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SUPPLEMENTARY INFORMATION: In May of 2002, a workshop on Theory and Modeling in Nanoscience was held in San Francisco, sponsored by the Basic Energy Sciences and Advanced Scientific Computing Research Advisory Committees to the Office of Science of the U.S. Department of Energy. The charge to the workshop was to identify challenges and opportunities for theory, modeling and simulation in nanoscience and nanotechnology, and to investigate the growing and promising role of applied mathematics and computer science in meeting those challenges. The final report of the workshop can be found at http://www.sc.doe.gov/bes/Theory_and_Modeling_in_Nanoscience.pdf.

Background: The Revolution in Theory, Modeling and Simulation

The past two decades have seen the fundamental techniques of theory, modeling and simulation undergo a revolution that parallels the experimental advances on which the new field of nanoscience is based. This period has seen the development of density functional algorithms, quantum Monte Carlo techniques, *ab initio* molecular dynamics, advances in classical Monte Carlo methods and

mesoscale methods for soft matter and fast-multipole and multigrid algorithms. The application of these and other new theoretical capabilities are providing quantitative understanding of the novel behavior of nanoscale systems. The same two decades have also seen dramatic advances in computing hardware, which have increased raw computing power by four orders of magnitude. The combination of new theoretical and computational methods with increased computing power has made it now possible to simulate systems with millions of degrees of freedom.

The application of new experimental tools to nanosystems has created a concurrent need for a quantitative, predictive understanding of matter at the nanoscale. The absence of quantitative models that describe newly observed phenomena increasingly limits progress in the field. Without reliable, robust predictive tools and models for the quantitative description of structure and dynamics at the nanoscale, the research community will miss important scientific opportunities in nanoscience. The lack of such tools inhibits widespread applications in fields of nanotechnology ranging from molecular electronics to biomolecular materials. New investments in both human and computational resources are required to maintain the creative pace of nanoscience and nanotechnology.

The Opportunity and the Challenge

The nanoscale is not just another step towards miniaturization. It is a qualitatively new scale where materials properties depend on size and shape, as well as composition, and differ significantly from the same properties in the bulk or in isolated molecules. It is at this scale where one crosses over from the smallest scales, where a quantum mechanical description is required, to the larger scales, where a classical description is often adequate. All approximations and assumptions used previously are suspect for systems at this scale and must be reexamined. Fundamental methods for theory, modeling and simulation developed for larger of smaller scales will need to be modified, extended, and sometimes combined into a more complete description.

Completely new methods may be required. Synergism created within a team of researchers from nanoscience, computational science and applied mathematics can accelerate progress and broaden insight. Thus, the current solicitation for applications allows for and encourages the building of teams of theorists, computational scientists,

applied mathematicians, and experts in high-performance computing. There are many theory, modeling and simulation challenges in the broad topical areas of: (1) Nano building blocks (nanotubes, quantum dots, clusters and nanoparticles); (2) complex structures and interfaces involving such building blocks; and (3) the assembly and growth of nanostructures, including (but not limited to):

- Determining the essential science of transport mechanisms at the nanoscale.

- Devising theoretical and simulation approaches to study nanointerfaces, which dominate many nanoscale systems and are highly complex and heterogeneous.

- Simulating, with reasonable accuracy, the optical properties of nanoscale structures and modeling nanoscale opto-electronic devices.

- Simulating complex nanostructures involving "soft" biological or organic structures, and "hard" inorganic ones, as well as nanointerfaces between hard and soft matter.

- Simulating self-assembly and directed self-assembly.

- Bringing from length- and time-scales appropriate for electronic motion to those needed for larger scale phenomena—all the way up to macroscopic properties.

- Devising theoretical and simulation approaches to quantum coherence, decoherence, and spintronics.

- Devising self-validating and benchmarking methods.

Each of these challenges represents an opportunity for theory, modeling and simulation to provide new insights into the dynamic behavior of nanoscale systems.

Investment Plan of the Office of Science

A new investment in theory, modeling and simulation in nanoscience will have a major impact on the national nanoscience initiative, by stimulating the formation of alliances and teams of experimentalists, theorists, applied mathematicians and computer and computational scientists to meet the challenge of developing a broad quantitative understanding of structure and dynamics at the nanoscale. The Department of Energy is uniquely situated to build such a program in theory, modeling and simulation in nanoscience. First, DOE currently supports much of the nation's experimental work in nanoscience, and new facilities dedicated to nanoscience research are currently being built at the DOE national laboratories. Second, the Department maintains an internationally renowned program in applied mathematical sciences research,