced polymer composites offer a 50 to 60 percent reduction [Carpenter *et al.*, 2008].

The barrier to such replacements is simply the price tag. Using present technology to manufacture components with such lightweight materials, in fact, can increase the costs of the parts by 50 to 200 percent compared to today's standard materials. Reducing the costs must be a major objective of any science and technology program, and it will be difficult to achieve with "single-phase" materials, such as aluminum, magnesium and titanium, whose properties and production routes are well known and capped by the limited variability of their compositions and structures. Therefore, we believe the greatest long-term basic research and long-term applied research opportunities for lightweight materials lie in composites and nanostructured materials with tailored properties [Tjong and Ma 2000; Wang *et al.*, 2002].

Composites are still in their infancy and comprise a wide range of potential material constituents, morphologies, compositions, and internal structures. Additionally, composites can exhibit properties that are normally contradictory, such as high strength and flexibility; optical transparency and electrical conductivity; or high ductility and stiffness. With so many variables in play, there are many possibilities for low-cost manufacturing and new, desirable properties.

The carbon nanotube provides one example of the wide array of opportunities for lightweight new materials. This simple material has a tensile strength of 65 gigapascals (GPa), approximately 100 times greater than steel, combined with a density one-fifth to one-sixth lower than that of steel.

The carbon nanotube demonstrates but one instance of the combination of properties that can be accessed with new materials. We believe that the innovation opportunities are immense, and that applied research into new lightweight composite and nanostructured materials with tailored properties has a very high potential to improve energy efficiency in transportation.

7. Advanced Windows

Developing more efficient windows with higher insulation values and selective control of the solar spectrum has been the goal of considerable research in recent years. It is now possible to construct windows that exhibit a net energy gain during the winter if they are properly oriented. Such windows allow the solar energy entering a room to exceed the heat energy that leaves it.

But additional research is needed to make the high-performance windows affordable for retrofit applications, especially in the case of residential buildings. Using nanotechnology to produce transparent high-R-value panels offers one possible path forward.

Future window systems and active façades have the potential to achieve net energy gains during the winter and substantially reduce air conditioning loads in the summer. They would adjust daylighting, solar gains and ventilation in response to detailed monitoring of interior conditions. In the case of commercial structures, innovative materials and mirrored systems offer the possibility of distributing daylight much deeper into the building interiors, with projected reductions of 50 percent in average lighting energy usage.

8. Advanced Ventilation

Natural ventilation systems can reduce the seasonal cooling energy requirements by 50 percent or more in many U.S. climates, while improving human comfort and satisfaction, according to research findings. But natural ventilation requires a façade that has controllable apertures and an interior design that ensures adequate airflow throughout the structure. For a mixed-mode building, that is not an easy undertaking.

To ensure sufficient airflow for all interior spaces while meeting indoor air quality and fire code standards requires a detailed understanding of fluid dynamics, turbulent flow and thermal behavior in a large multiconnected space under a variety of heat loads and wind conditions. But

finding a complete solution to the equations governing turbulent flow in a large, complex building is a daunting task, and simple computational models may introduce unacceptable errors.

There is a serious need to develop straightforward, mixed-mode, natural-ventilation design tools for building architects and engineers. There is also a need to develop effective ways to control natural-ventilation systems under a wide range of conditions.

The influence of indoor air quality on health and productivity is an important issue that is now receiving significant public scrutiny. Further research is needed to identify pollutants, the sources of the pollutants, the limits on acceptable concentration levels and whole-building control measures for volatile organic compounds, mold and other asthma triggers.

9. Ultrathin Insulators

Insulating materials in common use today are limited in their effectiveness due to the heat transfer characteristics of the gases contained in their interiors. As a result, the exterior walls of buildings and the walls of refrigerators must be relatively thick to achieve high levels of insulation. Aerogels represent the first advance in developing materials that utilize submicron-sized pores to limit the heat transfer through gas molecules in their interiors.

Nanopore materials hold the promise of reducing both thermal radiation and conduction energy transfer. They offer the possibility of developing thin, rigid, high-R-value insulation panels suitable for retrofitting the interior surfaces of exterior walls in existing homes without requiring a major renovation of the interior geometry. They could also find applications in appliances such as refrigerators and ovens.

Current windows have far lower insulation levels than the adjacent walls. Oriented nanostructures hold the possibility for developing transparent panels that substantially increase insulation levels while maintaining sufficient clarity for window applications.

In the high-performance thermal insulation materials currently in use, heat transfer by means of radiation plays an important role. For example, at room temperature, infrared radiation accounts for one-third to one-half of the total heat transfer in foam and fiberglass insulation. Tailored nanoparticles added to such insulation could act as reflectors of infrared radiation, substantially reducing the radiative heat loss and increasing the R-value of the material by as much as 100 percent.

10. Thermodynamic Cycles

Heating represents the largest single energy use in residential buildings, and burning fossil fuels for low-temperature applications is a very inefficient use of the commodity from the standpoint of thermodynamics. Combining heat and power systems at the single building or community level can provide substantial energy savings. Heat pumps can also provide greater efficiency.

But today, heat pumps have a coefficient of performance—the ratio of thermal energy delivered to electrical energy consumed—of only 2.5 to 3. By contrast, the ideal reversible heat pump, a “Carnot cycle,” has a coefficient performance of 14 for the same limits between ambient and interior temperature. The large efficiency losses in existing heat pumps are caused, in part, by the sizeable temperature differences that occur across the heat-transfer surfaces in the evaporators and condensers. Improving the heat exchangers is a major research challenge.

Techniques currently being explored for cooling integrated circuits in computers offer a possible approach to the problem. In the case of integrated circuits, surfaces with microgrooves have displayed a tenfold improvement over conventional heat transfer devices. Other techniques include boundary layer enhancement, such as that used in improved cooling of interiors of gas turbine blades;

nanotechnology applications, such as those considered for improving thermal conductivity of thermal fins; and nanofluids, such as those envisioned for enhancing overall convective heat transfer.

Considerable work, especially in Europe, has identified ways to reduce building energy used in cold climates. But finding ways to accomplish that in warm and humid climates is a more challenging problem. As the population continues to increase in such regions, the need for a solution grows.

Finally, the amount of energy consumed in cooling large computer server facilities—now equal to the energy used by the computers themselves—is a mounting problem. The development of a novel system integration of heat pumps and air conditioners within the computer facility could generate considerable energy savings. For example, systems using liquid-cooled radiant panels along with intelligent controls and variable speed compressors could reduce overall energy requirements for air conditioning by one-third or more. The development of dehumidification technologies would also be extremely beneficial.

11. Behavioral Research

Consumers, companies and governments frequently use criteria other than energy efficiency in arriving at decisions and formulating policies involving energy. Often cost or convenience is the driving factor, with energy efficiency relegated to a lower priority. A survey conducted in 2007, at a time when gas prices already exceeded \$3 per gallon, showed that new car buyers still ranked energy efficiency sixteenth in priority, well below leading factors such as reliability, safety and purchase price [German, 2007]. With gasoline costing more than \$4 per gallon today, consumer sentiment has changed.

The efficiency of energy usage ultimately depends on the judgments millions of corporate, government and citizen decision-makers reach in their daily activities, in their homes and on their jobs. Improving end-use energy efficiency requires an understanding of how people arrive at their judgments. Therefore, we believe that social research into human behavior and decision-making must be a high priority.

Although a wide array of factors clearly influence how people reach their decisions involving energy usage, the availability of information is surely one of them. But understanding how the information is best presented, how the consequences of personal and public decisions are best explained and how people are likely to process the knowledge they acquire are essential to the success of any attempt to improve end-use energy efficiency.

Behavioral research into the way energy decisions are made, implemented and accepted, including economic, cultural and psychological factors that affect priority setting, would contribute significantly to designing incentives for increased energy efficiency, facilitating the performance of markets and arriving at regulatory practices where they are needed.

Many of the challenges presented in these endnotes are described more comprehensively in the 2002-2007 U.S. Department of Energy's Basic Energy Needs Workshop Series (www.sc.doe.gov/bes/reports/list.html) and in the 2008 Materials Research Society report, *Harnessing Materials for Energy* [Arunachalam and Fleischer, 2008].

CHAPTER 4 REFERENCES

- V. S. Arunachalam and E. L. Fleischer, eds., *MRS Bulletin* **33** (4), (2008).
- J. A. Carpenter, Jr., J. Gibbs, A. A. Pesaran, L. D. Marlino and K. Kelly, “Road Transportation Vehicles,” *MRS Bulletin* **33** (4), 439 (2008).
- G. W. Crabtree and M. S. Dresselhaus, “The Hydrogen Fuel Alternative,” *MRS Bulletin* **33** (4), 421 (2008).
- C. K. Chan, H. Peng, G. Liu, K. McIlwrath, X. F. Zhang, R.A. Huggins and Y. Cui, “High-Performance Lithium Battery Anodes Using Silicon Nanowires,” *Nature Nanotechnology* **3**, 31 (2008).
- F. J. DiSalvo, “Thermoelectric Cooling and Power Generation,” *Science* **285**, 703 (1999).
- M. S. Dresselhaus, G. Chen, M. Y. Tang, R. G. Yang, H. Lee, D. Z. Wang, Z. F. Ren and J. P. Fleurial, P. Gogna, “New Directions for Low-Dimensional Thermoelectric Materials,” *Advanced Materials* **19**, 1043 (2007).
- B. C. Gates, G. W. Huber, C. L. Marshall, P. N. Ross, J. Sirola and Y. Wang, “Catalysts for Emerging Energy Applications,” *MRS Bulletin* **33** (4), 429 (2008).
- J. German, quoting Strategic Vision, 2007 New Vehicle Experience Study, American Honda Motor Co. (2007).
- T. C. Harman, P. J. Taylor, M. P. Walsh and B. E. LaForge, “Quantum Dot Superlattice Thermoelectric Materials and Devices,” *Science* **297**, 2229 (2002).
- C. Humphreys, “Solid State Lighting,” *MRS Bulletin* **33** (4), 459 (2008).
- D. A. Kraut, K. S. Carroll and D. Herschlag, “Challenges in Enzyme Mechanism and Energetics,” *Annu. Rev. Biochem.* **72**, 517 (2003).
- PCAST (President’s Council of Advisors on Science and Technology), The Energy Imperative. Technology and the Role of Emerging Companies (2006), www.ostp.gov/PCAST/pcast.html.
- V. R. Stamenkovic, B. Fowler, B. S. Mun, G. Wang, P. N. Ross, C. A. Lucas and N. M. Markovic, “Improved Oxygen Reduction Activity on Pt₃Ni (111) via Increased Surface Site Availability,” *Science* **315**, 493 (2007).
- J.M. Tarascon and M. Armand, “Issues and Challenges Facing Rechargeable Lithium Batteries,” *Nature* **414**, 359 (2001).
- S. C. Tjong and Z.Y. Ma, “Microstructural and Mechanical Characteristics of *In Situ* Metal Matrix Composites,” *Materials Science and Engineering* **29**, 49 (2000).
- Y. Wang, M. Chen, F. Zhou and E. Ma, “High Tensile Ductility in a Nanostructured Metal,” *Nature* **419**, 912 (2002).
- K. Wipke, S. Sprik, H. Thomas and J. Kurtz, Learning Demonstration Interim Progress Report—Summer 2007, National Renewable Energy Laboratory tech. rep no. 560–41848, 2007; www.nrel.gov/docs/fy07osti/41848.pdf (accessed January 2008).