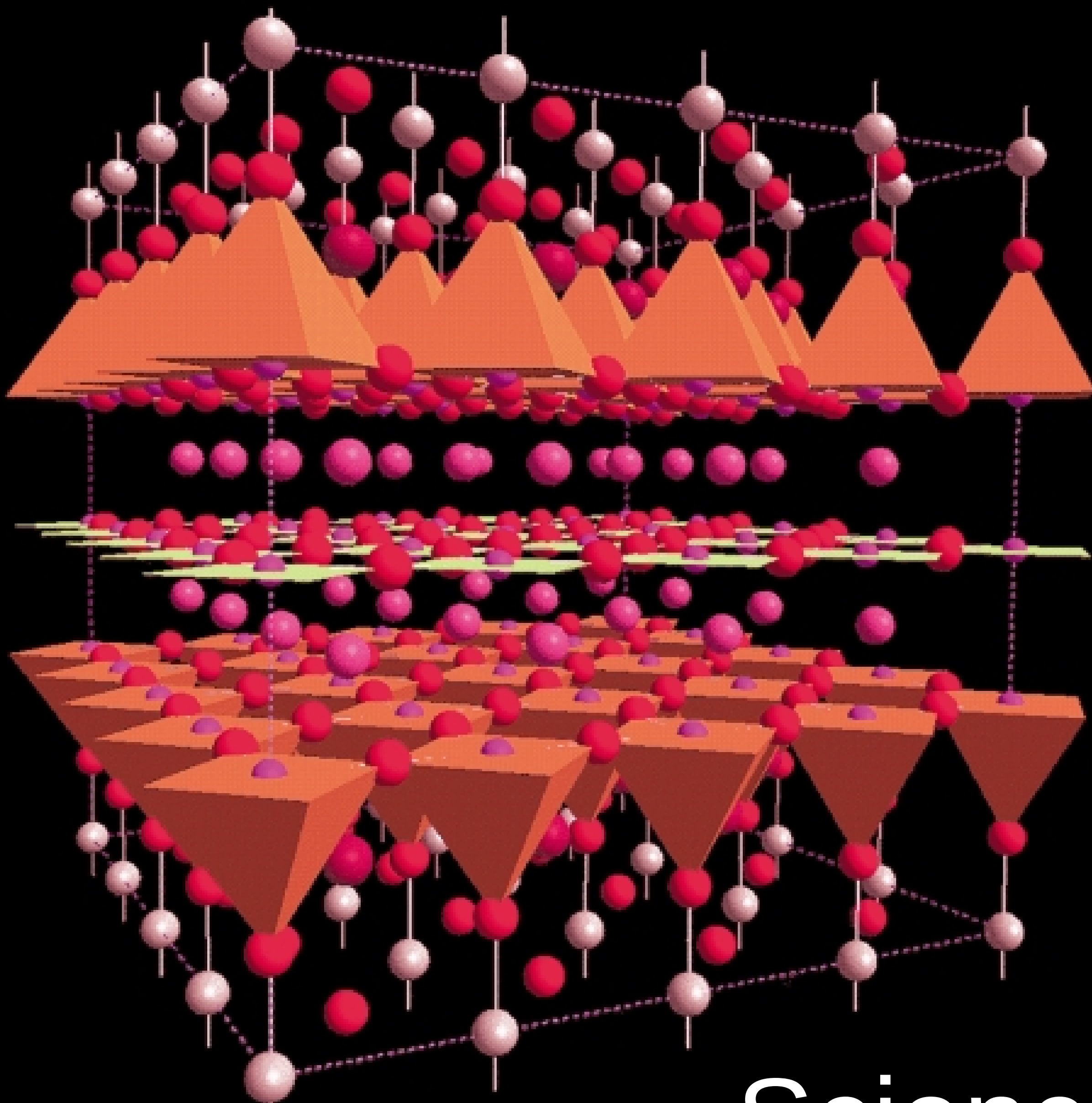
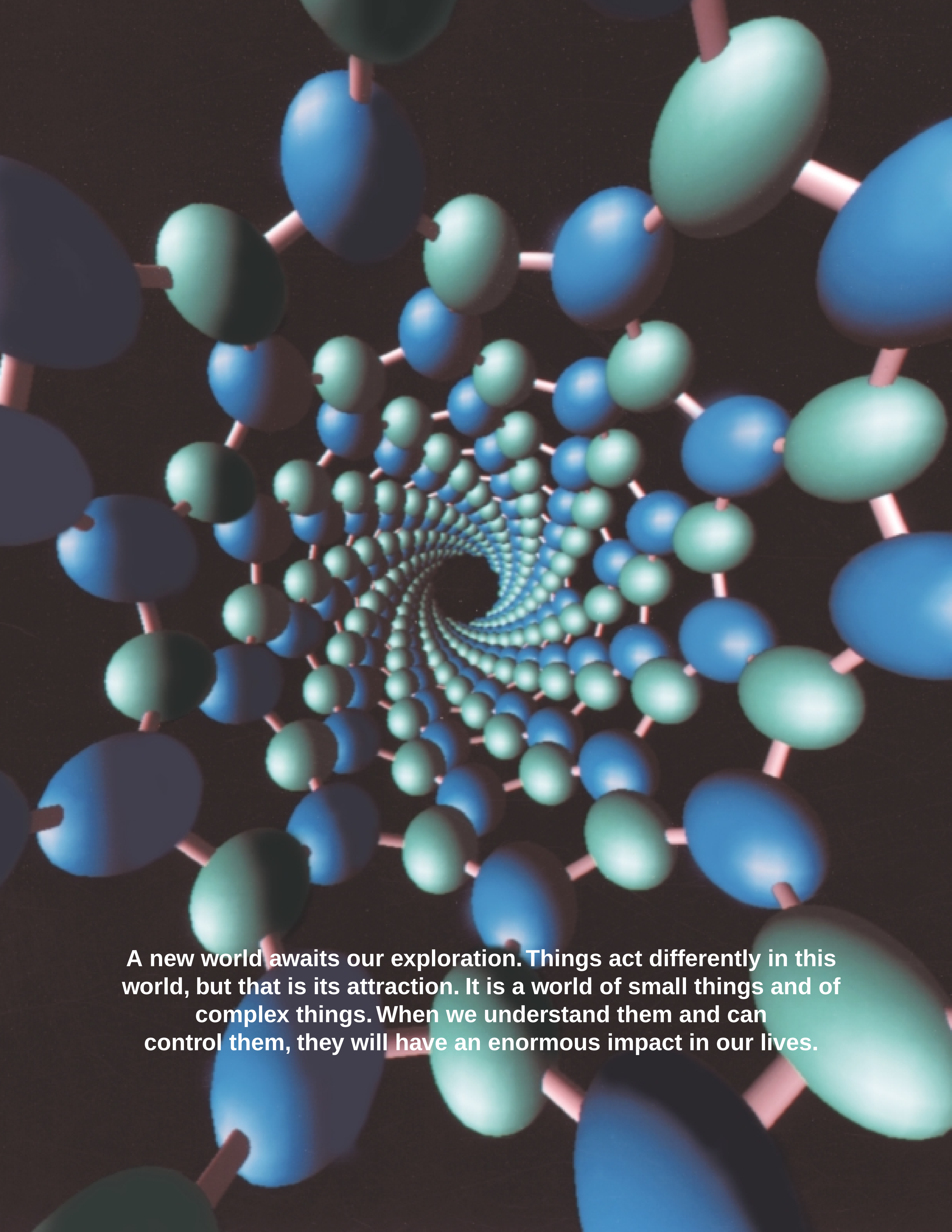
Complex Systems



Science for the 21st Century

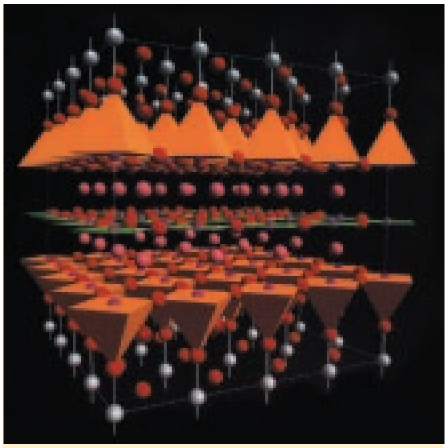

A new world awaits our exploration. Things act differently in this world, but that is its attraction. It is a world of small things and of complex things. When we understand them and can control them, they will have an enormous impact in our lives.

Complex Systems

Science for the 21st Century

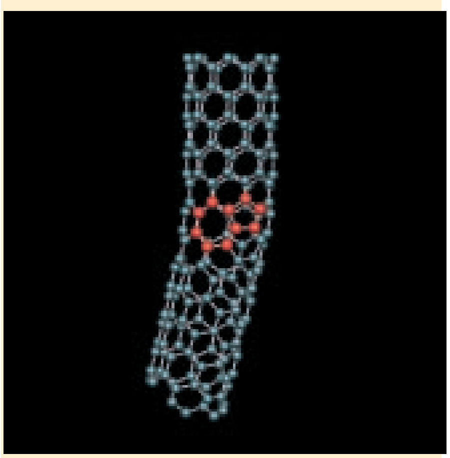
A U.S. Department of Energy, Office of Science Workshop

Complex Systems
Science for the 21st Century
Executive Summary



Collective Phenomena—*Can we achieve an understanding of collective phenomena to create materials with novel useful properties?*

Materials by Design*—Can we design materials having predictable, and yet often unusual properties?*



Functional Systems*—Can we design and construct multicomponent molecular devices and machines?*

As we look to the next century, we find science and technology at yet another threshold: the study of simplicity will give way to the study of "complexity" as the unifying theme.

The triumphs of science in the past century, which improved our lives immeasurably, can be described as elegant solutions to problems reduced to their ultimate simplicity. We discovered and characterized the fundamental particles and the elementary excitations in matter and used them to form the foundation for interpreting the world around us and for building devices to work for us. We learned to design, synthesize, and characterize small, simple molecules and to use them as components of, for example, materials, catalysts, and pharmaceuticals. We developed tools to examine and describe these "simple" phenomena and structures.

The new millennium will take us into the world of complexity. Here, simple structures interact to create new phenomena and assemble themselves into devices. Here also, large complicated structures can be designed atom by atom for desired characteristics. With new tools, new understanding, and a developing convergence of the disciplines of physics, chemistry, materials science, and biology, we will build on our 20th century successes and begin to ask and solve questions that were, until the 21st century, the stuff of science fiction.

Complexity takes several forms. The workshop participants identified five emerging themes around which research could be organized.

Collective Phenomena—*Can we achieve an understanding of collective phenomena to create materials with novel, useful properties?* We already see the first examples of materials with properties dominated by collective phenomena—phenomena that emerge from the interactions of the components of the material and whose behavior thus differs significantly from the behavior of those individual components. In some cases collective phenomena can bring about a large response to a small stimulus—as seen with colossal magnetoresistance, the basis of a new generation of recording memory media. Collective phenomena are also at the core of the mysteries of such materials as the high-temperature superconductors.

Materials by Design—*Can we design materials having predictable, and yet often unusual properties?* In the past century we discovered materials, frequently by chance, determined their properties, and then discarded those materials that did not meet our needs. Now we will see the advent of structural and compositional freedoms that will allow the design of materials having specific desired characteristics directly from our knowledge of atomic structure. Of particular interest are "nanostructured" materials, with length scales between 1 and 100 nanometers. In this regime, dimensions "disappear," with zero-dimensional dots or nanocrystals, one-dimensional wires, and two-dimensional films, each with unusual properties distinctly different from those of the same material with "bulk" dimensions. We could design materials for lightweight batteries with high storage densities, for turbine blades that can operate at 2500˚C, and perhaps even for quantum computing.

Materials by Design: Supramolecular assembly. Reprinted from cover with permission from *Science*, vol. 276, 4/18/97; ©1997, American Association for the Advancement of Science, New York, NY.

Functional Systems—*Can we design and construct multicomponent molecular devices and machines?* We have already begun to use designed building blocks to create self-organized structures of previously unimagined complexity. These will form the basis of systems such as nanometer-scale chemical factories, molecular pumps, and sensors. We might even stretch and think of self-assembling electronic/photonic devices.

Nature's Mastery—*Can we harness, control, or mimic the exquisite complexity of Nature to create new materials that repair themselves, respond to their environment, and perhaps even evolve?* This is, perhaps, the ultimate goal. Nature tells us it can be done and provides us with examples to serve as our models. We learn about Nature's design rules and try to mimic green plants which capture solar energy, or genetic variation as a route to "self-improvement" and optimized function. These concepts may seem fanciful, but with the revolution now taking place in biology, progressing from DNA sequence to structure and function, the possibilities seem endless. Nature has done it. Why can't we?

New Tools—*Can we develop the characterization instruments and the theory to help us probe and exploit this world of complexity?* Radical enhancement of existing techniques and the development of new ones will be required for the characterization and visualization of structures, properties, and functions—from the atomic, to the molecular, to the nanoscale, to the macroscale. Terascale computing will be necessary for the modeling of these complex systems.

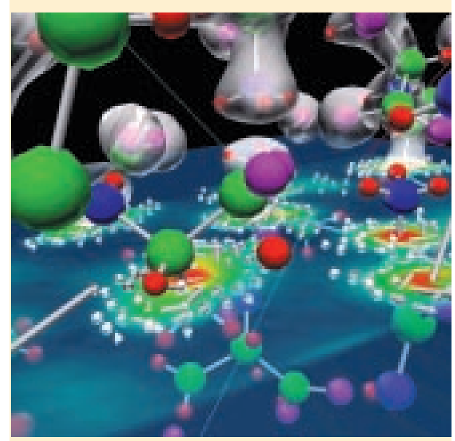
Now is the time. We can now do this research, make these breakthroughs, and enhance our lives as never before imagined. The work of the past few decades has taken us to this point, solving many of the problems that underlie these challenges, teaching us how to approach problems of complexity, giving us the confidence needed to achieve these goals. This work also gave us the ability to compute on our laps with more power than available to the Apollo astronauts on their missions to the moon. It taught us to engineer genes, "superconduct" electricity, visualize individual atoms, build "plastics" ten times stronger than steel, and put lasers on chips for portable CD players. We are ready to take the next steps.

Complexity pays dividends. We think of simple silicon for semiconductors, but our CD players depend on dozens of layers of semiconductors made of aluminum, gallium, and arsenic. Copper conducts electricity and iron is magnetic. Superconductors and giant magnetoresistive materials have eight or more elements, all of which are essential and interact with one another to produce the required properties. Nature, too, shows us the value of complexity. Hemoglobin, the protein that transports oxygen from the lungs to, for example, the brain, is made up of four protein subunits which interact to vastly increase the efficiency of delivery. As individual subunits, these proteins cannot do the job.

The new program. The very nature of research on complexity makes it a "new millennium" program. Its foundations rest on four pillars: physics, chemistry, materials science, and biology. Success will require an unprecedented level of interdisciplinary collaboration. Universities will need to break down barriers between established departments and encourage the development of teams across disciplinary lines. Interactions between universities and national laboratories will need to be increased, both in the use of the major facilities at the laboratories and also through collaborations among research programs. Finally, understanding the interactions among components depends on understanding the components themselves. Although a great deal has been accomplished in this area in the past few decades, far more remains to be done. A complexity program will complement the existing programs and will ensure the success of both. The benefits are, as they have been at the start of all previous scientific "revolutions," beyond anything we can now foresee.

***Nature's Mastery**—Can we harness, control, or mimic the exquisite complexity of Nature to create new materials that repair themselves, respond to their environment, and perhaps even evolve?*

***New Tools: Instruments**—Can we develop the characterization instruments to help us probe and exploit this world of complexity?*



***New Tools: Computer-Based Theory and Simulation**—Can we develop the theoretical tools to describe and predict the properties of increasingly complex phenomena?*

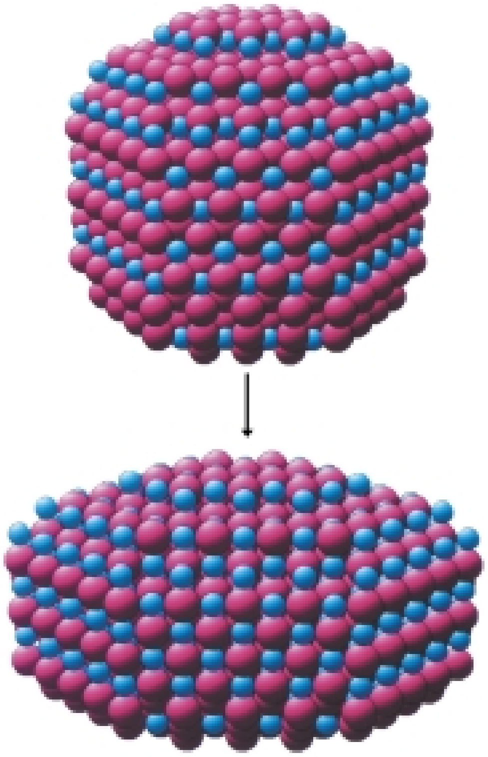
Complex Systems

The goal of science is to understand and appreciate Nature and to use that understanding to create materials and devices that enhance our lives.

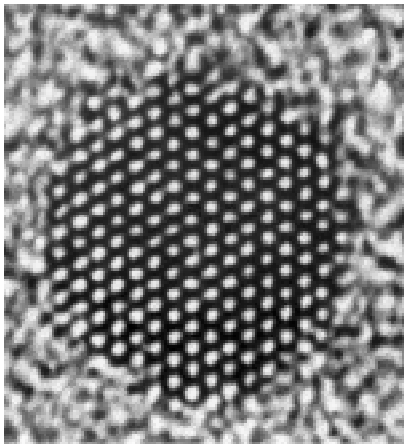
We can learn much from Nature. Certainly we can learn how she approaches problems. We can also learn how she solves specific problems—sensing, repairing damage, creating mechanical strength. Beyond that, our study of organisms tells us what can be achieved, what problems can be solved, where we can set our goals in exploiting this understanding to benefit society.

Nature's approach to building complex structures and functions is hierarchical. This guides us in two ways.

On a practical level, we can mimic this scheme by building our own structures hierarchially: combining simple molecules to fashion more complex ones, then combining those, repeatedly, until very complex structures with greatly enhanced properties emerge. Collagen, for example, has a tensile strength comparable to that of steel wire, yet it is fundamentally just a single strand of amino acids linked through single covalent "peptide bonds." It gains its strength, however, through the association of three single polymeric chains to make triple strands, which associate to make stronger microfibrils, which then associate to make still stronger fibrils, which aggregate to form the collagen fiber.



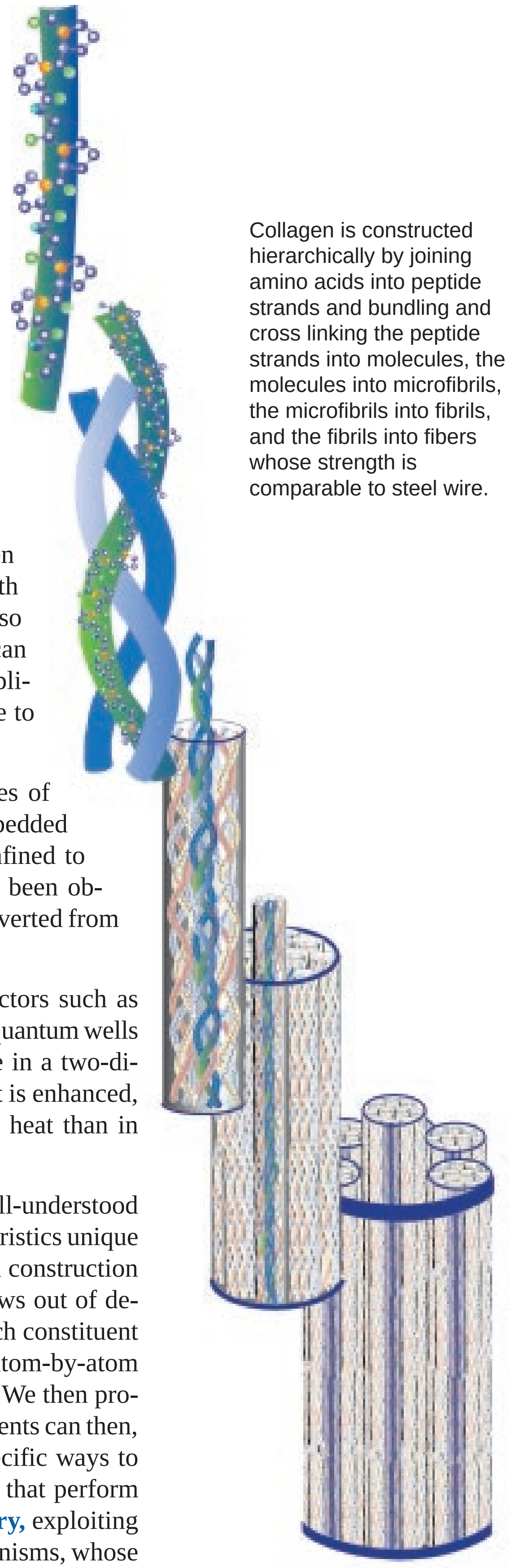
Nanocrystals of the semiconductor cadmium selenide with a radius between 1 and 10 nanometers can take two crystal forms (above), depending on applied pressure. Because of their "low dimensionality," their properties, such as melting point and color, depend on their size. An electron micrograph, below, shows columns of individual atoms and facets of nanocrystal surfaces.



At the conceptual level, Nature can be our guide in designing a multicomponent research program to mirror this hierarchy. At the base of this program is the continuing study of simple structures and phenomena—continuing because there is still much to learn, and because it provides the fundamental building blocks for the study of complexity.

While it is intuitive that large, more complicated, multicomponent structures can provide enhanced properties and functions, recent discoveries have shown that exploration of the "nano" world—structures with length scales between one and 100 billionths of a meter, 1000 times smaller than a human hair—is equally important. Such structures can be made either through self-assembly processes or through controlled deposition of the components of the material, for example, by lithography or molecular beam epitaxy. Crystals of these sizes contain as few as a thousand atoms and have remarkable and potentially valuable characteristics—most notably, properties that vary with the size and pattern of the structure. Surface effects dominate: while an ice cube melts at the same temperature as an iceberg, a 2-nm-diameter crystal of the semiconductor cadmium selenide melts at a lower temperature than a 4-nm-diameter crystal of the same material. These nanocrystals can be made to emit light, and again, in sharp contrast to larger structures, the quantum confinement resulting from their reduced dimensions causes the color of the light they emit to depend on their size. Single nanocrystals have been incorporated into structures patterned using the same lithographic techniques employed by chip designers and are able to act as nano-transistors, allowing the passage of only one electron at a time. The impact of these materials and devices on the development of computers, which owe their extraordinary advances to continual miniaturization, is incalculable, although not achievable without much additional research.

The discovery of "bucky" balls and tubes is another manifestation of Richard Feynman's 1959 prediction that there "is room at the bottom." Spheres of 60 carbon atoms have already been incorporated into photovoltaic devices, which capture solar energy as electricity. Even smaller balls, containing only 36 atoms, have been made and shown to be superconducting when "doped" with metal atoms. Carbon tubes of nanoscale dimensions have also been made. These are the strongest known fibers and can absorb large amounts of mechanical energy. Proposed applications range from lightweight armor to hydrogen storage to battery components.

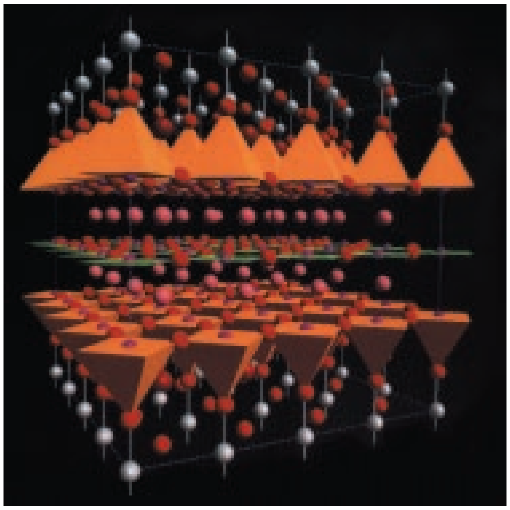


Collagen is constructed hierarchically by joining amino acids into peptide strands and bundling and cross linking the peptide strands into molecules, the molecules into microfibrils, the microfibrils into fibrils, and the fibrils into fibers whose strength is comparable to steel wire.

Other one-dimensional structures include molecular wires of 10-to-120-nm diameter, for example, bismuth threads embedded in channels in an alumina film. With charge carriers confined to this narrow "wire," novel thermoelectric properties have been observed, and there is evidence that the bismuth has been converted from a semimetal to a semiconductor.

Finally, layering of nanometer-thick films of semiconductors such as indium arsenide and aluminum indium arsenide can create quantum wells in which electrons are again confined, although this time in a two-dimensional plane. New properties arise—electron transport is enhanced, and laser light is emitted with the generation of far less heat than in conventional lasers.

More complex are **Collective Phenomena,** individual, well-understood components interacting with each other to exhibit characteristics unique to the combination. Beyond this is the rational design and construction of far more complicated structures. Defined function grows out of defined structure, the blueprint governing the location of each constituent atom. In **Materials by Design,** we formulate a structure atom-by-atom in order to allow it to perform a specific desired function. We then proceed to synthesize it, according to that plan. These components can then, through self-assembly or directed fabrication, link in specific ways to produce **Functional Systems,** motors, pumps and others that perform useful tasks. At the top of the pyramid is **Nature's Mastery,** exploiting all of these stages to produce extraordinarily complex organisms, whose very existence provides us with goals—and the knowledge that they can be achieved.



High-T_C superconductor $HgBa_2Ca_2Cu_3O_{8-\delta}$. This material conducts electricity without loss at temperatures up to –40˚C, higher than any other known material. The goal: room-temperature superconductors.

Collective Phenomena

The interaction of objects obeying simple rules can produce remarkably complex and yet organized behavior. Electrons interacting with each other and their host lattice in a solid can give rise to magnetism and superconductivity. Chemical constituents interacting in solution can give rise to complex pattern formation and growth. Birds flying in the sky give rise to flocking behavior. Some of these behaviors, and their relation to the underlying microscopic laws, are now understood, but many of the most interesting and important cases remain mysteries. Learning how to understand and control these emergent behavior patterns will provide the foundation upon which to build complex systems.

Strongly interacting electronic systems

The origin of high-temperature superconductivity remains a mystery, as do many aspects of the behavior of magnetoresistive materials. These materials have been extensively studied, and many of the important parameters governing their behavior have been experimentally identified. However, models based on the weakly interacting particles have failed to describe their behavior.

—New concepts and techniques based on a radically different point of view are necessary to describe these materials. Numerical studies on ever-larger systems will be used to support and guide these investigations. New experimental probes will be required to investigate both the microscopic and emergent order in these systems.

Phase transitions and responsive systems

Systems that are close to a classical or quantum phase transition can exhibit large responses to small external signals. These external signals can drive the system from one phase to the other, dramatically changing the properties of the material.

—To utilize the potential of responsive materials, a dramatic increase in our understanding of phase transitions is necessary, particularly ways to harness these transitions to perform useful activities. Examples include percolative networks that can sense changes in temperature, humidity, or chemical environment and materials that convert one type of signal to another, e.g., electrical to mechanical.

Coherence in complex systems

Coherence is central to many emergent properties of collective systems, including Bose–Einstein condensation, quantum computing, and quantum interference devices.

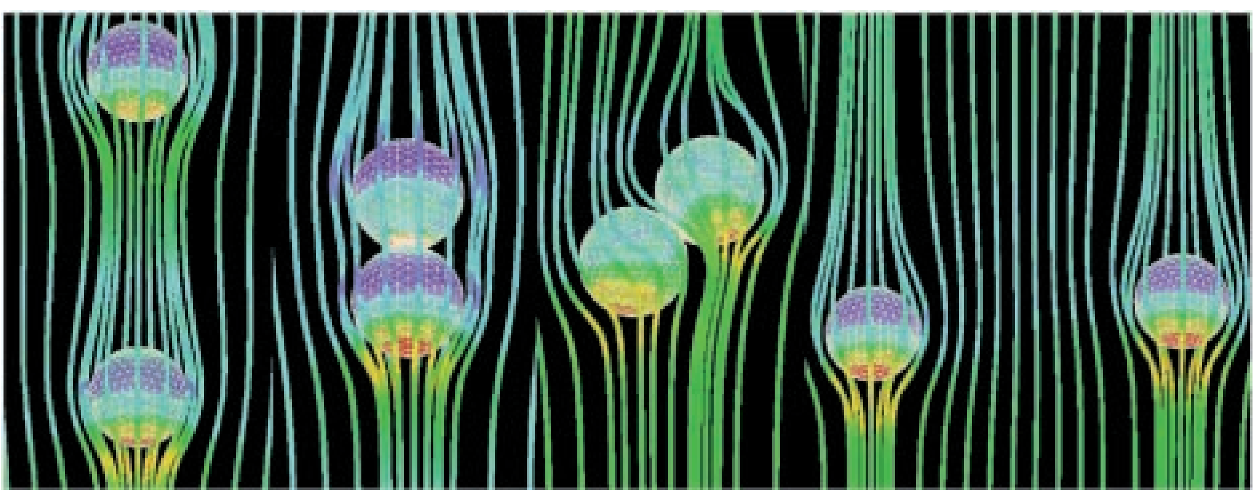
> — *While coherence in a single object such as an atom, quantum dot, or photon is now well understood, the behavior of collections of coherent interacting objects remains largely unexplored. Exploring the uses of coherence in such a complex environment is a tremendous challenge. New techniques and approaches must be developed to create and interact with these coherent systems. Improved computational techniques must be developed to model the effects on coherence.*

Bose–Einstein condensate of supercooled magnetically trapped atoms. The atoms move at identical speeds and in identical directions, defying the laws of classical physics. It has been suggested that this could be the basis for lasers for use in the nanoscale sculpture of circuitry.

Emergent properties of active objects

Interactive, mobile objects obeying simple rules for interacting can generate complex behaviors that range from flocking to spatial pattern formation. These emergent patterns interact strongly with their external environment.

> — *To understand, classify, and make use of these phenomena, the principles of statistical physics must be expanded to include systems composed of active elements. Such systems can be the basis of smart materials that respond collectively to external stimuli in a coherent and coordinated fashion.*



Drafting Kissing Tumbling Equilibrium

Simulation of particles in flowing liquids will aid our understanding of complex processes occurring in sedimentation columns, fluidized beds, slurries, and hydraulic fracturing.

Model of a supramolecular assembly of 100 triblock polymeric molecules of defined structure. Such supra-molecular materials could affect the technologies of sensors, biomaterials, waveguides, lubricants, catalysts.

Materials by Design

One of the most immediate and noticeable impacts of the development of complex materials will be the availability of new materials with properties that are greatly enhanced compared to those of materials available today. The complexity that gives rise to those enhanced properties will, at the same time, present significant design and synthesis challenges.

Compositional Control

Design and synthesis of complex materials will be radically changed. Design will be at the atomic level, starting with the electronic structure of the elements. This fundamental knowledge will be coupled with precise synthesis and fabrication techniques to translate that specific design into a material. The result will be the fabrication of materials with precisely defined, predetermined properties.

—A thorough understanding of the properties of the elements and, more importantly, their interactions over short and long distances in structures, will be required for the design of materials with specified properties. Targets for complex materials such as these include extremely lightweight batteries for use in electric automobiles and other applications. Turbine blades that can operate at extremely high temperatures with minimal failure rates would greatly increase the efficiency of fuel-burning engines. Quantum coherent materials; advanced photonic and electronic materials; and superhard, strong, fatigue-resistant, and corrosion-resistant materials would also have a great impact on energy efficiency, pollution prevention, and information storage and handling.

—Development of novel systems will require sophisticated synthetic tools. In some cases this will require the development of new chemistries, involving novel reactions and reaction conditions to synthesize structures of defined design. In other cases physical techniques such as deposition or lithography will be required.

Custom designed molecules (blue and pink) self-assemble to form a structure that specifically binds to a target molecule (green). Structures designed to be capable of binding each other are the basis for the development of large functional assemblies.

Unusual conditions

The properties of materials are very much a function not only of their compositions but also of the conditions under which they have been synthesized and the conditions under which they are used.

—Greatly increased exploration of materials made or used under unusual conditions is required. Techniques to create and maintain those conditions during synthesis and to model and characterize the resulting materials must be devised and implemented. Conditions in question include nonequilibrium, high pressure, high magnetic field, and high energy density. In addition, materials with large numbers of component elements, with controlled doping, chirality, and complex layering will be required to achieve the enhanced properties envisioned. Low-dimensional materials—"nanostructures"—whose properties do not scale with size will be synthesized and characterized. The extraordinary dependence of the properties of these materials on their size provides the materials designer with an entirely new palette of "colors" with which to work.

Parallel synthesis of members of a spatially addressable library of high-temperature cupric oxide superconductors allows rapid screening of thousands of materials to identify the compositions with optimized properties.

Library of high-temperature cupric oxide superconductors. Reprinted cover with permission from *Science*, vol. 260, 6/23/95; © 1995, American Association for the Advancement of *Science*, New York, NY.

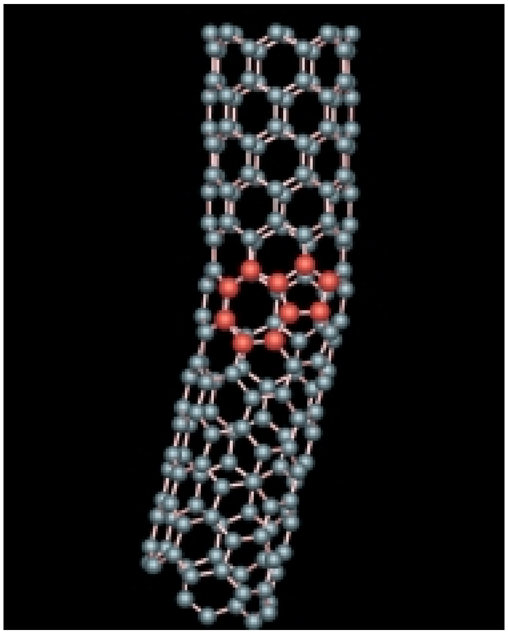
Parallel fabrication/characterization

While modeling techniques are being developed to allow the atomic-level design of materials with optimized properties, massively parallel combinatorial approaches will be applied to identify new materials.

—Systems need to be designed to synthesize huge numbers of materials with slightly different amounts of each of the constituent elements. These systems must also be able to achieve parallel synthesis under a wide variety of conditions, for example, variable oxygen pressure in superconductor synthesis. Characterization tools capable of rapid analysis of large numbers of small samples are needed. The combinatorial approach is not "hit or miss" but rather requires the same type of theoretical understanding as does conventional synthesis—each group of compositions used for synthesis must be selected through modeling and theory. The breakthrough is that thousands of compounds are synthesized at once rather than one by one. As modeling and prediction improve, the combinatorial approach will continue to be of value, allowing analysis of samples in narrower composition and condition regimes to achieve successively greater degrees of optimization of properties. Theory development will benefit from the enhanced database of structures with characterized properties.

Functional Systems

Nature assembles atoms to produce materials with required properties—optical, mechanical, catalytic, electrical, tribological. This entails the precise construction of those materials, with the selection of appropriate atoms and their arrangement in three-dimensional space. Nature has also learned how to combine materials and structures to build molecular-level machines. Some serve as pumps, moving material across barriers, often against a concentration gradient. Others serve in locomotion, moving molecules, structures, or whole cells. Others control processes acting as regulatory systems. Still others produce or transduce energy. We can learn from Nature to develop the tools to design and build our own complex materials and machines.



Nanotube formed by joining an "even" rolled graphite sheet (above joint) which is predicted to be semiconducting, to a "spiral" rolled sheet (below joint) which is predicted to show metallic behavior. Theory predicts that this would act as "nano-diode."

Complex multicomponent structures

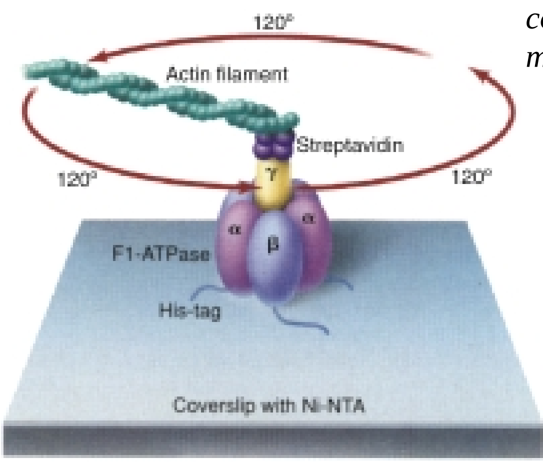
Complex structures will be multicomponent, yet nano- or meso-scale in dimension. Hybrid materials will combine organic and inorganic components or living and nonliving components.

—Reliable joining of dissimilar materials would allow synthesis of hybrid structures, with properties unachievable in less complex architectures. These could provide the critical link between many of the new materials to be developed in these programs and the silicon-based world of electronics and computing. New tools will be required to characterize these materials.

Building blocks/assemblies

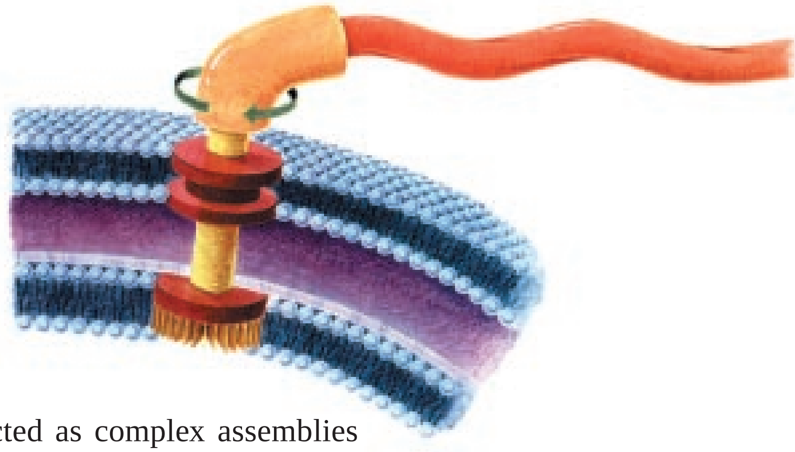
Complex, functional structures or assemblies are constructed from building blocks at both the nano- and the meso-scale. Structure development is driven by self-organization.

— Theoretical tools must be developed and used to design the minimal set of building blocks. These building blocks would incorporate into their structure not only the required functionality, but also the interfaces that will allow their assembly. Again, synthesis will require the development of new techniques, whether chemical, involving reactions and reaction conditions, or physical, involving deposition or lithographic techniques. Controlled self-assembly will require theory development and new tools to study interactions among molecules. This in turn will provide the basis for designing more sophisticated building blocks that, once assembled, have the required features and properties.



Multicomponent fabricated molecular rotor. Filament of a structural protein, actin, has been attached to the rotating γ subunit of the enzyme ATP synthase, which has been immobilized on the glass substrate. The filament rotates counterclockwise with the γ subunit in increments of 120˚, one step per molecule of ATP hydrolyzed by the enzyme.

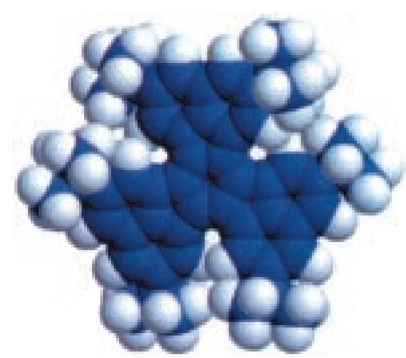
Bacteria "swim," propelled by their flagella, which are spun by a motor whose rotation is powered by the electrochemical gradient maintained across the bacterial plasma membrane.

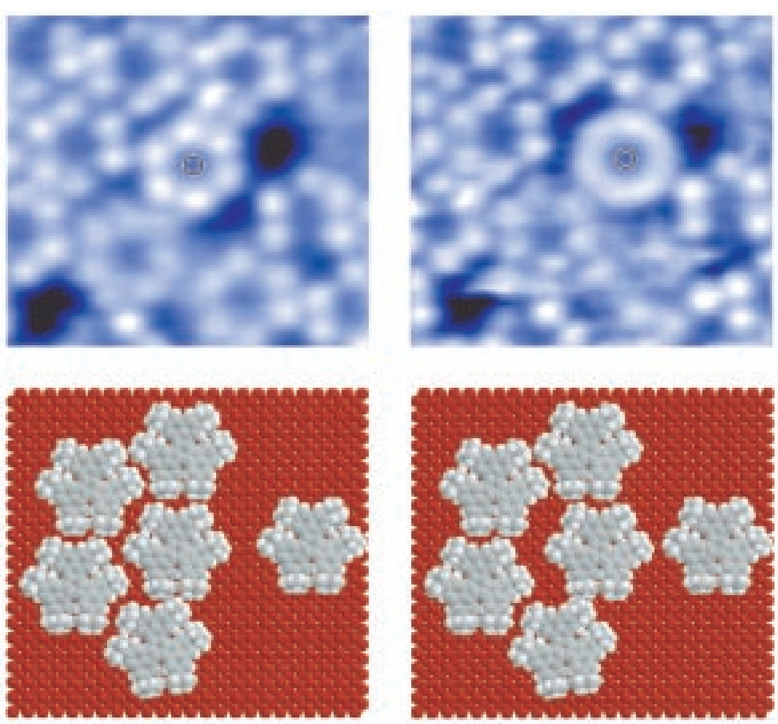


Machines

Functional "machines" are constructed as complex assemblies whose individually inactive components work together to perform a defined function. For example, the individually inactive protein subunits of ATP synthase spontaneously assemble to create a multi-subunit structure with channels, binding sites, and catalytic activity, which functions to link the exergonic passage of hydrogen ions through the channel with the endergonic catalytic synthesis of ATP at the binding sites.

> *— Design and synthesis of building blocks that can assemble to achieve system function require exquisite control of both function and surface interaction of component structures. Target functions include controlled transport across membranes, sensing of analytes, photosynthetic devices, and coatings, as well as displays that respond to external stimuli. In the longer run, chemical factories and pumps, actuators, and multifunctional electro/photonic devices would be fabricated.*





Propeller-shaped single molecule "rotor" of hexa-*tert*-butyl decacyclene (above) within a supramolecular "bearing." The molecule is locked in position (left-hand images), but once moved to a more "open" space, using a scanning tunneling microscope (STM) tip, it can freely rotate (right).

The intricate, controlled assembly of an inorganic shell over a precisely defined organic scaffold creates a structure that protects its inhabitant while allowing it to move about and continue all essential life functions.

Nature's Mastery

Living organisms represent the most sophisticated use of the elements to create materials, materials systems, and functional complexes. They operate under the same thermodynamic constraints that govern all materials; thus the study of Nature's achievements can allow us to set achievable goals for artificial systems. Enormous energy savings, pollution reduction, and productivity increases would be achieved by the development of materials and systems with the enhanced properties seen in Nature, including the ability to self-assemble, self-repair, sense, respond, and evolve. In many cases, accomplishment of these goals may appear to be beyond our reach, but no more so perhaps than optical tweezers, cloning, polymerase chain reaction, or gene therapy appeared a few years ago. We may or may not be able to reproduce all the characteristics of natural systems and tailor them to nonbiological needs. However, the study of Nature can clearly guide us and lead to achievements of great value that would not otherwise be made. Nature's achievements are therefore benchmarks for our increasing control of materials and materials systems.

Nature responds to its environment

Cellular components sense their surroundings and report to other components. Nature's structures sense damage and repair themselves. They respond to the environment, alternating among a variety of states in response to short-term changes in conditions. They evolve, altering properties to suit long-term changing environments.

—The mechanisms by which living things sense their environment and respond to it must be explored as models for artificial systems. Sensors linked to feedback systems that control functions must be developed.

Model of HSP16.5, a protein that helps other proteins maintain their proper 3-D structure. Its 24 identical protein chains form a hollow sphere with eight triangular and six square "windows." These serve, it is thought, as attachment points for the proteins to be protected.

Nature creates complexity via self-assembly

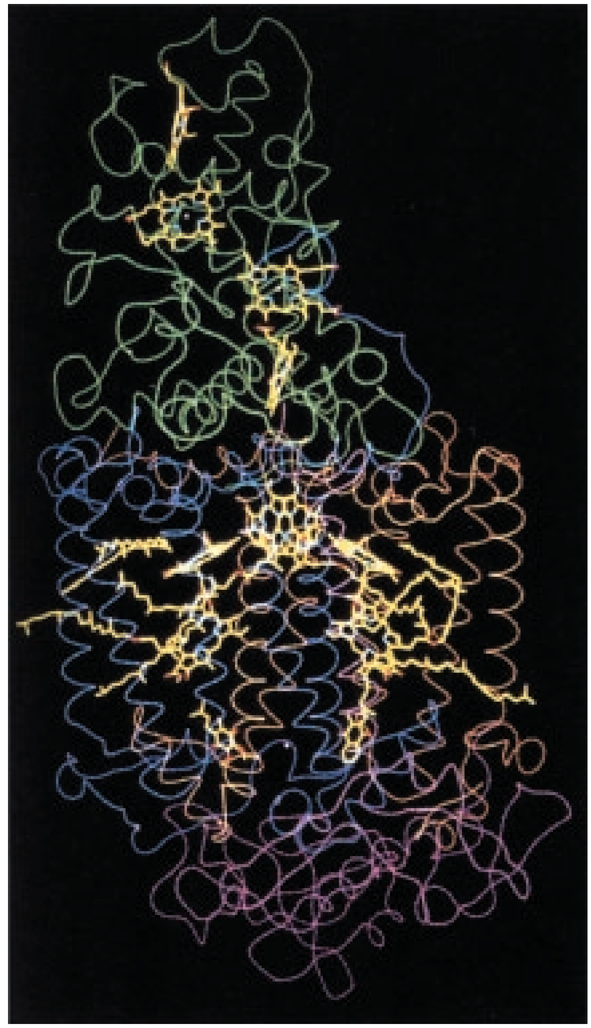
Components of systems are synthesized independently and then assemble themselves into precisely defined structures following the laws of thermodynamics.

—The surface science of molecules and structures needs to be studied so that the interactions among them can be understood, allowing controlled design of surfaces for spontaneous interaction and binding.

Nature fabricates hierarchically

Nature creates building blocks designed for linkage into polymers, which join in assemblies, and eventually into functioning organs, and then into organisms.

—Control of self-assembly is required to allow stepwise construction of increasingly complex structures. Components at each level of the hierarchy must be designed such that they join together in a structure with the required functions. At the same time, unwanted interactions between incomplete structures are blocked.



Photosynthetic reaction center is a self-assembled complex of four proteins containing 1190 amino acids, four molecules of chlorophyll, two molecules of a modified chlorophyll, one molecule of ubiquinone, one of menaquinone, and numerous iron and magnesium atoms. It harvests light to produce nutrients and energy for plants.

Nature discovers new structures

Through combinatorial synthesis and selection, billions of antibody molecules are constructed simultaneously by rearranging their building blocks. The "correct" structure is selected and then copied on the basis of how well it performs in its required function.

—Theory is required to direct the selection of components to use in a combinatorial materials discovery effort. Robotic mixing techniques and characterization tools for rapid screening of small samples are required.

Nature uses templates

Templates are used to build molecules for which there is no thermodynamic or kinetic selection. DNA directs the construction of proteins so that only the desired, functional sequences will be produced.

—Templates, whether surfaces or three-dimensional structures, must be developed to control the construction of complex materials or systems.

Nature uses thermodynamics

Entropy disfavors the ordering of components in a complex structure, but it is, for example, the entropy of the water in which they reside that drives the organization and the stability of proteins, membranes, and functional biological structures.

—A more complete understanding of the fundamental laws of structure development is required, whether it be the still incompletely understood structure of water or the folding of proteins. These would be used as guides for the design of artificial structures that can form stable structures.

Advanced Photon Source, Argonne National Laboratory. The APS provides high brightness x-rays for the elucidation of detailed atomic structure and dynamics.

New Tools

New tools drive scientific revolutions. They allow the discovery of phenomena not previously seen and the study of known phenomena on shorter time scales, at shorter distances, and with greater sensitivity. The telescope, the microscope, the laser, x-ray diffraction, and recombinant DNA are a few of the many examples.

The study of complex systems will place extraordinary demands on both theory and modeling, and also on experimental characterization. We need to radically improve the capabilities of existing instruments and develop those that allow novel observations or the manipulation of structures in new ways. Prediction of structures and phenomena can direct the experimentalist. The ability to explain the experimentalist's data in terms of theoretical models greatly accelerates the rate of discovery.

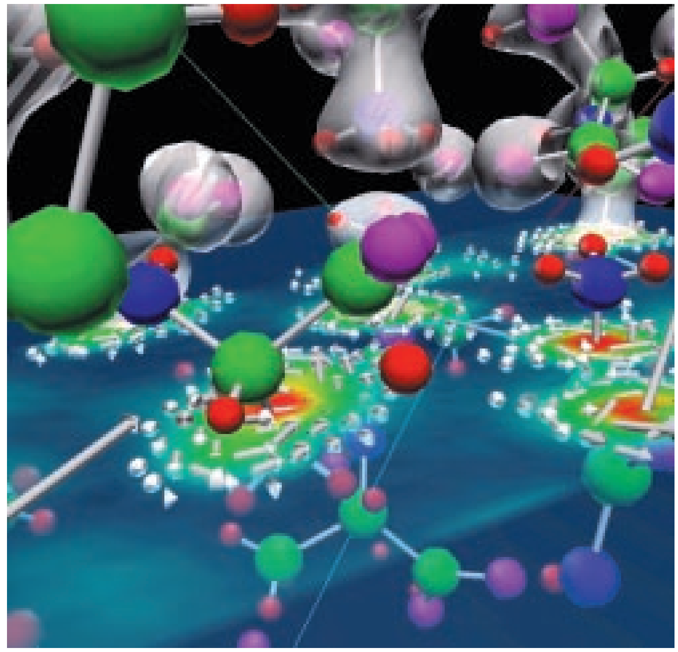
Experimental characterization

The novel and diverse phenomena associated with strongly coupled materials involve a complex interplay among magnetic, charge, and structural properties, and influence spatial scales from the macroscopic to the atomic. Required instrumentation will necessarily involve the enhancement of conventional techniques (steady-state and time-resolved optical spectroscopies, high field NMR, ESR, mass spectrometry, scanning-probe microscopies, table-top x-ray) for detailed characterization of the diverse properties of these materials with regard to shorter spatial scales, faster time scales, and properties that emerge under extreme conditions of temperature, pressure, and electric and magnetic fields. Characterization of these materials will also depend heavily on revolutionary experimental tools, including techniques for the active control of growth with parallel analysis using multiple probes and the capability to sample very small volumes.

The National Center for Electron Microscopy, Lawrence Berkeley National Laboratory. Its newest microscope can resolve atoms that are less than 0.1nm apart.

The high brightness, and spatial and energy resolution of synchrotron sources provide a means for the simultaneous measurement of the macro- and microstructure of materials. Neutron scattering, reactor or spallation-based, provides a means for the study of the structure as well the energetics of systems. Advances in x-ray and neutron detector technology should provide the means for the gathering of measurements on fast time scales. Advances in electron microscopy will shed light on dynamic structural characteristics.

Among the newly developed tools, atomic force and optical tweezer techniques promise the investigation of the nanoforces of individual atomic bonds. Spectroscopic information on single molecules is becoming feasible and should also benefit from the use of high-brightness synchrotron and free-electron laser sources. We need to develop instrumentation and techniques capable of triggering, isolating, or activating single molecules or independently addressing multiple molecules in parallel processing fashion. We must be able to transfer one or more photons or other controlled forms of energy to a single molecule, as well as to trigger a molecular activator. New tools must be developed to harvest the energy output of a molecular machine. Novel synthetic tools will include stereo- and site-specific isotopic labeling of complex structures for spectroscopic studies.



Simulation, on a Cray T3E supercomputer, of the response of a crystal of the amino acid glycine to the magnetic field applied during nuclear magnetic resonance spectroscopy (NMR) studies. The field induces a current (arrows) and a charge density (colored and gray surfaces) that depend on the environment of each atom and which affect the NMR signal from that atom. This provides information about the structure of the material.

Theory and modeling

New generations of theory and computational tools are required. At present, we have no theory for complex systems. We need a framework for understanding multilevel systems of many interacting objects with individual states.

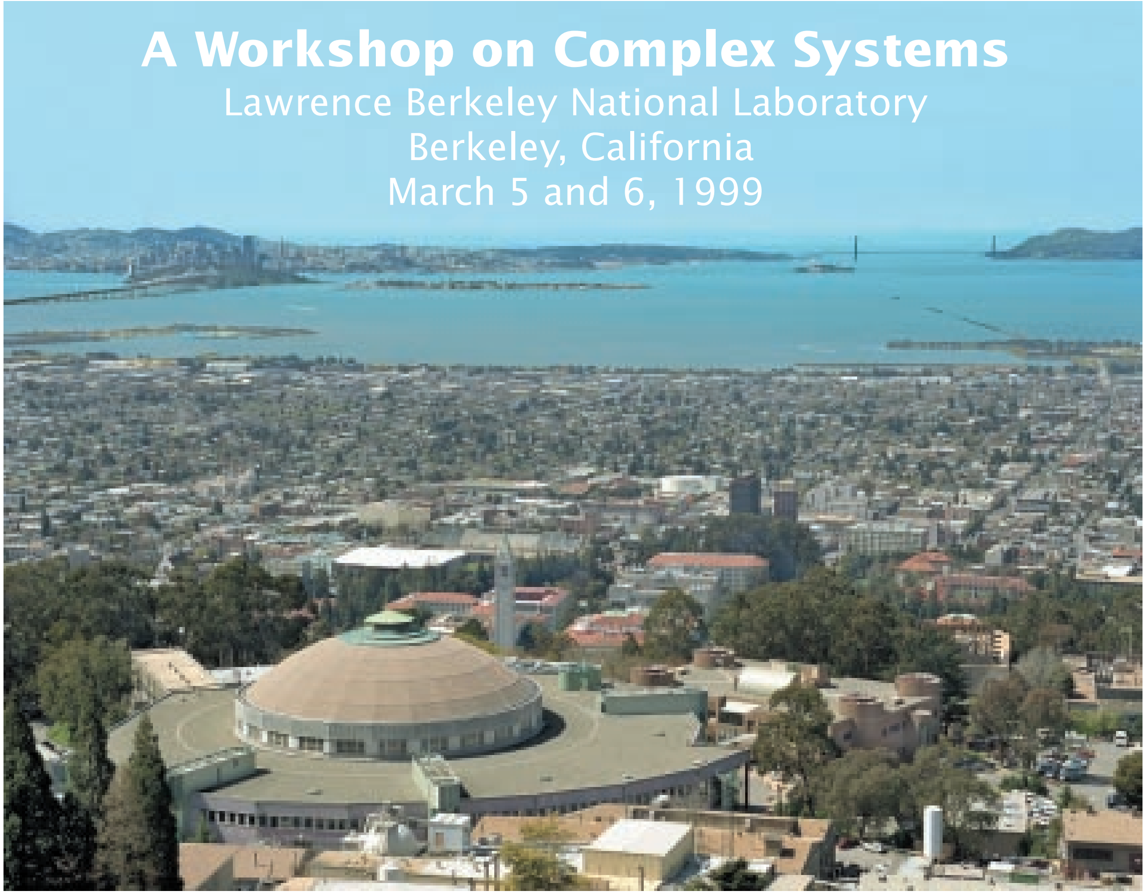
Theoretical and computational advances will be required to study self-assembling systems, to predict interactions of known surfaces, and to predict surfaces for defined interactions. To design novel materials capable of performing interesting and well-determined functions, it is critical to have a theoretical framework that defines the minimal building blocks necessary to generate particular structures. The problems encountered in predicting protein structures from amino acid sequences are examples of the challenges awaiting attempts to analyze motifs with more complex sets of building blocks and perhaps even “active” synthetic steps.

This same type of theory and modeling will be critical for the design and synthesis of functional synthetic structures. A combination of simple models and detailed atomistic simulators could jointly be used to determine the dominant energetic and entropic components that control these processes.

Larger and faster computers would expand the time and length scales that can be achieved by first-principles simulations. Future computers may also integrate hardware and software to allow coupling of very different computational tasks within a single framework (for example, allow reconfiguration of the computational architecture as a function of the dynamics in a simulation). This may open new avenues for simulation of multilevel dynamics. Ultimately, some of the complex materials to be synthesized may be used as the very hardware of future generations of computers.

A Workshop on Complex Systems

Lawrence Berkeley National Laboratory
Berkeley, California
March 5 and 6, 1999



Workshop Chair

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David Awschalom, University of California, Santa Barbara
Moungi Bawendi, Massachusetts Institute of Technology
Jean Fréchet, Lawrence Berkeley National Laboratory
Donald Murphy, Lucent Technologies
Sam Stupp, Northwestern University
Peter Wolynes, University of Illinois

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p. 2. *Top:* Superconductor. ISIS. Andrew Taylor, Rutherford Appleton Laboratory, UK. *Center:* Supramolecular assembly. *Science*, vol. 276, 4/18/97, cover image; © 1997, AAAS. *Bottom:* Nanotube. Steven Louie and Marvin Cohen, Lawrence Berkeley National Laboratory (LBNL); Vincent H. Crespi, Pennsylvania State University.

p. 3. *Top:* Fossilized ammonite shells. Martin Dohrn/Science Photo Library/Photo Researchers, New York, NY. *Center:* Advanced Photon Source, Argonne National Laboratory. *Bottom:* Simulation of glycine crystal response to magnetic field in NMR spectroscopy. National Energy Research Scientific Computing Center (NERSC).

p. 4. *Top:* CdSe nanocrystals. *Bottom:* Electron micrograph of nanocrystal. Both images, Paul Alivisatos, LBNL.

p. 5. Collagen. Margaret C. Holm, LBNL.

p. 6. Superconductor (see page 2 reference).

p. 7. *Top:* Bose-Einstein condensate. *Science*, vol. 270, 12/22/95, cover image; © 1995, AAAS. *Bottom:* Particle motion simulation. Daniel Joseph, Univ. of Minnesota, and NERSC.

p. 8. *Top:* Supramolecular assembly (see page 2 reference). *Bottom: Science*, vol. 270, 12/1/95, cover image; © 1995, AAAS.

p. 9. Library of Superconductors. *Science*, vol. 260, 6/23/95, cover image; © 1995, AAAS.

p. 10. *Top:* Nanotube (see page 2 reference). *Bottom.* Molecular Rotor. *Science*, vol. 282, 12/4/98, page 1844; © 1998, AAAS.

p. 11. *Top:* Flagella motor, p. 1139, Fig. 34-74, Biochemistry, Donald Voet and Judith Voet; © 1990 by John Wiley & Sons, Inc., reprinted by permission of John Wiley & Sons, Inc., New York, NY. *Bottom:* Molecular rotor. *Science*, vol. 281, 7/24/98, pages 531-532; © 1998, AAAS.

p. 12. *Top:* Fossilized ammonite shells (see page 3 reference). *Bottom:* Model of HSP 16.5, Sung-Hou Kim, LBNL.

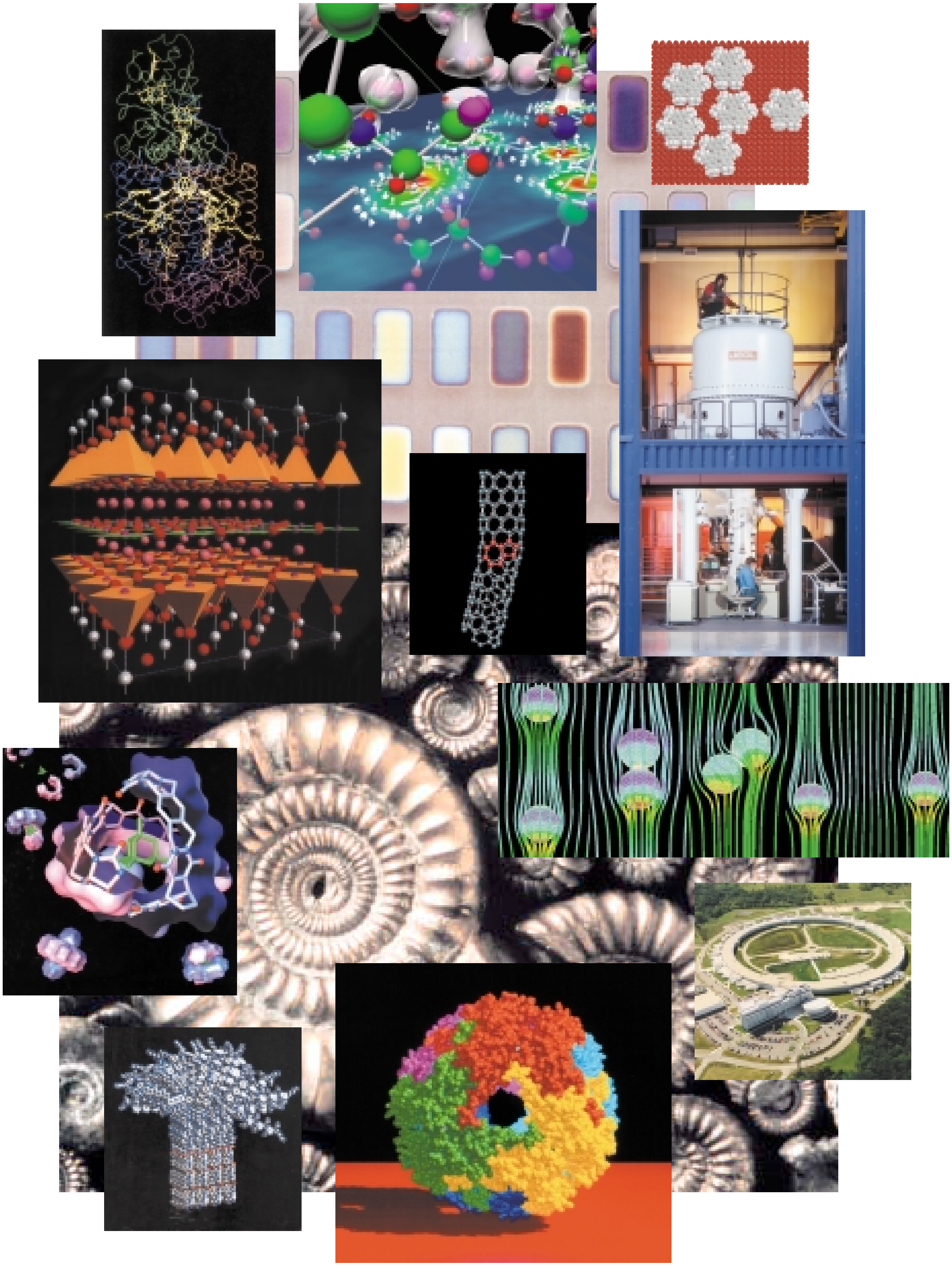
p. 13. Photosynthetic reaction center. Johann Deisenhofer and Hartmut Michel, Les Prix Nobel, 1989; © 1989 The Nobel Foundation, reprinted by permission of The Nobel Foundation, Stockholm, Sweden.

p. 14. *Top:* Advanced Photon Source, Argonne National Laboratory. *Bottom*. National Center for Electron Microscopy, LBNL.

p. 15. Simulation of glycine crystal response to magnetic field in NMR spectroscopy (see page 3 reference).

Front cover. Superconductor (see page 2 reference). **Inside front cover.** View down center of boron nitride nanotube. Steven Louie and Marvin Cohen, LBNL; Vincent H. Crespi, Pennsylvania State University.

Ernest Orlando Lawrence Berkeley National Laboratory is operated for the U.S. Department of Energy under Contract No. DE-AC03-76SF00098. PUB-826.



(Above) With new tools, new understanding, and a developing convergence of the disciplines of physics, chemistry, materials science, and biology, we will build on our 20th century successes and begin to ask and solve questions that were, until the 21st century, the stuff of science fiction.

(Back Cover) Dynamics of Discovery: Through computational technologies, scientists from a range of disciplines tame many pathways to discovery. Here, the streamline of fluid dynamics swirl into the smooth mathematical surface of the Mobius strip, while around them float molecular structures from chemistry and the double helices of biology. Robert H. Russ, an SDSC animator and artist now at Pixar, used SGI workstations and Alias/Wavefront PowerAnimator Software to create this 3-D image. Image provided courtesy of the San Diego Supercomputer Center.