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Don't Forget Long-Term Fundamental Research in Energy

George M. Whitesides^{1*} and George W. Crabtree²

Achieving a fundamental understanding of the phenomena that will underpin both global stewardship and future technologies in energy calls for a thoughtful balance between large-scale immediate solutions using existing technology and the fundamental research needed to provide better solutions in the 50-year period.

Energy and climate change are now preoccupations shared by science, engineering, and society. There is a range of views on energy and almost religious levels of advocacy for particular technologies. There is also surprisingly broad (although not universal) agreement that there is no single solution to the dual problems of meeting future demands for energy and managing the environmental consequences of energy production. Whatever strategy emerges will be a quilt made up of patches representing almost every imaginable technology.

The energy problem is often phrased in terms of developing a strategy that roughly doubles the global production of energy by 2050 (from 13 to about 30 terawatts) (Fig. 1) (1–9). The problem of climate change includes two especially important components: (i) understanding the relationship between the climate and the chemistry of the atmosphere and oceans and (ii) predicting the impact on climate of different strategies for energy production. Because atmospheric CO₂ is the dominant greenhouse gas, and because coal is the carbon-rich fossil fuel whose use can most readily be expanded (especially in the rapidly growing economy of China), understanding the linkage between coal and climate is particularly important (6).

There is a pervasive sense that “We must do something *soon*.” This urgency may be justified, but we must also remember that the problems of providing energy and maintaining the environment are not about to go away, no matter how hard we try using current technologies. In the rush to do something—to find technological solutions to global-scale problems—we should not forget that we must ultimately *understand* them, if we are to find the most effective, sustainable solutions. Fundamental research in science and engineering is important. Understanding phenomena relevant to energy and the environment leads to new technologies and to the ability

to control the economic and environmental outcomes of their applications (7).

The cost of large technology demonstration projects is enormous and the time to develop them decades, and it is easy to overlook the fundamental research that nourishes them. Today, we have a growing thicket of energy and environmental problems and great enthusiasm for solving them quickly. In fact, 50 years from now, most of these problems (and more) will still remain unsolved. Developing the best patches we can for the immediate problems is one approach. Understanding the underlying problems is another, and one that is at least as important, much less expensive, and perhaps ultimately time-saving. Energy and climate are problems that will extend over decades or centuries, and the unimaginable technologies of 100 years from now will rest on fundamental research that must start now.

What follows is a sketch of nine representative long-term problems in research that are vital to the development of future technology for energy. We emphasize that this list is personal and idiosyncratic; it tends to emphasize materials. Others might select differently, although most lists would probably have areas of broad overlap.

The Oxygen Electrode Problem

A hydrogen fuel cell operates by extracting electrons from H₂ and transferring them through an external circuit to O₂ (to generate H₂O). If the H₂ is generated electrochemically, the reverse reactions take place. In either event, the transfer of electrons from H₂O to one electrode and to O₂ from another are slow reactions and lower the efficiency of practical fuel cells (considering the free energy of the reactions involved). The slow rates of interconversion of 4 e⁻ + O₂ + 4 H⁺ and 2 H₂O exemplify a broader class of reactions in which a single process requires the transfer of multiple electrons. Understanding these reactions and finding strategies for circumventing their limitations are important in developing new, more practical procedures for reactions ranging from the electrochemical production of H₂ and the use

of O₂ in fuel cells to the reduction of nitrogen to ammonia.

Catalysis by Design

Many of the reactions that occur in the production of energy involve catalysis: the full set used in the processing of crude oil to fuels; all of the biological reactions involved in photosynthesis, in fixing CO₂, and in biodegradation; the hydration of CO₂ to carbonate ion; the movement of electrons in batteries; the operation of fuel cells; the cleanup of exhaust gas from internal combustion engines; and many others. Given the enormous importance of catalysis in the production and storage of energy, in the production of petrochemicals and the materials derived from them, and in all biological and most geochemical processes, it is astonishing (and a little disheartening) how little is known of the fundamentals of catalysis: how catalysts operate, how to control them, and especially how to generate new ones. Catalysis by design has periodically been embraced as a grand challenge, and periodically abandoned as too difficult, but nanoscience and surface science offer new approaches to this problem. The fundamental study of catalysis must be reanimated across the full spectrum of processes involved in energy and the environment.

Transport of Charge and Excitation

Photoexcitation of the semiconductor or dye component of a solar cell creates an exciton: a separated but associated hole and electron (4, 5). To generate current, the electron must move to one electrode, and the hole to the other, before they combine. These processes are inefficient in materials that might make inexpensive photocells: defective, polycrystalline, disordered, or quantum-dot semiconductors (whether inorganic or organic). Understanding them and circumventing their deficiencies is one key to cost-effective solar cells.

Chemistry of CO₂

CO₂ is a key molecule in global warming (6), in chemical and biological fuel production, and in fuel use. We must know everything possible about its physical and chemical interactions. Important topics include new uses of CO₂ in large-scale chemistry (where it has the attractive feature that it has negative cost), new chemical reactions of CO₂, the movement and reactions of CO₂ in the earth, the role of CO₂ in determining the behavior of the atmosphere and oceans, and the chemistry and properties of CO₂ at high pressures. For decades, there has been little research, whether fundamental or exploratory, in this area; it was considered a solved problem.

Improving on Photosynthesis

The process of uptake and fixation of CO₂ in biological photosynthesis is not an optimized

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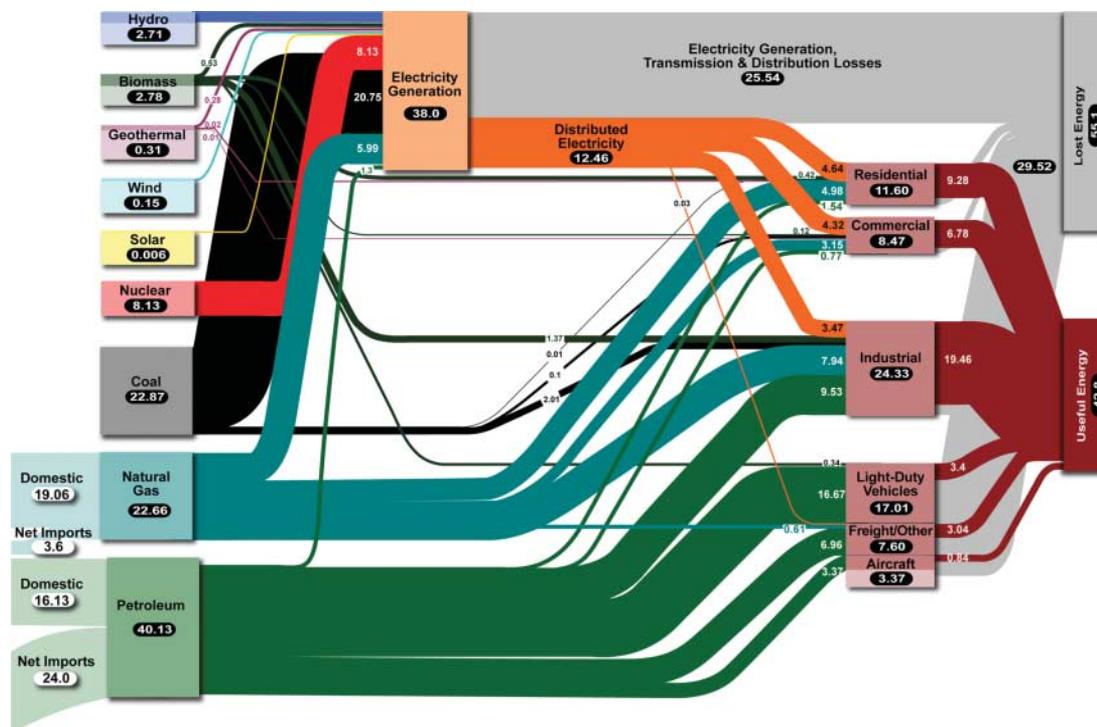


Fig. 1. The complex system of energy flows in the United States in 2005 (1). More than half of the energy produced is wasted. Units are in quads; 1 quad = 10^{15} British thermal units = 1.055 exajoules. [Figure prepared by Lawrence Livermore National Laboratory, University of California, and the U.S. Department of Energy]

marvel: It is fairly inefficient thermodynamically, and several key reactions [for example, the key step involving the reaction of CO_2 with ribulose diphosphate (with its competing reaction with O_2)] have a surprisingly poor yield. These inefficiencies are an opportunity. Photosynthesis has immense appeal for the closed-cycle capture of energy from the Sun in forms that are useful as fuels (4). The prospects of re-engineering biological photosynthesis for greater efficiency, maximizing metabolic flux through specific biosynthetic pathways, growing plants in regimes of temperature or salinity where they normally do not flourish, and directly producing fuels such as H_2 , CH_4 , or alcohols are all alluring ones, but ones that will require decades of imaginative research to realize. The prospect of non-biological photosynthesis (where “photosynthesis” might include bio-inspired physical and chemical reactions or more straightforward photochemical or photothermal processes that generate fuels or store energy) also warrants new research.

Complex Systems

Understanding energy and the environment analytically poses a series of problems that we presently have neither the mathematical tools nor the data to solve. Most global systems are “complex” in physicists’ definition of the word: They comprise many components, with many degrees of freedom, usually interacting non-

linearly. These systems are the natural home of big surprises—often referred to as emergent behavior. Our difficulty in understanding and modeling these systems leads to uncertainties that cloud most discussions of energy and the environment and of the costs and impacts of almost any technology (5). What really is the cost of a kilowatt produced by silicon solar cells? How important will the burning of coal be to global warming? What, in detail, are the global sources and sinks for carbon and how do they interact? What can one say about the impact of technologies for generating nuclear power on the potential for proliferation of nuclear weapons? Development of the theory of complex systems to the point where it gives reliable results (or at least results whose reliability can be quantified) remains a key enabling capability, and is probably the best way of minimizing the potential miseries of the law of unintended consequences.

The Efficiency of Energy Use

Increasing the efficiency of energy conversion and storage is a major opportunity. Many of our standard energy conversion routes are far from their Carnot efficiency limits: Electricity production with the present mix of fuels is only 37% efficient on average, the typical automobile engine is perhaps 25% efficient, and an incandescent bulb is only 5% efficient for producing visible light. Increasing effi-

ciency requires understanding the fundamental phenomena of existing and alternative energy conversions. Solid-state lighting, for example, can achieve efficiencies of 50% or more, provided that we understand the mechanisms controlling the conversion of electronic energy to photons. New understanding of mechanisms of friction, wear, and corrosion also provides new strategies for reducing losses.

The Chemistry of Small Molecules

The chemistry of small molecules dominates many aspects of energy and climate: H_2O , H_2 , O_2 , CO_2 , CO (for Fischer-Tropsch chemistry), NO_x , O_3 , NH_3 , SO_2 , CH_4 , CH_3OH , HCl , and others are all vitally important components of these discussions. There remains a wide range of information about these molecules and their combinations that is needed to understand the complex systems of which they are a part.

New Ideas: Separating Wheat from Chaff

The spectrum of ideas for dealing with problems of energy and global stewardship is not complete, based just on what we now know. We need new ideas, and we need to know which of the current smorgasbord of unexplored and unproved ideas will work (9). Developing affordable technologies for removing carbon from the atmosphere (for example, by growing biomass and converting it to a stable form of carbon) must be explored now, if they are to be options in the future. Changing the albedo of Earth, stimulating photosynthesis in the oceans by the addition of essential trace elements such as iron, developing new nuclear power cycles, a hydrogen economy, new methods for separating gases (such as CO_2 from air) and liquids, room-temperature superconductivity to carry electric power without loss, biological H_2 production, new concepts in batteries, and nuclear fusion—all must be explored fundamentally and realistically.

These problems all require long-term, patient investment in fundamental research to yield new and validated ideas. These problems are also, in some cases, sufficiently technical that their importance is most obvious to specialists. The oxygen electrode (as one example) might seem an exotic problem in science, but it is hard to

believe that a hydrogen economy that used electrolysis to generate H₂ and O₂ from water, and a fuel cell to convert H₂ and O₂ back to water and electrons, could make a substantial contribution to global energy without a much-improved oxygen electrode. The identification of this problem is not in any sense new: The redox chemistry of oxygen has been a subject of active interest (but limited success) for decades. We simply need new ideas.

Another reason to work on these big problems is that they will attract the most talented young people. Over the past 30 years, the National Institutes of Health has used stable and generous support to recruit and build a very effective community of biomedical scientists.

Solving the problems of energy and global stewardship will require the same patient, flexible, and broadly based investment, if society believes that the problems in these areas are sufficiently important to provide a life's work for its most talented young people.

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PERSPECTIVE

Toward Cost-Effective Solar Energy Use

Nathan S. Lewis

At present, solar energy conversion technologies face cost and scalability hurdles in the technologies required for a complete energy system. To provide a truly widespread primary energy source, solar energy must be captured, converted, and stored in a cost-effective fashion. New developments in nanotechnology, biotechnology, and the materials and physical sciences may enable step-change approaches to cost-effective, globally scalable systems for solar energy use.

More energy from sunlight strikes Earth in 1 hour than all of the energy consumed by humans in an entire year. In fact, the solar energy resource dwarfs all other renewable and fossil-based energy resources combined (1). With increasing attention toward carbon-neutral energy production, solar electricity—or photovoltaic (PV) technology—is receiving heightened attention as a potentially widespread approach to sustainable energy production. The global solar electricity market is currently more than \$10 billion/year, and the industry is growing at more than 30% per annum (2). However, low-cost, base-loadable, fossil-based electricity has always served as a formidable cost competitor for electrical power generation. To provide a truly widespread primary energy source, solar energy must be captured, converted, and stored in a cost-effective fashion. Even a solar electricity device that operated at near the theoretical limit of 70% efficiency would not provide the needed technology if it were expensive and if there were no cost-effective mechanism to store and dispatch the converted

solar energy upon demand (3). Hence, a complete solar-based energy system will not only require cost reduction in existing PV manufacturing methods, but will also require science and technology breakthroughs to enable, in a convenient, scalably manufacturable form, the ultralow-cost capture, conversion, and storage of sunlight.

One key step is the capture and conversion of the energy contained in solar photons. Figure 1 shows the fully amortized cost of electricity as a function of the efficiency and cost of an installed PV module (2, 4). Because the total energy provided by the Sun is fixed over the 30-year lifetime of a PV module, once the energy conversion efficiency of a PV module is established, the total amount of “product” electricity produced by the module at a representative mid-latitude location is known for the lifetime of the system. The theoretical efficiency limit for even an optimal single-band gap solar conversion device is 31%, because photons having energies lower than the absorption threshold of the active PV material are not absorbed, whereas photons having energies much higher than the band gap rapidly release heat to the lattice of the solid and therefore ultimately contain only a useful internal energy equal to that of the band gap (2). Small test cells have demonstrated efficiencies of >20%, with the remaining losses almost en-

tirely due to small reflection losses, grid shading losses, and other losses at the 5 to 10% level that any practical system will have to some extent. Shipped PV modules now have efficiencies of 15 to 20% in many cases. At such an efficiency, if the cost of a module is ~\$300/m² (2), and if we take into account the accompanying fixed costs in the so-called “balance of systems” (such as the inverter, grid connection, etc.), which add a factor of ~2 to the total installed system cost), then the sale price of grid-connected PV electricity must be \$0.25 to \$0.30 per kilowatt-hour (kWh) to recover the initial capital investment and cost of money over the lifetime of the PV installation (2, 4). Currently, however, utility-scale electrical power generation costs are much less, with current and new installations costing ~\$0.03 to \$0.05 per kWh (1). Hence, for solar electricity to be cost-competitive with fossil-based electricity at utility scale, improvements in efficiency are helpful, but manufacturing costs must be substantially reduced.

In current manufacturing schemes for Si-based solar cells, the cost of the processed and purified Si is only about 10% of the final cost of the PV module. Some of the Si is lost in cutting up boules into wafers, and other costs are incurred in polishing the wafers, making the diffused junction in the Si into a photovoltaic device, fabricating the conducting transparent glass, masking and making the electrical contacts, sealing the cells, connecting the cells together reliably into a module, and sealing the module for shipment. Hence, in such systems, the energy conversion efficiency is at a premium so as to better amortize these other fixed costs involved with making the final PV module.

Improvements in efficiency above the 31% theoretical limit are possible if the constraints that are incorporated into the so-called Shockley-Queisser theoretical efficiency limit are relaxed (2). For example, if photons having energies greater than the band gap of the absorbing material did not dissipate their excess energy as heat, but instead produced more voltage or

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