Investment Mode 1: Fundamental Nanoscale Science and Engineering Research—Knowledge Generation

Interdisciplinary fundamental research offers a productive fusion of traditional ideas that frequently leads to unanticipated results and significant breakthroughs. By exploiting the opportunities afforded by the nanoscale instrumentation for analysis and manipulation of matter, interdisciplinary fundamental research will foster the development of unifying principles, phenomena, and tools.

Specific areas of focus that draw on multiple disciplines include:

- Novel phenomena, material structures, processes, and properties
- Nano-biosystems
- Nanoscale devices and system architecture
- Theory, modeling, and simulation

Agency Participation

(lead in bold)

DOD	National security
DOE	Energy, national security, and the environment
IA	National security
NASA	Aeronautics and space exploration
NIH	Biological phenomena
NIST	Basic nanoscale measurement science
NSF	Traditional discipline-based research as well as multidisciplinary research in biological sciences; computer and information science and engineering; education and human resources; engineering; mathematical and physical sciences; and, social, behavioral, and economic sciences
USDA	Biological and agricultural production systems

Novel Phenomena, Material Structures, Processes, and Properties

Opportunity

The discovery of the novel phenomena and material structures that appear at the nanoscale will affect the entire range of applications that the grand challenges identify, and more.

Priorities

Research in this area supports the discovery of the fundamental physics, chemistry, materials science, and mechanics of nanostructures; the development of new experimental tools to characterize and measure nanostructures and phenomena;

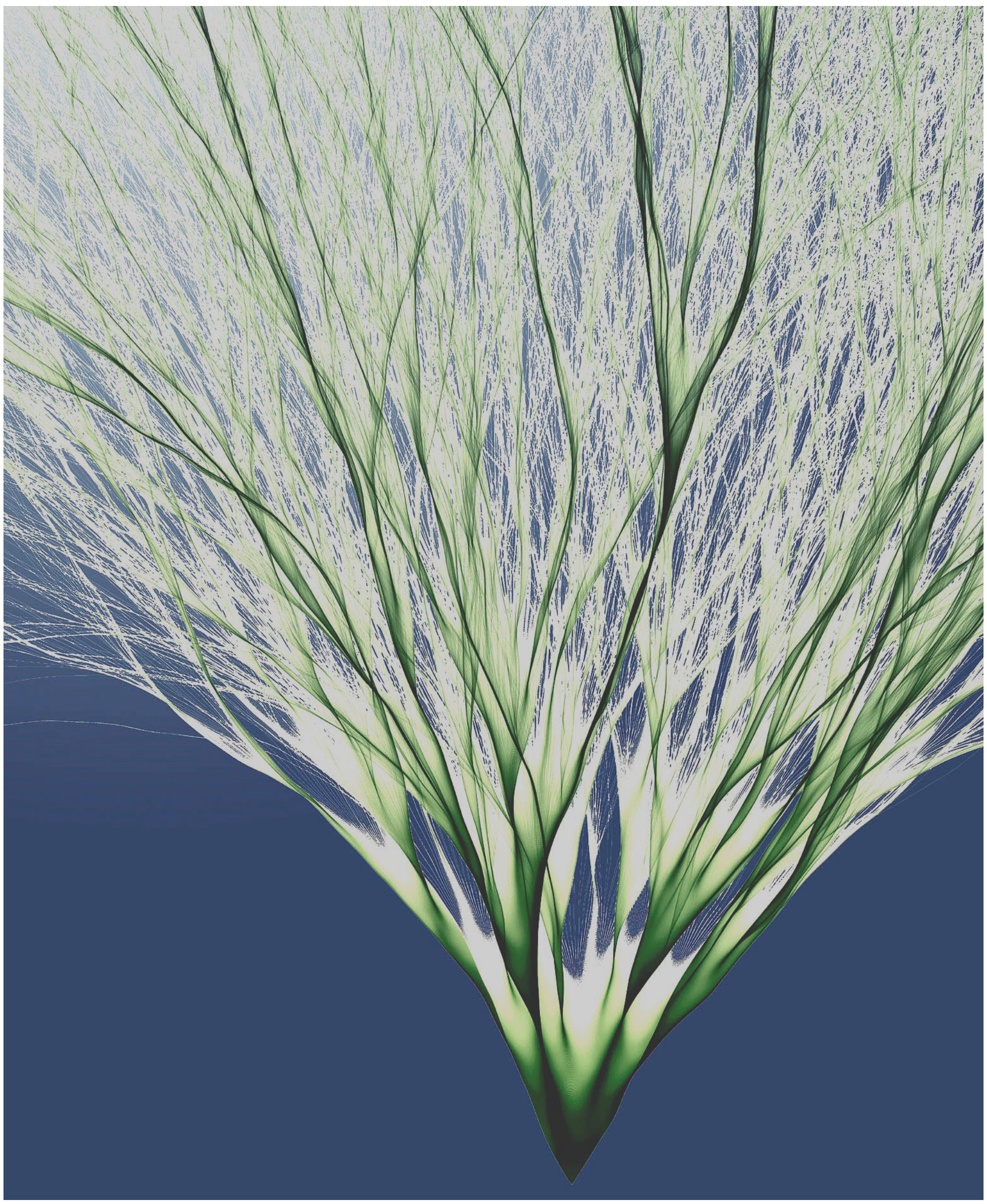

Figure 3a. Theoretical simulations of electron flow in nanostructures: Two-dimensional flow of electrons injected at the bottom of the image. (courtesy E.J. Heller, Harvard University).

novel synthesis or fabrication techniques; and the development of new mathematical and simulation tools to aid our understanding of nanoscale phenomena.

Research Example: Imaging Coherent Electron Flow in Nanostructures (supported by NSF)

As electronic devices get smaller, electron-transport properties will play an increasingly important role in device operation and performance. At the nanometer scale, real surfaces have imperfections that affect electron flow patterns. A Harvard group is conducting systematic investigations on the flow of electrons in nanostructures (Figures 3a and 3b). This research will provide a foundation for the design of electronic circuits in future nanodevices.

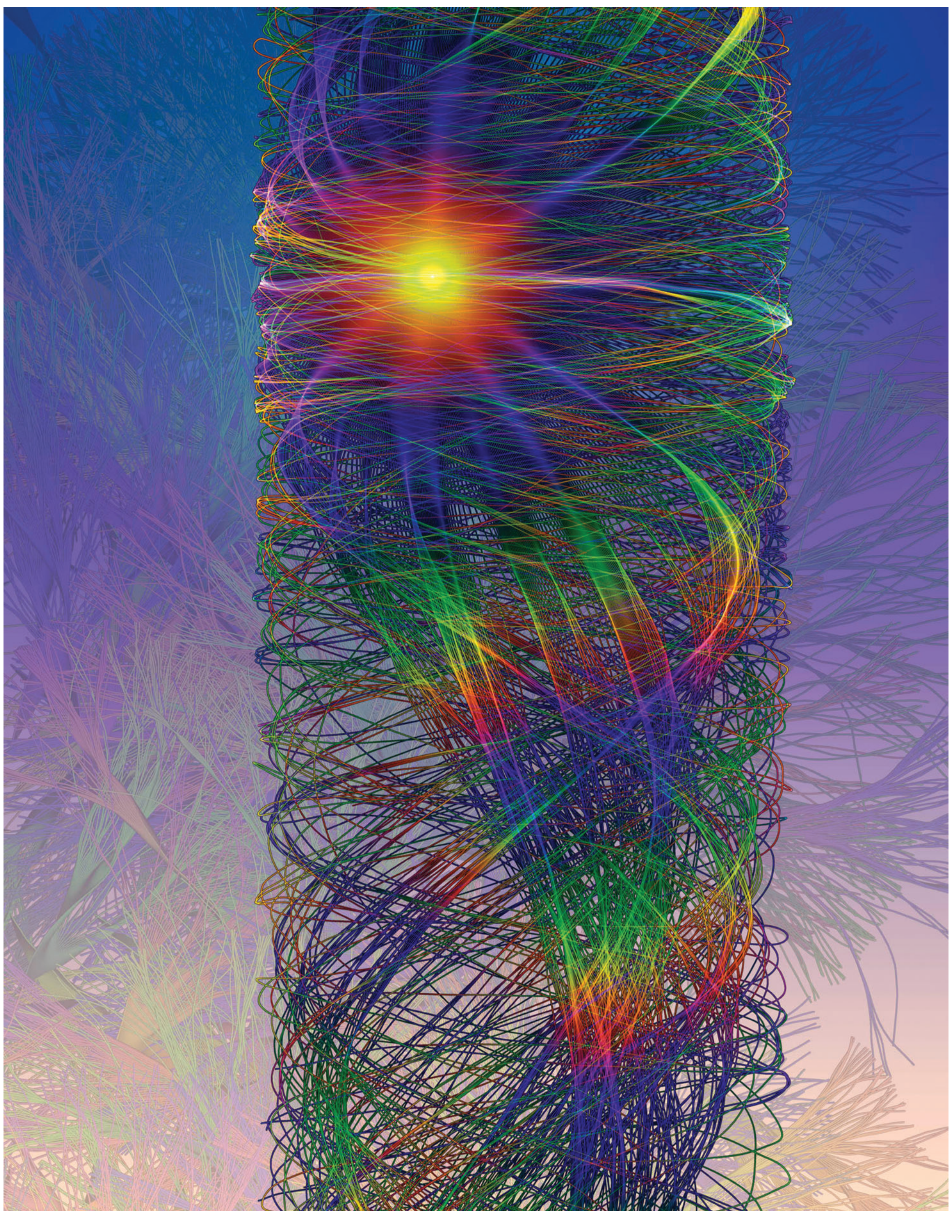

Figure 3b. Theoretical simulations of electron flow in nanostructures: Flow of electrons injected at the "bright spot" into a 500 nm diameter "nanowire." Electrons are scattered due to interactions at the wire surface. Variation in the quantum phase of the scattered electron waves is indicated by changes in color. The dynamics of such electron scattering affects the electronic properties of the wire, its resistance, the speed of response to external stimuli, and coherence of information flow along its length (courtesy E.J. Heller, Harvard University).

Nano-Biosystems

Opportunity

A cell is a micrometer-sized factory with molecular machinery operating on the nanometer scale. Thus, a fundamental understanding of nano-biostructures and processes will open broad opportunities in nano-biotechnology, nano-medicine, and biomaterials.

Priorities

Priority areas include developing an understanding of the relationships among composition, structure, single molecule behavior, and biological function. Additional research areas include the study of organelles and subcellular complexes such as ribosomes and molecular motors; construction of nanometer-scale probes and devices for research in genomics, proteomics, cell biology, and nanostructured tissues; and synthesis of nanoscale materials based on the principles of biological self-assembly.

Research Example: Nature's Tools to Assemble Materials with Atomic Precision (supported by NSF)

Among the basic assembly processes nature uses are nanoscale self-assembly, molecular recognition, self-correction, and nano-structural regularity. Researchers at the University of Texas at Austin have developed new assembly techniques, based on biomolecular recognition. Using this technique, amino acids, such as those in simple peptides or on the surfaces of viruses, are designed to recognize and bind to specific nonbiological electronic and magnetic materials. Complex structures can be assembled by tailoring the biomolecules appropriately, as shown in Figure 4. One advantage is that such processes take place at near-ambient conditions. In the future, biologically inspired assembly may provide cost-effective alternative manufacturing processes.

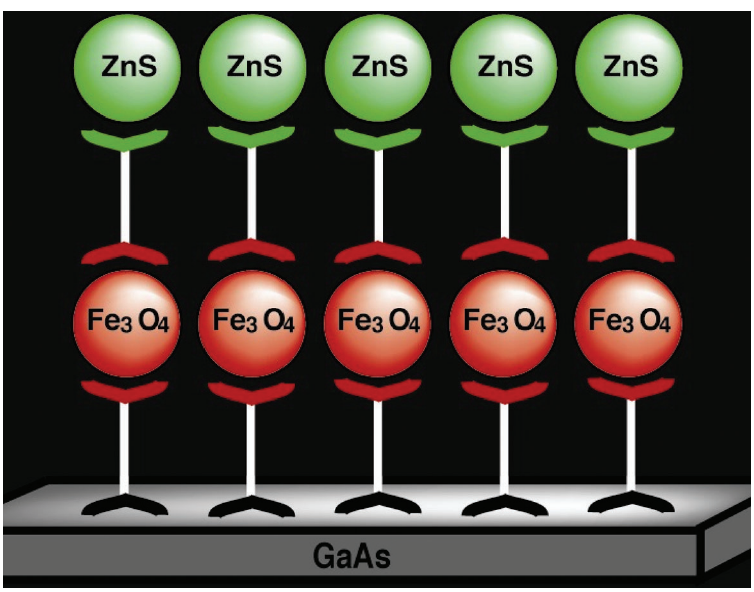

Figure 4. Illustration of how biomolecular recognition processes may be used to assemble a magneto-electronic structure composed of zinc sulfide (ZnS) and iron oxide (Fe_3O_4) nanoparticles. Two tailored bifunctional peptides, one that binds the gallium arsenide substrate to iron oxide, and the other that binds the iron oxide particle to zinc sulfide, control the formation of the layered structure. Such directed self-assembly processes have the potential to replace far more complex processes used in conventional micro- and nano-electronic manufacturing (courtesy A.E. Belcher, now at Massachusetts Institute of Technology).

Nanoscale Devices and System Architecture

Opportunity

New concepts and design methods are needed to create new nanoscale devices, assemble them into functional systems, and create architectures compatible with various operational environments.

Priorities

Research in this area includes the development of (a) new tools and techniques for sensing, manipulating, and assembling; (b) architectures that integrate across multiple length scales; (c) software for automated design of specialized nanosystems; and (d) design automation tools for assembling large numbers of heterogeneous nanocomponents into a system.

Research Example of a Nanoscale Device: Molecular Transistor (supported by NSF)

Researchers at Cornell University have demonstrated a transistor-like device with the principal functional element being just one molecule (Figure 5). The device is fabricated from two gold electrodes separated by a very narrow gap that is bridged by a single molecule containing a cobalt atom. The flow of electrons from one electrode to the other, which occurs by an electron hopping on and off the cobalt atom, is controlled by the voltage on a third electrode near the bridging molecule. The electrical characteristics of the transistor can be varied by making chemical changes to this molecule, such as lengthening the molecule's connecting "arms." This research demonstrates that electron devices ~10,000 times smaller than present devices are possible.

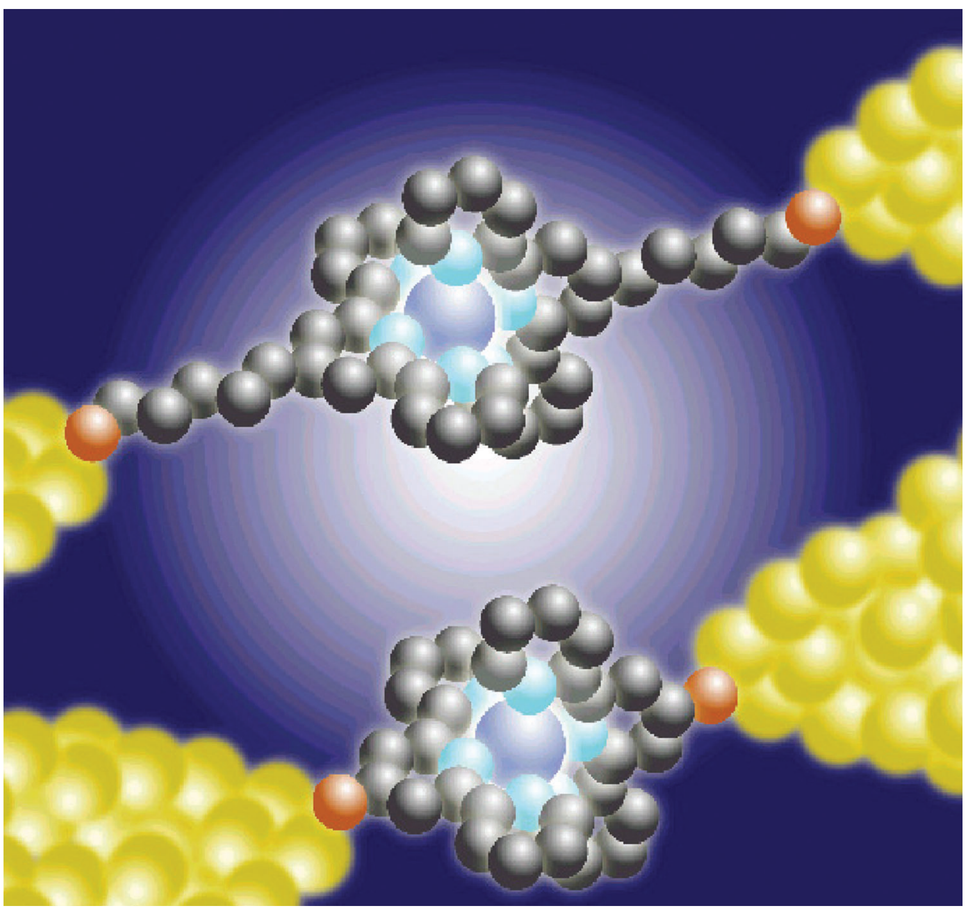

Figure 5. Artist's rendition of a molecular transistor ~10,000 times smaller than present devices. The flow of electrons (current flow) through the molecule bridging between the two gold electrodes is controlled by the voltage on a third electrode, not shown. The electric field from the third electrode determines the rate electrons can hop on and off a cobalt atom (dark blue) in the bridging molecule. The well-defined and deliberately designed molecular configuration is attached to the gold electrodes by sulfur atoms (red) (courtesy P. McEuen, Cornell University).

Theory, Modeling, and Simulation

Opportunity

The emergence of new behaviors and processes in nanomaterials, nanostructures, nanodevices, and nanosystems creates an urgent need for theory, modeling, large-scale computer simulation, and new design tools in order to understand, control, and accelerate development.

Priorities

Research on mathematical methods to model and simulate physical, chemical, and biological systems at the nanoscale will include techniques such as quantum mechanics and quantum chemistry, multi-particle simulation, molecular simulation, continuum-based models, stochastic methods, and nanomechanics. Approaches that integrate more than one such technique will play an important role in this effort.

Modeling and simulation of the time variation of processes in nanostructures is also an urgent need. Current research is limited to modeling only a relatively small number of time increments of process variation and dynamics of complex structures, such as shown in Figure 6. Improved computational methods and tools will enable more realistic time scales of process variation to be modeled.

Research Example: Modeling and Simulation of Biological Ion Channels to Cure Illnesses (supported by NSF and DOD)

Researchers from the Network for Computational Nanotechnology at the University of Illinois at Urbana-Champaign and Stanford University, in collaboration with Rush Medical Center, have simulated transport through nanoscale biological ion channels (Figure 6). Ion channels regulate the transport of ions in and out of cells, which is essential to proper cell function. In turn, understanding cellular processes is critical to understanding and treating diseases at the cellular level.

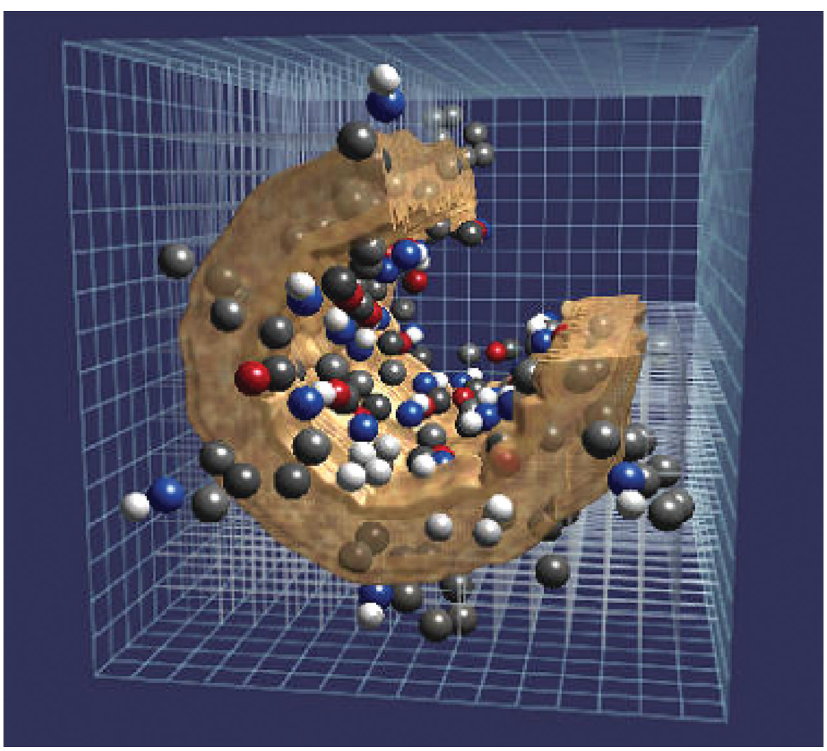

Figure 6. Computer simulation of biological ion-channel pore formed by the antibiotic gramicidin. Formation of ion channels through bacteria cell membranes is one mechanism by which antibiotics kill bacteria. The simulated pore is approximately 3 nanometers long and 0.5 nanometers in diameter. The different colored spheres represent specific atoms in the proteins constituting the wall of the ion channel (courtesy K. Hess and U. Ravaioli, University of Illinois).