Grand challenges in basic energy sciences

Graham R. Fleming and Mark A. Ratner

Research focused in five related areas will allow unprecedented control over the microscopic world and could be the key to a sustainable future.

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A new report compiled for the Office of Science of the Department of Energy emphasizes the advent of control science, poses five specific grand challenges to science and the imagination, and suggests ways in which DOE can lead the effort to solve them. The report had its origin in a request from Raymond Orbach, the director of DOE's Office of Science, to John Hemminger, chair of the Basic Energy Sciences Advisory Committee (BESAC), to hold a workshop to identify and articulate for the broader scientific community the most important scientific questions and science-driven technical challenges facing the disciplines supported by the DOE Office of Basic Energy Sciences.[1] The request also asked for recommendations on what new theories, instruments, facilities, computational capabilities, and education and workforce development would be needed to address those questions and challenges.

Rather than hold a workshop, BESAC convened a committee cochaired by us to carry out an extended study. In this article we present a summary of our committee's report, with much of the material drawn from the introductory chapter. The report uses sidebars to expand and illustrate specific points—boxes 1 and 2, adapted from two of those sidebars, exemplify the style.

Why now?

The report is timely for reasons of necessity and opportunity. From prehistoric times to the present, progress has been marked by increasingly advanced technologies designed to make use of the planet's bounty. As the 21st century progresses, natural resources are declining, and many technologies are adversely affecting the environment. Whereas it was once axiomatic that civilization would continue to advance, questions of sustainability now arise. In the US, it has been taken for granted that science and technology will solve such problems. Science and technology can be the keys to a better tomorrow, but the scientific community faces significant intellectual challenges.

Balancing the necessity of sustainable advancement is the opportunity created by the newfound ability to probe and understand the microscopic quantum world. Our committee concluded that science has now reached the point at which scientists may move beyond simple observation and take the steps that will enable the direction and control of matter and energy at the quantum level. With that end in mind, we propose five grand challenges that together define the forefront of basic energy sciences and that we hope will inspire and energize the scientific community.

Making the leap from observation to control requires a threefold attack: new approaches to training and funding, theories and concepts beyond those currently available, and instruments that are more precise and flexible than those now in use. (Directing and controlling the properties of materials for a desired outcome requires the ability to see functionality at the relevant length, time, and energy scales.) The final chapter of the report takes up those topics and suggests ways in which DOE can provide leadership to the scientific community in solving grand-challenge problems.

The five grand challenges

To define grand challenges for basic energy sciences, our committee set the following criteria:

A grand challenge must

- be scientifically deep and demanding,
- be clear and well defined,
- be relevant to the broad portfolio of basic energy sciences, and
- promise real dividends in devices or methods that can significantly improve the quality of life and help provide a secure energy future for the US.

We began by asking members of the community to describe their "big questions." From about 100 responses received, several scientific areas emerged in which current knowledge and capability were seriously deficient. Underlying and linking those areas are a number of scientific themes, as illustrated in figure 1, from which the committee identified the following five grand challenges.

1. Control material processes at the level of electrons.[2] In the coming decades, basic energy sciences will shift from the study of how quantum systems are organized to the study of how they work and, ultimately, how to make such systems work for a desired outcome. Controlling electron behavior in matter at the attosecond time scale is a key component of that challenge. To date, the equations behind quantum mechanics have been far too difficult to solve, and the experimental methods for probing strong quantum correlations have been too crude. It will be necessary to overcome those limits and improve understanding of such quantum concepts as coherence and coherent interactions between matter and energy.

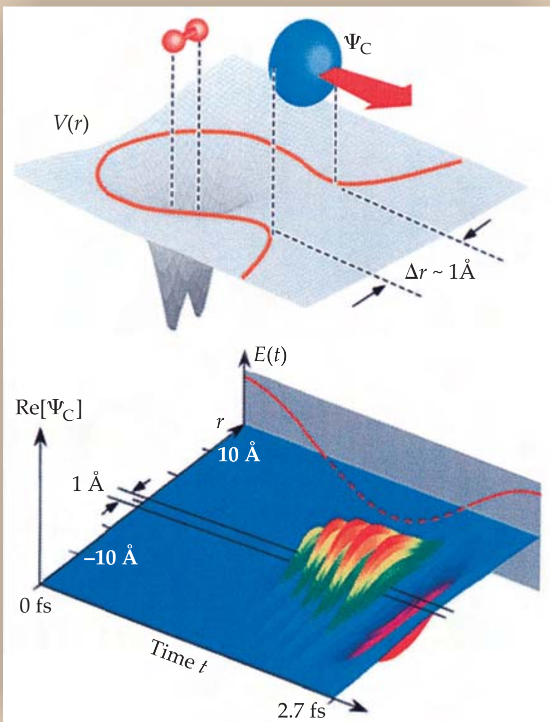
Coherence in quantum mechanics is a measure of the extent to which a wave field vibrates in unison with itself at neighboring points, enabling it to produce interference effects. Although quantum coherence only becomes evident on the microscopic scale of atoms and electrons, it can dominate

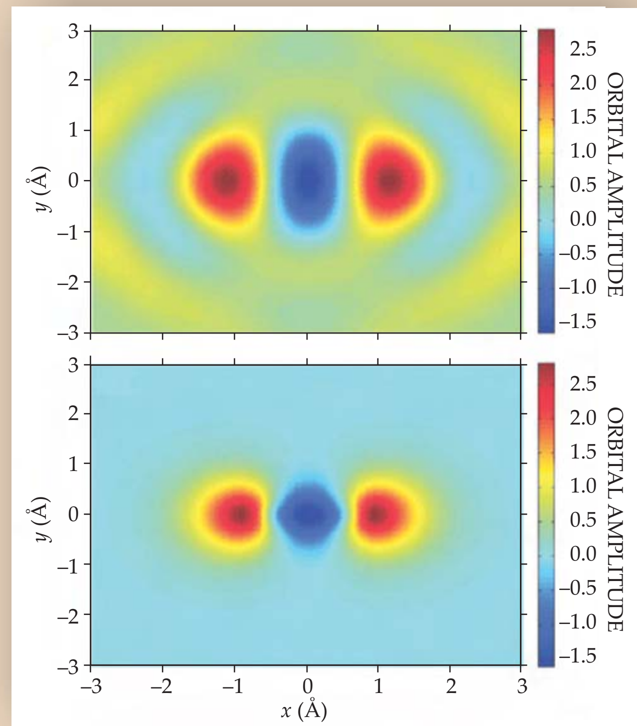
Box 1. Quantum electron scattering

Chapter 2 of the Department of Energy report on five challenges in basic energy sciences[2] describes a new approach to controlling the quantum world that bypasses the woefully inadequate supercomputers by asking the quantum system to find the control solutions. A similar approach may allow imaging on the quantum scale by asking the atom or molecule to image itself. The advantage here is that the quantum system has access to quantum-phase information that is hidden from classical measurement tools.

Quantum imaging has already been developed for simple molecules. For example, if an intense femtosecond laser is focused onto a molecule, an electron may be field ionized and then recollide half an optical cycle later. The electron becomes the probe to interrogate its parent molecule. It can scatter coherently from the molecule or may be captured in the process that produces high harmonics. Either way, the emitted photon or electron will provide phase-coherent information on the electronic structure of the molecule.

The figure on the left is an illustration showing collection of an image of a nitrogen molecule as it undergoes strong-field ionization and recollision. The image on the right was collected from the radiation produced in the recollision (top) and a calculation of the most loosely bound ground-state electron in nitrogen (bottom). (Figures adapted from Committee on AMO 2010, National Research Council, *Controlling the Quantum World: The Science of Atoms, Molecules, and Photons*, National Academies Press, Washington, DC, 2007.)





the macroscopic properties of materials. For example, quantum coherence is responsible for superconductivity, the resistance-free flow of electrical current. Control of quantum coherence will allow the development of highly desirable materials and processes in the 21st century.

Elements of quantum control are exhibited in nature in various physical processes, including the harvesting of light during photosynthesis. Research in catalysis, photochemistry, molecular biology, and device physics could build on nature's techniques to achieve quantum-level control in human technologies. How can energy be produced in ways that are renewable and environmentally benign? How can computers be made smaller, faster, and better—the spintronics device in figure 2 represents one possibility—and what are their true physical limits?

2. Design and perfect atom- and energy-efficient syntheses of new forms of matter with tailored properties.[3] The terms "Stone Age," "Bronze Age," and "Iron Age" refer to humans' increasing mastery over those materials. Likewise, in the "Control Age," researchers will direct the movement of electrons during the ungluing and regluing of atoms in chemical reactions and processes. That control will enable the creation of new materials with properties tailored to meet the changing needs of civilization. The creation of new materials and processes has always progressed hand-in-hand with advances in the ability to define the arrangements and transformations of atoms and electrons in matter and advances in the theories that explain and predict such phenomena. That only a tiny fraction of all possible chemical compounds have been prepared and studied suggests that great discoveries and technological payoffs will come from further advances in knowledge, if researchers can efficiently find or make the compounds they want.

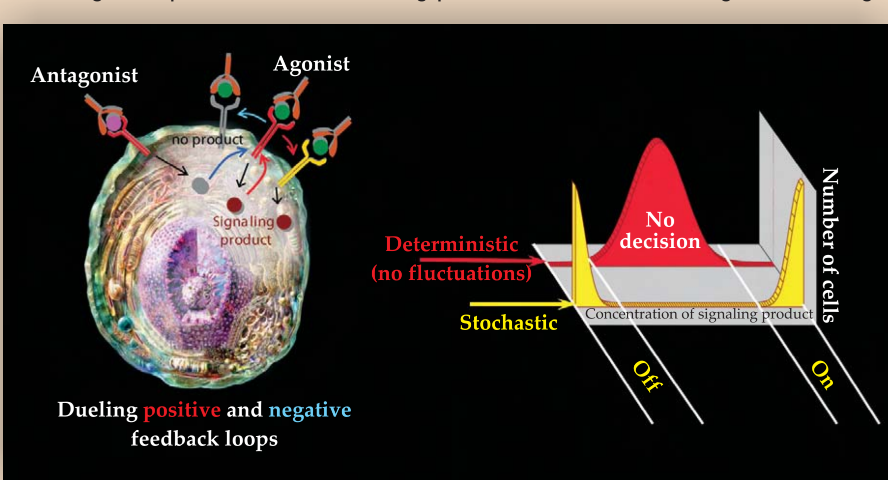
Science is now tantalizingly close to the so-called directed synthesis, guided by predictive design, of some materials with tailored properties (such as those of the sea sponge skeleton shown in figure 3). How mechanically strong can materials be while remaining lightweight? How durable can they be? How

Box 2. Noise can be useful

Immune cells make definite decisions when dealing with noisy data. Cells must often make decisions based on fluctuating (noisy) chemical concentrations in their environment. For example, the T lymphocytes of the immune system must determine whether peptides are foreign pathogens or self-peptides. It has recently been shown that dueling positive and negative feedback loops can be used by T cells to produce digital signals in the presence of stochastic fluctuations in the concentrations of agonist and antagonist ligands. (Agonist ligands bind to a receptor and stimulate production of signaling molecules, while antagonist ligands also bind to receptors but shut off signaling induced by agonists.) If the agonist stimulates a positive feedback loop that further provokes production of the signaling molecule, and if the antagonist initiates a negative feedback loop that inhibits production of the signaling molecule, stochastic fluctuations influence the duel between the two loops in a remarkable way.

In a deterministic (mean-field) picture, each cell always produces an intermediate amount of the signaling molecule when confronted with a mixture of agonists and antagonists in its environment. In other words, the cell makes no decision because a threshold amount of signaling product is required to initiate gene transcription and the consequent immune response. In the presence of fluctuations due to small numbers of agonists and antagonists (the real-world situation), for identical conditions that lead to no decision in a deterministic world, each cell makes a clear decision—it is either on or off. The proportion of cells that are on or off depends on the ratio of agonists to antagonists in the cell's environment.

The figure depicts the decision making process when the ratio of agonist to antagonist is about 1:1. The cells exploit stochastic fluctuations to make decisions that lead to clear functional outcomes, not confusion. That kind of digital signaling has been seen in T lymphocytes. The conditions necessary for stochastic effects resulting in binary cellular decisions are ubiquitous in cell biology, so the phenomenon may be prevalent in both natural and engineered systems. (Figure on left courtesy of A. Chakraborty, MIT; right, M. N. Artyomov et al., *Proc. Natl. Acad. Sci. USA* **104**, 18958, 2007.)



resistant to extreme conditions of temperature, corrosion, or radiation? How electrically and thermally conductive? How transparent? How magnetic? How sticky? How biocompatible? Can researchers learn from nature how to make substances that repair themselves? Can materials be made to modify themselves in response to a changing environment?

Those questions cannot be answered now, but they set the stage for the grand challenge of designing new materials with tailored properties to meet human needs. Over the next few decades, advances in theoretical understanding and computational power and methodologies may well turn the design rules for materials upside down. For example, the reverse design of materials might become commonplace. Beginning with a set of desired properties, the atomic arrangement needed to achieve them will be determined by computer simulation. With that estimate as a guidepost, material designers will then be able to produce truly extraordinary materials with properties that can now only be guessed at.

3. Understand and control the remarkable properties of matter that emerge from complex correlations of atomic and electronic constituents.[4] So-called emergent phenomena, in which the correlated behavior of many particles leads to an unexpected collective outcome, are of great significance across a broad swath of science and engineering. In basic energy sciences, the particles may be microscopic like atoms, molecules, or electrons, or they may be larger entities such as sand grains, cells in an organism, or magnetic rocks in Earth's crust. One can readily find emergence in a multitude of phenomena, including crystalline materials, superconductivity (as illustrated in figure 4), phase transitions, plasmas, climate change, self-assembly, cell colonies, and life itself. The human brain is one of the most stunning displays of emergent properties. It contains about 100 billion neurons that transmit and receive electrochemical signals. Each neuron exists as an individual and rather simple cell, but from billions of them acting collectively there emerges the human mind.

Uncovering the fundamental rules of correlations and emergence is the first part of the challenge. The second part is achieving control over those correlations, a prospect that can be contemplated because the tools now exist to probe and affect particles and their correlations on the nanoscale. The potential applications are as rich and diverse as the variety of emergent phenomena, but the collective properties of electrons in solids are of special importance to basic energy sciences. For example, today's information technology is based on semiconductors that under normal conditions are weakly correlated materials, meaning that the motion of one electron is influenced by other electrons only in a relatively simple way. That simplicity has been a great benefit for modeling the function of semiconductors, but it also has limited that functionality. Strongly correlated materials, on the other hand, display collective electronic phenomena—such as magnet-

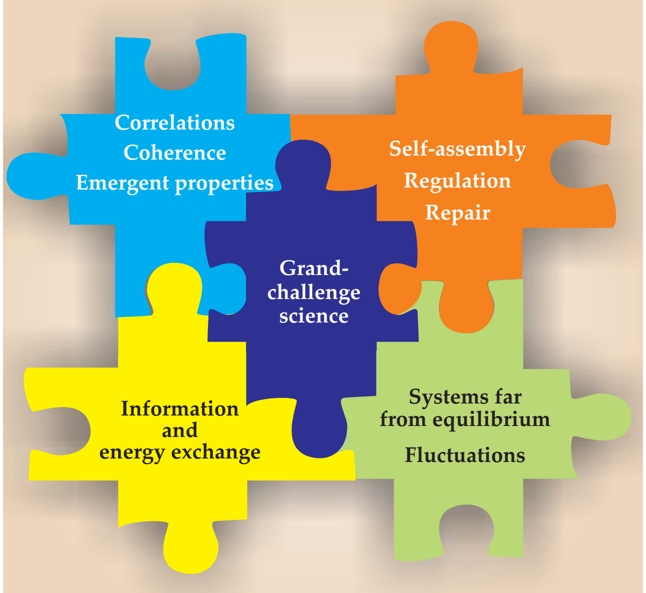


Figure 1. Scientific themes underlying and connecting the five grand challenges.

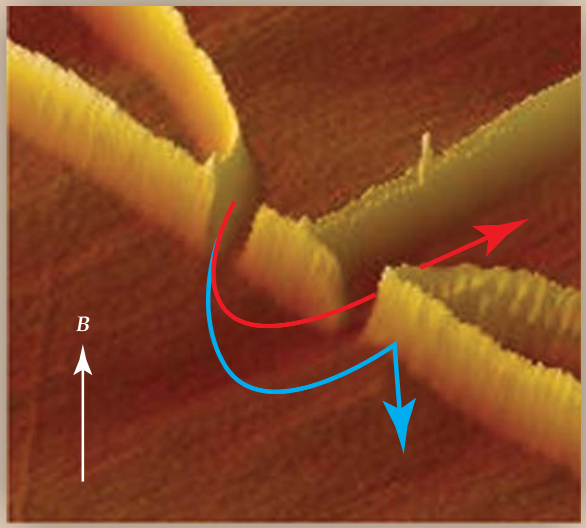


Figure 2. An atomic force micrograph of a device used to separate electrons according to their spin, a feature that could be used in next-generation spintronics. Two point contacts act as a monochromatic source of ballistic holes; with a narrow detector in a magnetic focusing geometry, they act as a tunable spin filter. The red and blue lines show the different pathways that spin-up and spin-down electrons follow. The magnetic field B is perpendicular to the surface, and the lithographic separation between point contacts is roughly 1 μm. (From L. P. Rokhinson et al., *Phys. Rev. Lett.* **93**, 146601, 2004.)

ism, superconductivity, and ferroelectricity—even under ordinary conditions.

If researchers could achieve for strongly correlated materials the same level of understanding, precise processing, and control that they routinely achieve for semiconductors, it would open up remarkable technological possibilities—for example, essentially lossless transmission of energy across the continents. The grand challenge of understanding and controlling collective phenomena and emergent properties will require the extension of existing theories to new regimes, the development of fundamentally new theories, and the building of new instruments to control directly the atomic-level dynamics.

4. Master energy and information on the nanoscale to create new technologies with capabilities rivaling those of living things.[5] Biological systems are built from the same fundamental elements of matter and follow the same laws of physics as inorganic and human-engineered materials. Biological energy and chemical transduction, communication, adaptation, self-repair, and reproduction are all emergent properties. Look closely at biological nanomachines such as rotary molecular motors, and they appear to resemble their human-engineered counterparts. However, biological machinery often works in ways dramatically different from those of synthetic devices. In most cases biological mechanisms hinge on physical behaviors that exist only at the nanoscale. Learning how biosystems use energy and fluctuations can lead directly to new human-engineered devices.

Design and fabrication of devices on the nanometer scale using solid-state electronic materials is becoming possible, but many biological systems currently exceed human-engineered nanotechnologies—by a great margin—in what they can do. Biological systems are the proof of concept for what can physically be achieved with nanotechnology. Consider, for example, the ease with which biological systems transform and store energy, or their ability to perform self-repair and to adapt to changing external conditions. The ways in which energy, entropy, and information are manipulated within the nanosystems of life provide lessons on what humans must learn to do to develop similarly sophisticated technologies. To bring that level of nanotechnology under human control, several questions must be answered. Can the long-standing approach of top-down engineering be extended to the molecular level? That is, is it possible to construct functional interfaces between biological and synthetic systems that can direct the biological capabilities to suit human purposes? Or is it necessary to pursue a bottom-up approach, whereby synthetic devices are constructed with the functionalities of living systems?

Harnessing nanoscale phenomena will entail interfacing biological and nonbiological systems, which in turn will require communication—that is, using the chemical language of cells to convey information to them and ultimately domesticate them. It is also necessary to understand living systems' hardware configurations and to connect nanoscale functions with the macroscopic world. Energy and information will need to be controlled on the nanoscale, and new nanoscale devices must be fabricated and implemented. The size of nanoscale objects makes it feasible to use large numbers of them, which could result in radically new emergent properties. Meeting that challenge of energy and information on the nanoscale paves the way for artificial, self-regulating, adaptive interactive devices.

Living systems of necessity exist away from equilibrium and constantly use energy to maintain that condition. The remarkable ways in which biology uses fluctuations around a steady state are key to many of its control processes. Those concepts also underlie the next and last grand challenge.

5. Characterize and control matter away—especially far away—from equilibrium.[6] A system is in equilibrium when it does not change with time. All natural and most human-caused phenomena occur away from equilibrium.

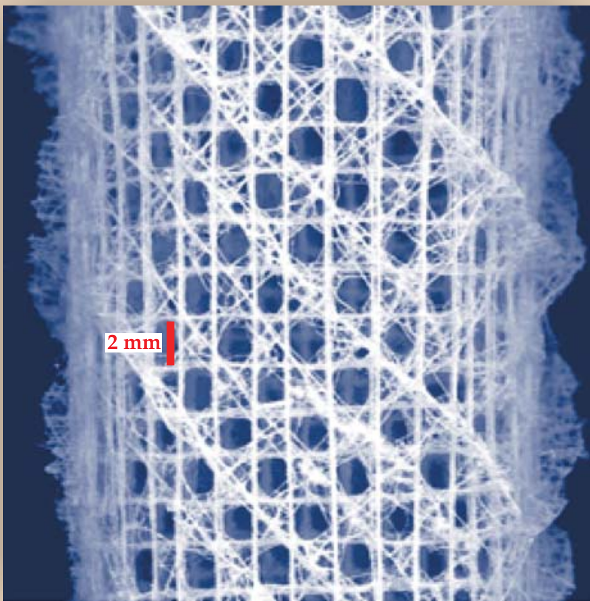


Figure 3. Skeletal structure of a natural sea sponge, produced by protein templating of mineral growth in an aqueous marine environment under mild conditions. Sea sponges, and many other biological materials, are examples of nanocomposite materials, which grow under conditions controlled at the nanometer scale, and are an elegant example of the potential for designed materials. (From J. Aizenberg et al., *Science* **309**, 275, 2005.)

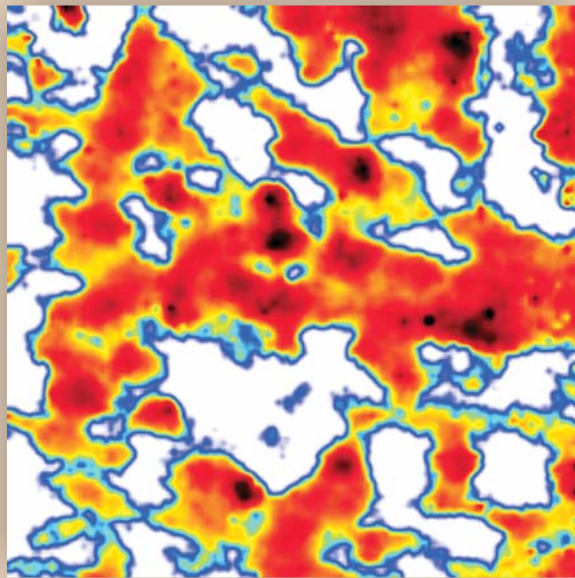


Figure 4. Scanning tunneling microscope data for a high-temperature superconductor, showing large local variations of the energy gap, the energy required to remove or add an electron. The area shown is 30 nm square, and the color scale varies from a gap of zero (white) to approximately 100 meV (black). Remarkably, the image was taken at 120 K, well above the 93 K superconducting transition temperature of the sample. Clearly, some sort of gap persists above the transition. Imaging local functionality, as demonstrated here, is a crucial route to understanding emergent properties. (From K. Gomes et al., *Nature* **447**, 569, 2007.)

Nonequilibrium systems can range in scale from the microscopic (such as nanostructures and bacteria) to the enormous (such as seismic fault zones), and away-from-equilibrium processes occur on time scales ranging from nanoseconds to millennia. Despite the pervasiveness of nonequilibrium systems and processes, most of the current understanding of physical and biological systems is based on equilibrium concepts.

It has long been recognized that understanding matter and information systems away from equilibrium is a grand challenge to science and engineering. Understanding the nonequilibrium behavior of physical, chemical, biological, atmospheric, geological, and even astronomical systems promises huge advances in the ability to manufacture super-hard, super-strong, and self-repairing materials, and in a great many other areas as well, from earthquake and tide prediction to the control of complex structures and even phase stability. Understanding nonequilibrium phenomena will also help to optimize processes for obtaining and transducing energy from wind, geothermal, nuclear, fossil-fuel, and other sources.

A real understanding of nonequilibrium phenomena will require answers to a number of complex questions. What are the general rules that apply to microscopic relaxation on extremely long time scales? How can nonequilibrium processes be directed at the nanoscale? How do systems search free-energy landscapes? Can efficiency measures be developed for cellular and artificial cellular processes and for highly nonequilibrium processes? Can machines be designed to operate far from equilibrium to produce power efficiently? Can artificial systems be designed to mimic nonequilibrium processes in biology? Can multiple-temperature phenomena be exploited for energy control? Can matter be stabilized in nonequilibrium states, such as metamaterials, high-strength glass, or graded structures? Is it possible to understand and control turbulent flows that pertain to phase transitions, diffusion, and chemical reactions? Because of the pervasiveness of nonequilibrium phenomena, mastering them should pave the way for dealing effectively with a host of issues facing civilization, including energy, climate, materials, biology, and even security.

Recommendations

The science we have described is inherently multidisciplinary and will require sustained efforts over long periods of time before society will reap the benefits. Based on the committee's input, we propose that DOE adopt a three-pronged approach to training and supporting scientists for grand-challenge and energy-security sciences:[7]

▶ A DOE energy institute, to support creativity and accomplishment by the most promising and productive researchers.

▶ An energy sciences study group, to approach problems requiring science and technology to meet energy-security challenges.

▶ A DOE fellows program, to train and inspire young scientists.

We envision the DOE energy institute to be modeled after the Howard Hughes Medical Institute's investigator awards. Investigators would be supported at a significant level and the funds would be unrestricted, but the projects funded must be long term and broadly related to energy sciences. The goal is to change the prestige and impact of university research supported by the Office of Basic Energy Sciences. The energy sci-

Box 3. Subcommittee on grand challenges for basic energy sciences

Graham Fleming (cochair), Mark Ratner (cochair), Paul Alivisatos, Leon Balents, David Bishop, Philip Bucksbaum, Jay Groves, John Hemminger, Michael Hochella, Walter Kohn, Tobin Marks, Paul McEuen, Joel Moore, Thomas Moore, Cherry Murray, Daniel Nocera, Teri Odom, Julia Phillips, Peter Schultz, Robert Silbey, John Spence, Stanley Williams, Jun Ye.

ences study group would aim to make its young participants conversant with the scientific and technical dimensions of national energy research and to convey an appreciation for the interdisciplinary nature of energy sciences. The DOE fellows program would help improve the training of young scientists via summer energy experiences, grand-challenge workshops, and network energy teams that would allow scientists to customize their training and begin their own collaborative group at an early and significant career stage.

The theoretical challenges described in the report cannot simply be reduced to ever larger computations—in many cases the theory is not yet formulated well enough to compute anything at all. There is a need to attract the best theoretically inclined scientists to basic energy sciences to develop the new concepts needed to understand and control matter with precision. We envision an ambitious scientific culture that encourages high-risk, high-reward theoretical exploration focused on such issues as nonequilibrium phenomena, coherence, correlations, and the interconversion of energy and information.

On the experimental side, directing and controlling the properties of materials to achieve a desired outcome requires new tools to explore the length, time, and energy scales on which processes of interest take place. It is necessary to probe matter at a level much deeper than the macroscopic averages studied today, so that the properties of individual molecules or atoms of a material can be observed and controlled. Experimental researchers therefore need to develop and disseminate new tools capable of viewing such inner workings of matter as transport, reactivity, fields, excitations, and dynamics.

Richard Smalley won the 1996 Nobel Prize in Chemistry for his discovery of a new form of carbon. He argued that the problem of energy confronts the human race today with immediacy and danger. He felt that understanding and mastering energy sciences could have great positive effects on civilization, the economy, and all people. It is in that spirit that we pose our five grand challenges for science and the imagination.

We are grateful to the members of the Basic Energy Sciences Advisory Committee for their encouragement and helpful comments. We thank the members of the subcommittee, listed in box 3, for their creativity, courage, and hard work. We are indebted to Patricia Dehmer for her leadership, imagination, deep expertise, and unfailing support. We are grateful to Tiffaney Dressen, Art Robinson, and Lynn Yarris for their help with the wording, production, and organization of this article.

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