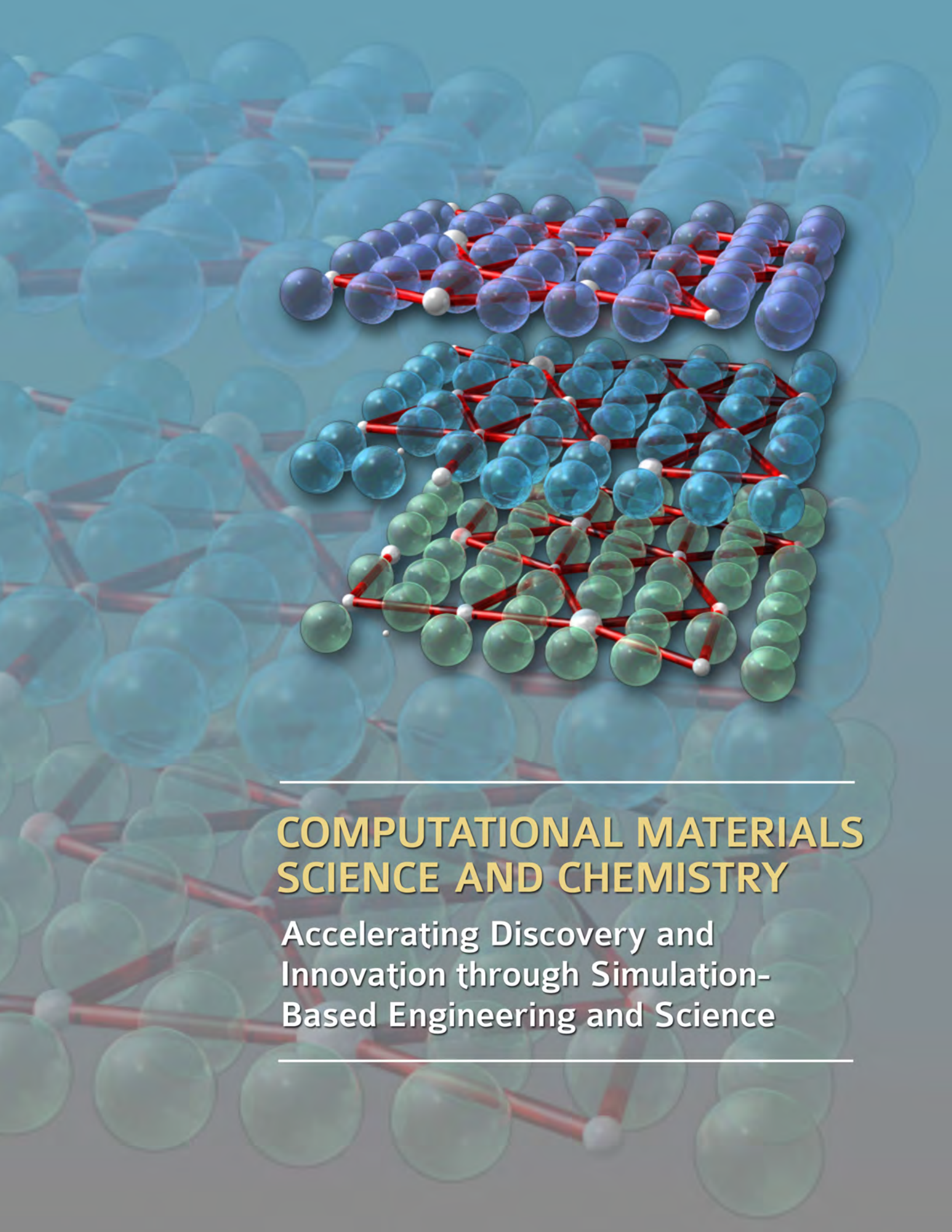


COMPUTATIONAL MATERIALS SCIENCE AND CHEMISTRY

Accelerating Discovery and Innovation through Simulation-Based Engineering and Science

Report of the Department of Energy Workshop on

Computational Materials Science and Chemistry for Innovation

July 26–27, 2010

Cochairs

George Crabtree, Argonne National Laboratory
Sharon Glotzer, University of Michigan
Bill McCurdy, University of California–Davis
Jim Roberto, Oak Ridge National Laboratory

Panel leads

Materials for extreme conditions
John Sarrao, Los Alamos National Laboratory
Richard LeSar, Iowa State University

Chemical reactions
Andy McIlroy, Sandia National Laboratories
Alex Bell, University of California–Berkeley

Thin films, surfaces, and interfaces
John Kieffer, University of Michigan
Ray Bair, Argonne National Laboratory

Self-assembly and soft matter
Clare McCabe, Vanderbilt University
Igor Aronson, Argonne National Laboratory

Strongly correlated electron systems and complex materials: superconducting, ferroelectric, and magnetic materials
Malcolm Stocks, Oak Ridge National Laboratory
Warren Pickett, University of California–Davis

Electron dynamics, excited states, and light-harvesting materials and processes
Gus Scuseria, Rice University
Mark Hybertsen, Brookhaven National Laboratory

Separations and fluidic processes
Peter Cummings, Vanderbilt University
Bruce Garrett, Pacific Northwest National Laboratory

U.S. DEPARTMENT OF ENERGY | Office of Science

Computational Materials Science and Chemistry: Accelerating Discovery and Innovation through Simulation-Based Engineering and Science

Executive Summary

The urgent demand for new energy technologies has greatly exceeded the capabilities of today's materials and chemical processes. To convert sunlight to fuel, efficiently store energy, or enable a new generation of energy production and utilization technologies requires the development of new materials and processes of unprecedented functionality and performance. New materials and processes are critical pacing elements for progress in advanced energy systems and virtually all industrial technologies.

Over the past two decades, the United States has developed and deployed the world's most powerful collection of tools for the synthesis, processing, characterization, and simulation and modeling of materials and chemical systems at the nanoscale, dimensions of a few atoms to a few hundred atoms across. These tools, which include world-leading x-ray and neutron sources, nanoscale science facilities, and high-performance computers, provide an unprecedented view of the atomic-scale structure and dynamics of materials and the molecular-scale basis of chemical processes. For the first time in history, we are able to synthesize, characterize, and model materials and chemical behavior at the length scale where this behavior is controlled. This ability is transformational for the discovery process and, as a result, confers a significant competitive advantage.

Perhaps the most spectacular increase in capability has been demonstrated in high-performance computing. Over the past decade, computational power has increased by a factor of a million due to advances in hardware and software. This rate of improvement, which shows no sign of abating, has enabled the development of computer simulations and models of unprecedented fidelity.

We are at the threshold of a new era where the integrated synthesis, characterization, and modeling of complex materials and chemical processes will transform our ability to understand and design new materials and chemistries with predictive power. In turn, this predictive capability will transform technological innovation by accelerating the development and deployment of new materials and processes in products and manufacturing.

Harnessing the potential of computational science and engineering for the discovery and development of materials and chemical processes is essential to maintaining leadership in these foundational fields that underpin energy technologies and industrial competitiveness. Capitalizing on the opportunities presented by simulation-based engineering and science in materials and chemistry will require an integration of experimental capabilities with theoretical and computational modeling; the development of a robust and sustainable infrastructure to support the development and deployment of advanced computational models; and the assembly of a community of scientists and engineers to implement this integration and infrastructure. This community must extend to industry, where incorporating predictive materials science and chemistry into design tools can accelerate the product development cycle and drive economic competitiveness.

The confluence of new theories, new materials synthesis capabilities, and new computer platforms has created an unprecedented opportunity to implement a "materials-by-design" paradigm with wide-ranging benefits in technological innovation and scientific discovery. The Workshop on Computational Materials Science and Chemistry for Innovation was convened in Bethesda, Maryland, on July 26–27, 2010, to assess the potential of state-of-the-art computer simulations to accelerate understanding and discovery in materials science and chemistry, with a focus on potential impacts in energy technologies and innovation. Sponsored by the Department of Energy (DOE) Offices of Advanced Scientific Computing Research and Basic Energy Sciences, the workshop brought together 160 experts in materials science, chemistry, and computational science representing more than 65 universities, laboratories, and industries, and four agencies.

The workshop examined seven foundational challenge areas in materials science and chemistry: materials for extreme conditions, self-assembly, light harvesting, chemical reactions, designer fluids, thin films and interfaces, and electronic structure. Each of these challenge areas is critical to the development of advanced energy systems, and each can be accelerated by the integrated application of predictive capability with theory and experiment.

The workshop concluded that emerging capabilities in predictive modeling and simulation have the potential to revolutionize the development of new materials and chemical processes. Coupled with world-leading materials characterization and nanoscale science facilities, this predictive capability provides the foundation for an innovation ecosystem that can accelerate the discovery, development, and deployment of new technologies, including advanced energy systems. Delivering on the promise of this innovation ecosystem requires the following:

- **Integration of synthesis, processing, characterization, theory, and simulation and modeling.** Many of the newly established Energy Frontier Research Centers and Energy Hubs are exploiting this integration.
- **Achieving/strengthening predictive capability in foundational challenge areas.** Predictive capability in the seven foundational challenge areas described in this report is critical to the development of advanced energy technologies.
- **Developing validated computational approaches that span vast differences in time and length scales.** This fundamental computational challenge crosscuts all of the foundational challenge areas. Similarly challenging is coupling of analytical data from multiple instruments and techniques that are required to link these length and time scales.
- **Experimental validation and quantification of uncertainty in simulation and modeling.** Uncertainty quantification becomes increasingly challenging as simulations become more complex.
- **Robust and sustainable computational infrastructure, including software and applications.** For modeling and simulation, software equals infrastructure. To validate the computational tools, software is critical infrastructure that effectively translates huge arrays of experimental data into useful scientific understanding. An integrated approach for managing this infrastructure is essential.
- **Efficient transfer and incorporation of simulation-based engineering and science in industry.** Strategies for bridging the gap between research and industrial applications and for widespread industry adoption of integrated computational materials engineering are needed.

Contents

Materials science and chemistry: Pathway to innovation

One can describe the history of civilization as a series of breakthroughs in materials science and chemistry. Beginning with the Stone Age, we have progressed through Bronze, Iron, Nuclear, and Silicon ages. Materials lend their names to ages because materials define technological capabilities. Advances in materials and chemistry have shaped history and the balance of economic and military power: iron and steel, gunpowder, ammonia synthesis, antibiotics, uranium and plutonium, silicon-based electronics. Materials and chemistry have enabled modern civilization, providing a pathway to innovation in industry, energy, agriculture, national security, health, and information technology.

Energy technologies

It has been more than 100 years since the first solar cell, the first electric car, and the first rechargeable battery. Fossil power plants operate at two-thirds of their optimal efficiency and release large quantities of greenhouse gases, and a half century after the first nuclear power plant we have yet to reach consensus on fuel cycles or the disposal of spent fuel. None of these technologies are close to meeting their full potential, and the availability of advanced materials and chemical processes is the principal technological barrier.

Advances in materials science and chemistry enable technological revolutions

Virtually all energy technologies are limited by the performance of materials. For fossil and nuclear electric power, we need materials that can operate at greatly increased temperatures in extreme environments of corrosion and radiation. Such materials could increase the efficiency of existing technologies by as much as a third. We need materials and chemical processes that can efficiently separate greenhouse gases from effluent streams in conventional fossil plants, and that can separate and safely store radioactive materials from nuclear plants. We need materials that drive down the cost of solar cells while increasing their efficiency. We need materials and chemical processes for batteries that enable utilization of electric vehicles and intermittent solar and wind energy by storing electrical energy at densities that rival liquid fuels. We need lightweight materials for transportation and catalysts for the direct conversion of sunlight to fuels. There are no known fundamental barriers to these innovations, but they represent significant challenges to our science and technology.

Industrial competitiveness

Materials science and chemistry also underpin industrial competitiveness. Pick a technology and you will find that progress depends on advances in materials and chemistry: electric motors on compact, high-field magnets; batteries on electrolyte materials and chemistries; solar cells on thin-film materials technology; computer chips on nano-materials fabrication; polymers and plastics on chemical catalysts; steel on alloy science.

Predictive capability will drive innovation and competitiveness

The company or nation with the best environment for discovering and deploying new materials and chemical processes that transform products and technologies will be more competitive than less innovative and agile companies or nations. These transformational advances will create new industries and force the evolution of others. They are rational scientific and technical goals that are well within sight. They will be achieved: The question is how quickly and by whom.

Simulation-based engineering and science offers a significant opportunity to increase industrial competitiveness by reducing design times, accelerating the development and incorporation of new materials and processes, and minimizing testing requirements. The development and application of a predictive capability to facilitate the development of industrial products, processes, and technologies are transformational. This can be seen in the early application of Integrated Computational Materials Engineering (ICME) in several industry sectors including aircraft, automobiles, and manufacturing. ICME, based on integrated simulation of complex materials and manufacturing systems, has reduced prototyping times and accelerated deployment. Reductions in testing requirements by factors of up to seven, acceleration of deployment times by factors of two to three, and cost savings of tens to hundreds of millions have been reported. Predictive capability for the performance of materials and chemical systems is essential to this process.

Predictive capability also drives technological innovation. Advanced technologies typically require increasingly complex materials systems and processes. This complexity is a challenge for traditional development strategies due to the extensive parameter space that must be explored. Predictive capability based on simulation-based engineering and science offers the opportunity to significantly expand this parameter space while lowering both costs and development times. This will accelerate the replacement of rare or nondomestic source materials (such as rare earths for magnets or lithium for batteries) with abundant materials, the discovery of new materials with tailored properties, the deployment of "green" technologies and processes with lower environmental impact and improved performance, and the development of advanced manufacturing technologies with improved efficiency and flexibility. By accelerating the development and deployment of complex materials systems and processes, predictive capability will drive innovation and economic competitiveness.

Accelerating discovery and innovation in materials science and chemistry

The challenge of complexity

Advanced materials share a common characteristic: They are complex. Achieving the required performance gains depends on exploiting the many degrees of freedom of materials development including multiple chemical components, nanoscale architectures, and tailored electronic structures. This introduces enormous complexity in the discovery process, complexity that must be understood and managed.

Early steels consisted of three to four essential chemical components and a relatively simple microstructure. Today's advanced high-strength, high-temperature steels average six to eight chemical components and require complex, multiphase nanostructures. The parameter space for exploration has increased enormously, making continued development by trial and error impractical.

New catalysts are needed to improve the efficiency of industrial processes, make effective use of bioenergy, and drive energy conversion and environmental mitigation processes. There are billions of options: chemical combinations, local morphologies, atomic-scale structure. Sifting through the options using predictive modeling is the only intelligent and efficient path forward.

The superconductors of the 1980s were typically two-component systems with a simple crystal structure. Today's high-temperature superconductors boast four or more chemical components, layered architectures, and sensitive electronic doping. This trend is also apparent in new high-field magnetic materials that derive their properties from the interaction of multiple chemical elements in complex microstructures. Again, high performance comes with a significant increase in complexity—and with a corresponding need to narrow discovery possibilities to a manageable number of the most promising options.

Leveraging new capabilities in nanoscale science and technology

Across the spectrum of new materials and chemical processes, discovery is increasingly confronted with complexity. We do not have the time or resources to explore all the options experimentally. The only solution is materials and chemistry by design, using new synthesis and characterization tools, theory, and simulation and modeling to understand complex materials and chemical systems and predict the most promising research directions.

> We do not have the time or resources to explore all the options by trial and error.

Over the past two decades, the United States has developed and deployed the world's most powerful collection of tools for the synthesis, processing, characterization, and simulation and modeling of materials and chemical systems at the nanoscale, dimensions of a few atoms to a few hundred atoms across. This length scale is critical, because the nanoscale is where the properties of materials and chemical reactions are determined. These tools, which include world-leading x-ray and neutron sources, nanoscale science facilities, and high-performance computers, provide an unprecedented view of the atomic-scale structure and dynamics of materials and the molecular-scale basis of chemical processes. For the first time in history, we are able to synthesize, characterize, and model materials and chemical behavior at the length scale where this behavior is controlled. This ability is transformational for the discovery process and, as a result, confers a significant competitive advantage.

The role of simulation-based engineering and science

Perhaps the most spectacular increase in capability has been demonstrated in high-performance computing. Over the past decade, computational power has increased by a factor of a million due to advances in hardware and software. This rate of improvement, which shows no sign of abating, has enabled the development of computer simulations and models of unprecedented fidelity and speed. We are at the threshold of a new era where the integrated synthesis, characterization, and modeling of complex materials and chemical processes will transform our ability to understand and design new materials and chemistries with predictive power. This has profound implications for the pace of discovery and the creation of new technologies.

> We are at the threshold of a new era where predictive modeling will transform our ability to design new materials and chemical processes.

Simulation-based engineering and science has accelerated progress in scientific understanding and technology development by enabling complex systems such as astrophysical and climate phenomena, aircraft wings, and integrated manufacturing to be explored rapidly and efficiently. This leads to new scientific understanding of systems that are too large for experimental study, reduced time and cost of prototyping, and accelerated deployment of new technologies. The United States has a commanding presence in computational science with leadership positions in high-end computing infrastructure and high-performance scientific applications, but the penetration of this capability has been slow and uneven. Harnessing the potential of computational science and engineering for the discovery and development of materials and chemical processes is essential to maintaining leadership in these foundational fields and their downstream energy and industrial applications.

Capitalizing on the opportunities presented by simulation-based engineering and science in materials and chemistry will require an integration of experimental capabilities with theoretical and computational modeling; the development of a robust and sustainable infrastructure to support the development and deployment of advanced computational models; and the assembly of a community of scientists and engineers to implement this integration and infrastructure. The experimental facilities are in place, and the computational power is available. The goal is leadership in predictive materials science and chemistry—predictive power to accelerate discovery and innovation in materials and chemical processes that enable energy technologies and drive industrial competitiveness.

Foundational challenges in predictive materials science and chemistry

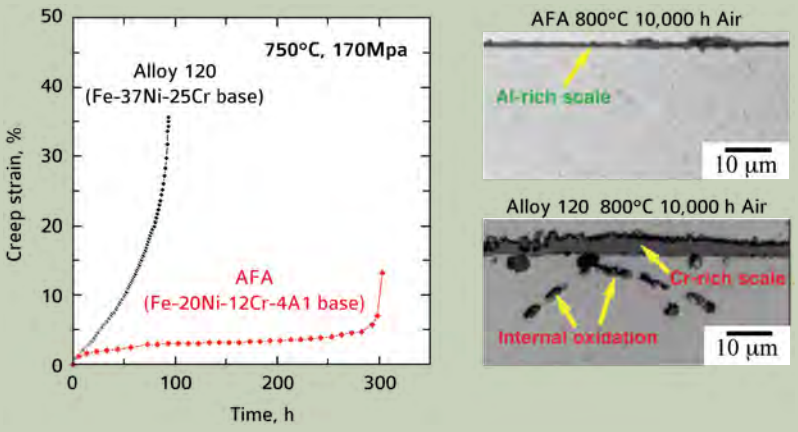
Materials for extreme conditions: Controlling microstructures

The availability of structural materials that can operate at extreme values of temperature, stress and strain, pressure, radiation flux, and chemical reactivity is the principal limiting factor in the performance of many energy systems. Fossil power plants, nuclear plants, and transportation systems all operate at lower efficiencies due to the limitations of existing structural materials. Impressive gains in efficiency of 30% and more can be achieved by the development of new materials capable of withstanding these demanding conditions.

The failure of materials, often at one-tenth or less of their intrinsic limits, is not understood. Understanding failure and achieving intrinsic properties require bridging length and time scales from molecular structures and their interactions to continuum models of bulk components. Central to this challenge is predicting and controlling the microstructure—the complicated arrangement of crystalline grains, defects, interfaces, and impurities that make up the microscale structure. Microstructure is key to understanding damage processes, preventing failure, and enhancing performance.

The design space of modern structural materials is huge—much too complex to explore by trial and error. Predictive modeling is needed to guide experiments in the most productive directions, to accelerate design and testing, and to understand performance. State-of-the-art computational tools allow scientists to calculate from first principles the interactions that dominate microstructural behavior, while experimental tools can now provide time-resolved measurements on real materials to validate these models. This integration of theory, simulation, and experiment will accelerate materials discovery and innovation. Key to achieving these advances is verification, validation, and uncertainty quantification of the computer models. Physical measurements must be made at relevant length and time scales and compared directly with theory and simulation.

The time is ripe for development of a sustained effort in integrated computational materials engineering. The lack of new materials is a critical factor in design and manufacturing, and a barrier to sustained competitiveness. The outcome of this effort will be the rapid development and deployment of new materials that can be incorporated in energy systems and manufacturing. This can increase the efficiency of power plants and transportation systems, significantly reduce requirements for physical testing, and increase competitiveness by achieving improved functionality and reduced time-to-market of a wide variety of products and technologies.



Computational techniques enabled the rapid development of alumina-forming austenitic (AFA) stainless steels with excellent creep resistance, ten times better corrosion resistance, and low alloy costs.

Courtesy of M. Brady, Oak Ridge National Laboratory

The microstructure of a material controls a wide range of important properties, including strength, fatigue, high-temperature performance, corrosion, and radiation resistance. While there is substantial qualitative understanding of microstructural evolution, there are no predictive models that link materials processing to resultant microstructures. Further, there is a lack of understanding of the connections between microstructure and materials performance. The new generation of synchrotrons, neutron sources, and synthesis and characterization equipment, together with recent computational and algorithm advances, provides an opportunity for the first time to envision designing microstructures for specific purposes and bringing them to fruition in real materials.

The potential impact of optimizing performance through engineered microstructures by design is huge. A recent National Academies report (see below) documents Ford's success in using integrated computational materials engineering to develop quantitative prediction of materials properties based on processing history. This has provided a substantial return on investment by reducing design times, lowering development costs, and accelerating the product cycle. The capability to tailor materials for specific applications, such as radiation environments, will become increasingly important as materials properties are pushed to their theoretical limits. Recent successes in demonstrating fourfold increases in the strength of advanced steels point to the dramatic gains that can be made.

Realizing this vision will require integrating and linking models that capture the multitude of individual physical phenomena that dictate material performance (microporosity, grain size, multiple phases, precipitates, etc.) and their effect on properties (fatigue, creep strength, corrosion, radiation resistance, etc.). This will also require close collaboration across the synthesis, characterization, theory, and computational communities, as well as sustained efforts in the related computer science, mathematics, and information science fields. Finally, integration with industry will be essential to develop and transfer the new computational tools and ensure their applicability to industry needs.

Early impacts of simulation-based engineering and science in industry (from top): virtual aluminum casting at Ford (7:1 return on investment), airframe design and manufacturing at Boeing (estimated 3–4 year reduction in material certification time), diesel engine brought to market solely with modeling and analysis tools at Cummins (reduced development time and improved performance), new tire design at Goodyear (threefold reduction in development time). From *Integrated Computational Materials Engineering: A Transformational Discipline for Improved Competitiveness and National Security*, National Academies Press (2008) and *Goodyear Puts Rubber to the Road with High Performance Computing*, Council on Competitiveness (2009).

Designing and engineering materials at the nanoscale: Understanding and controlling self-assembly

Designer materials made of pre-programmed building blocks that spontaneously organize into structures with unique and complex properties currently exhibited only by biological systems have long been a dream of technologists. Structures whose constituents can assemble, disassemble, and reassemble autonomously or on command enable materials capable of self-repair, multi-tasking, and even shape-shifting—properties known throughout the biological world. Imagine coatings that can change color or toggle between translucent and opaque on cue; sensors that can detect, trap, and dispose of pathogens; materials that can self-regulate porosity, strength, water or air resistance, elasticity, or conductivity—all these and much more are possible through self-assembly.

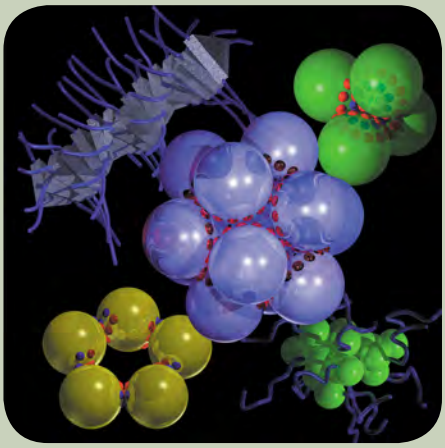
Importantly, self-assembly also permits material structures far more complex than traditional metals, ceramics, and polymers, with many levels of hierarchical organization and compartmentalization typical of biological structures such as cells and organelles. Such structural complexity is demanded by the sophisticated properties and behavior we desire of next-generation materials capable of meeting future energy demands—especially active materials, which must perform functionally in ways not possible today for traditional, nonbiological matter.

Over the past decade, investments and advances in nanoscience have made possible the creation, imaging, characterization, and manipulation of highly complex building blocks ranging from single molecules to supramolecular objects nanometers to microns in size—precisely the size range needed for the "bricks and mortar" of next-generation, self- assembled materials. Nanoparticles and colloids of nearly any shape, made of metals, semiconductors, and/or polymers, and functionalized with organic molecules and biomolecular ligands—including proteins, viruses, and DNA—as well as other chemical "hooks" are now possible. As a result, vast palettes of designer building blocks, in many cases coupled with solvents that play an active role in mediating interactions, are at hand, with the propensity for self-assembly into structures of unprecedented complexity and function.

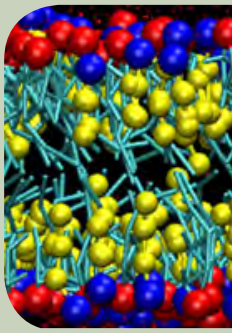
The design space for self-assembled materials is now so vast that computational tools are required for the rapid screening and prototyping of building blocks that will predictably self-assemble into desired structures. In recent years, promising new theoretical and computational approaches to the study of self-assembly have emerged to guide experiments, but these are in their infancy. At the same time, continued investments in high-performance computing (HPC) have produced computing platforms that are now fast enough to permit predictive simulations of self-assembly for complex building blocks, and new experimental probes promise the needed resolution of nanoscale structure to monitor assembly processes in situ, parameterize models, and validate simulations. These combined advances in synthesis, characterization, and modeling capabilities set the stage for a tipping point in our ability to discover the underlying principles controlling self-assembly, and to develop robust, predictive simulation-based tools to achieve materials by design.

Predictive capabilities for materials self-assembly

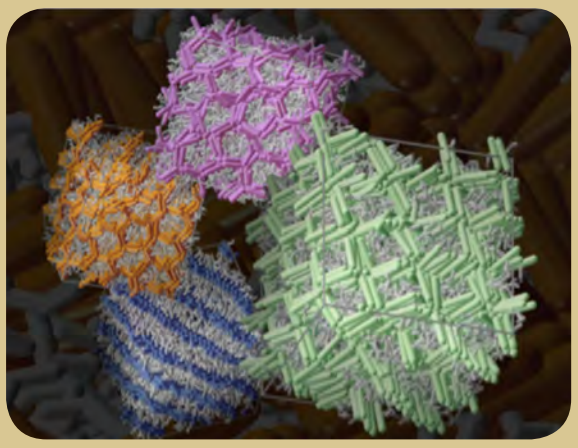
To fully master the science and engineering of self-assembly requires rapid and integrated progress on several related fronts of discovery and innovation. It requires harnessing the often competing theoretical



Scales of Assembly



These images show examples of assembly phenomena at various scales. (Left) Patchy particle nanocolloids and their assemblies predicted by coarse-grained models and Brownian dynamics simulations (courtesy of C. R. Iacovella and S. C. Glotzer, University of Michigan). (Right) Coarse-grained simulation of hexadecanic acid (yellow and dark blue) and cholesterol (red and turquoise) in water which represents a simple skin lipid material. The lipids self-assemble into an experimentally observed bilayer and demonstrate that shortening the acid tails destabilizes the bilayer due to decreased solubility of the acid, while longer acid tails lead to bilayer unzipping (courtesy of K. R. Hadley and C. McCabe, Vanderbilt University).



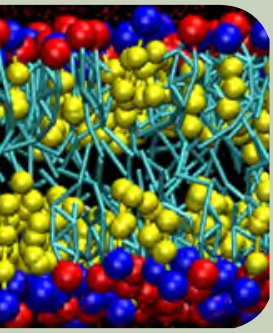
Self-assembly and reconfigurability of nanomaterials

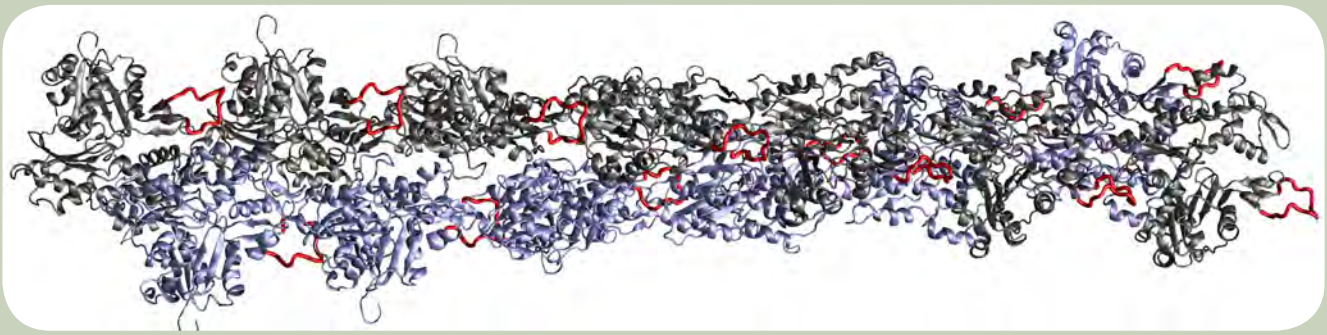
By combining organic and inorganic matter into hybrid building blocks, hierarchically ordered nanostructures can be achieved through self-assembly. The image at left shows the predictions of computer simulations of polymer-tethered rod-like nanoparticles. Depending on rod length, different structures result. Each structure exhibits different geometries and consequently different properties. By using "active" nanorods capable of lengthening and shortening, simulations show how the assemblies can be made to be reconfigurable, toggling among different structures on command.

Courtesy of T. D. Nguyen and S. C. Glotzer, *ACS Nano* 4(5), 2585–94 (2010).

principles of thermodynamics and kinetics in materials comprised of complex molecular and supramolecular building blocks whose shapes and interactions can result in kinetic traps that prevent assembly into equilibrium structures. It also requires discovering and applying the principles of statistical thermodynamics in active systems and systems driven far from equilibrium, as in biological systems, in which the constant input of energy creates and stabilizes structures. Finally, it requires developing simulation-based design tools that enable both the prediction of structures and their properties from building blocks and the rapid prototyping and reverse engineering of building blocks designed and pre-programmed to assemble into target structures.

Such advances are possible within the next few years due to the anticipated rapid convergence of synthesis capabilities, experimental probes, theoretical understanding, computing hardware, and scale-spanning algorithms. In particular, innovative high-resolution experimental probes (high-resolution X-ray and neutron scattering, super-resolution scanning optical microscopy, real-time 3D nanotomography, cryo-transmission electron microscopy, scanning probe microscopies, and others) allow for direct measurements of building block interactions and in situ, real-time monitoring of the various stages of self-assembly. Since many of the most interesting new building blocks (such as DNA-functionalized nanoparticles) combine biological and nonbiological matter, new experimental probes will be needed. On the HPC side, graphics processing units, or GPUs, developed by the billion-dollar video game industry already provide up to 1000-fold speedups in simulations that are highly "data parallel," including those used to study self-assembly (molecular dynamics, path sampling, phase diagram mapping, energy minimization, etc.). These architectures are ideal for rapid searching and optimizing of large design spaces, but significant code development will be required to utilize this new platform effectively as codes developed over the past one to two decades for serial or massively parallel CPU architectures cannot simply be ported to GPUs and perform optimally. Once rapid, high-throughput assembly prototyping for arbitrary building blocks is achieved, open databases and digital libraries for broad classes of self-assembling materials will be needed to expedite model and code validation. The new simulation capability that will result from these coordinated investments will revolutionize our ability to predict, model, and design self-assembled materials with desired functional properties for a broad host of energy and other applications.





(Above) Multimillion, all-atom molecular dynamics simulation of an assembled actin filament (shown in ribbon representation). The simulation results show that the conformation of the monomer binding loop (red) has dramatic effects on the structural and mechanical properties of actin (courtesy of J. Pfaendtner, D. Branduardi, T. D. Pollard, M. Parrinello, and G. A. Voth).

Light harvesting: Photons to energy

Developing future molecular, polymeric, and hybrid materials for harvesting and converting energy from sunlight requires sophisticated computational search strategies to find the optimal combination of organic and inorganic materials that can harvest light from the entire solar spectrum. Designing materials for such light collection requires capture of the infrared and ultraviolet parts of the solar spectrum and is expected to involve strategies based upon intermediate band gap materials, plasmonic excitations in clusters and molecules, and optimized thermoelectrical conversion complexes. Requisite to finding the optimal solar-harvesting "needle" in the materials genome "haystack" is the ability to accurately determine how any material specimen absorbs energy at every color of light (frequencies) delivered by the sun. Additional challenges are to determine the mechanisms by which the absorbed energy (exciton) migrates through the system prior to splitting into charges (electrons and holes) that are converted to electricity or chemical bonds.

In addition to the computational design of materials for solar cells, photosynthetic mimics, and photochemical pathways to fuels, the need to computationally predict and optimize a material's or chemical's propensity toward absorption and transfer of optical energy is ubiquitous and relevant to several energy technologies including

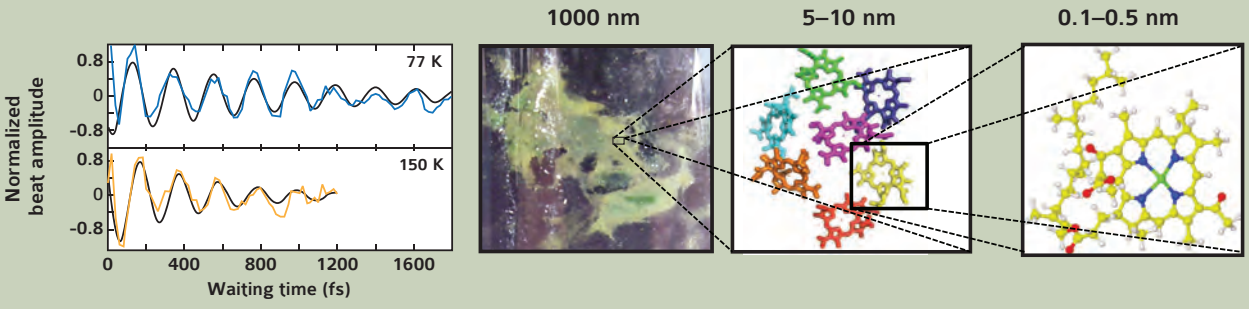
- radiative energy transfer in combustion,
- photocatalysis, and
- interfacial charge transfer.

Computer simulation and prediction of electronic excited states and their interactions with light and vibrations in molecules and materials can be pursued using several different techniques that have been developed during the past decade but need further refinement. Examples of such capabilities include the solution of the time-dependent hybrid density-functional theory coupled cluster equations, the Bethe-Salpeter equations, and the so-called GW equations. However widespread use of more than any one of these methods by experts in the fields of computational chemistry and materials science is rare, and significant but well-defined efforts are required to avail all electron dynamics and excited state methods to a broad swath of the academic, laboratory, and industrial-based scientific community.

For light-harvesting systems, interest is in understanding phenomena associated with timescales for charge/energy transport that are comparable to the reorganization time of the surrounding solvent. Accounting for such dynamics, especially in a realistic environment containing defects, is difficult but can be obtained from first-principles calculations such as quantum mechanics/molecular mechanics (QM/MM). However there is no *unified* or universal code that embodies these powerful methods, and the development of such a tool would enable the routine simulation of light harvesting in realistic systems. To directly simulate and understand the transfer of electrons from an adsorbed photoexcited dye molecule at the solid-liquid interface, semiclassical dynamical approaches relying upon publicly available force fields and quantum-mechanical methods are required. Additionally, one must account for dissipation and transport through the electrode.

National materials and chemistry computational networks

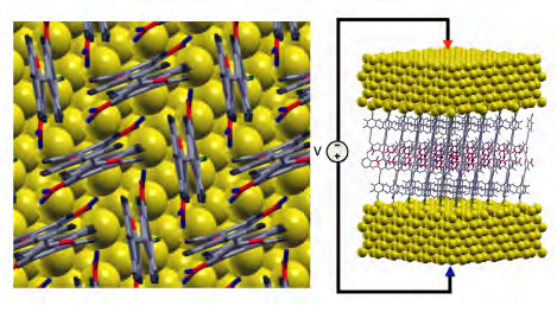
As shown in recent work by Ceder, Jacobsen, Norskov, and others, it is now possible to scan hundreds of thousands of possible combinations of elements across the entire periodic table, suggesting many new materials solutions that far exceed the traditional intuition of experts in



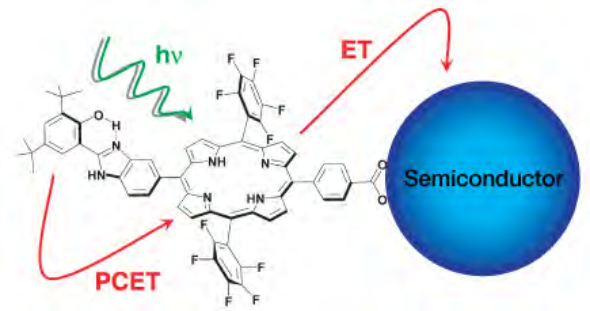
Design of molecular and polymer-based solar cells

Solar energy harvesting and processing requires understanding of phenomena mediated by exciton production, transfer, and splitting into carriers. Recent ultrafast experiments (above left) demonstrate unusually long-lived excitations in the light-harvesting bacteriochlorophyll complex which powers the green sulfur bacteria (two middle panels). These algae-like plants and their relatives effectively utilize the nonvisible parts of the solar

Materials for Light Harvesting and Charge Transport



Excited States for Photochemical and Voltaic Conversion



these fields. Even incomplete and low-level theories have suggested novel combinations of materials for new energy technologies. In principle, finding the best solution to solar harvesting and other issues related to composition-dependent process optimization can now be accomplished using this approach. The challenge of solar harvesting cross-cuts the traditional domains of chemistry and physics as it requires coupling together capabilities for localized excitations, band-to-band transitions, and electron transport. However, recent advances in theory, algorithms, hardware, and materials and chemical sciences are yet to be made available to the majority of scientifically and technically capable communities in the United States, especially those in the commercial sector—a situation which seriously threatens the realization of revolutionary breakthroughs in complex materials chemistry and materials design. With the exception of the highest-accuracy quantum-mechanical methods that are generally limited to small system sizes, other countries have far surpassed the United States in developing software for large-scale energy systems. This progress has been made possible by large groups of domain researchers that are networked together by schemes similar to those that were initiated in Europe 15 years ago. Because of its tradition of single principal investigator groups working on specific problems, the United States has no comparable infrastructure for scientific software development. As documented in a recent report (*International Assessment of Research and Development in Simulation-Based Engineering and Science*, World Technology Evaluation Center, 2009) almost all supported, user-friendly codes for many-atom systems now come from Europe. Reliance on access to nondomestic codes for technology vital to this nation's economic and security interests is untenable; therefore, the United States must rectify this situation or risk falling further behind technologically. Creation of national web-enabled networks would facilitate the coordination and sharing of information pertaining to materials data, scalable codes, and their implementation in new architectures. Networks would consist of one or two primary colocated groups that are linked together and include many single investigators. Through exchange programs they would provide expertise to experimentalists in academia, industry, and government. Such exchange would also lead to the creation of universal standards for materials reseach that would minimize the use of multiple codes and methodologies.

Images above (left to right): H. P. Cheng et al., cf. *J. Phys. Chem. C* **113**, 20713–20718 (2009); Moore et al., cf. *JACS* **130**(32), 10466 (2008).

spectrum. Recent observations of quantum beats in Fenna-Mathews-Olson photosynthetic complexes [Engel et al., PNAS (2010)] at different temperatures agree with a computational analysis [cf. Aspuru-Guzik et al., JCP 129 (2008)] that identified energy transfer pathways between neighboring chlorophylls in the complex. These computationally taxing methods demonstrate that theory can be used to understand this process but call for vastly increasing the computational efficiency and complexity of methods for predicting quantum-mediated transport and energy scavenging. A recent example of enhanced computational tools for multiscale computational methods and theories [cf. Wang et al., Nano. Lett. (2009)] demonstrated the ability to predict charge mobility in disordered conjugated polymers and can be extended to enable atomic-to-macroscale prediction and design of light harvesting in all types of materials such as the complex depicted here. At the molecular scale, quantum mechanics establishes the local properties and excited-state energies of the charge carriers. On scales of a few nanometers, the underlying molecular morphology determines sites for charge localization. Quantum mechanics also determines the rate at which the excited charges hop between locations. At scales larger than 10 nm, classical molecular-dynamical simulations and continuum approaches determine how the environment influences the active light-harvesting complexes. At scales of 100 nm or more, sophisticated sampling of carrier hopping rates gives a macroscopic mobility.

Controlling chemical reactions: Combustion and catalysis

The chemical bond represents the most compact non-nuclear energy storage medium known. Gasoline, for example, has more than 30 times the energy density of lithium-ion batteries. For this reason, chemical reactions hold center stage in the storage and release of energy in both current devices and those envisioned for a secure and sustainable future. The robust nature of chemical energy storage is embodied in the millennia between the photosynthesis of prehistoric plants, which stored the energy of the sun, and the recovery and combustion of the resulting fossil fuels today, which releases that energy. The challenge for the future is to capture, store, and release energy on an immediate timescale and in a sustainable way.

The predictive simulation of chemical transformations will accelerate the transition from utilizing energy stored in prehistory to establishing a sustainable cycle of energy storage and utilization. There are three principal areas of opportunity where design using predictive simulation will impact energy technologies:

- Artificial Photosynthesis and Solar Fuels
- Efficient Combustion of Low-Carbon Fuels
- Converting Biomass to Transportation Fuels

For the first of these, the sun offers an abundant and sustainable source of energy that can be used to convert water or water and carbon dioxide to fuels or intermediates used in the production of fuels. The essential barrier to developing this technology to industrial scales is finding appropriate photocatalysts that work together to perform the complete photosynthetic chemical cycle.

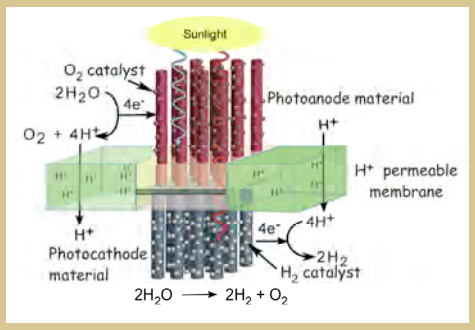
In the case of low-carbon fuels, efficient combustion technologies make use of turbulent reacting flows. Development of these technologies requires a combination of complex fluid flow simulations and high-accuracy chemical kinetic reaction mechanisms that capture the complex chemistry of current and future fuels: hundreds of reactants and thousands of reactions.

Finally, the challenge in the production of biofuels is to convert the principal components of biomass, a combination of cellulose, hemicelluloses, and lignin, into products that can be used as a substitute for gasoline and diesel fuel for various forms of transportation. The difficulty in meeting this challenge is the intrinsic complexity of biomass.

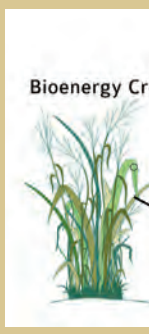
Further development of these three essential energy technologies requires predictive simulation that crosses many length and time scales. Combustion science is on the threshold of a new era of predictive modeling and simulation based on the convergence of new computer resources and the high-fidelity simulation codes ready to exploit them. Artificial photosynthesis, splitting water with sunlight, and biomass conversion into fuels all require new catalysts. The process of screening potential candidates, or synthesizing new ones, in the near future will be accelerated by predictive simulation of their properties.

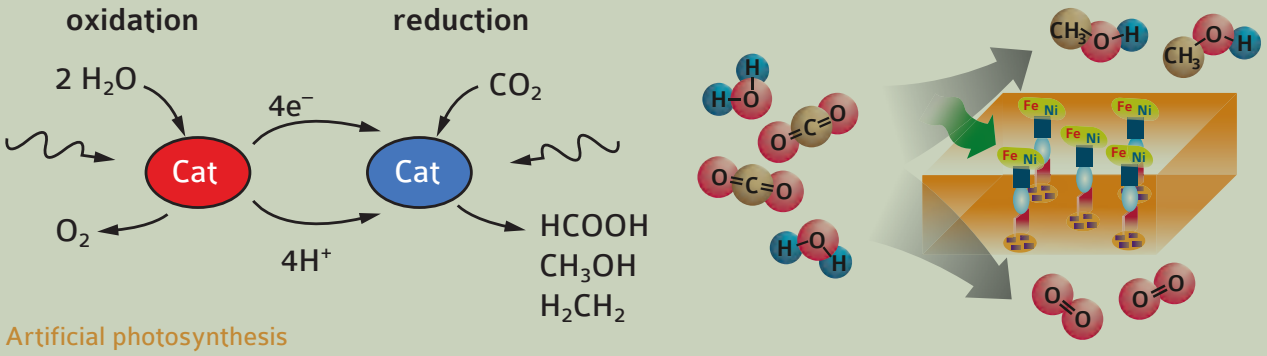
The computational science communities in each of these areas are poised to exploit existing computing technologies and extend their simulation algorithms and codes to dramatically shorten the time required to build a secure energy future.

Solar Fuels and Artificial Photosynthesis



Bioenergy Cr

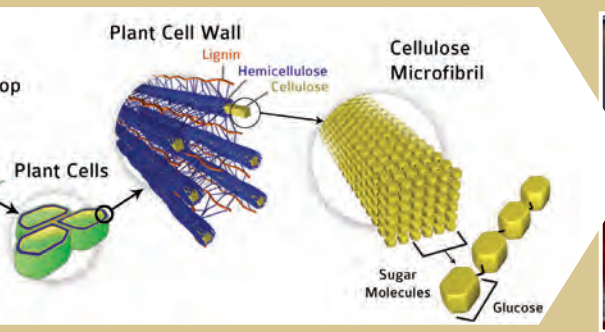




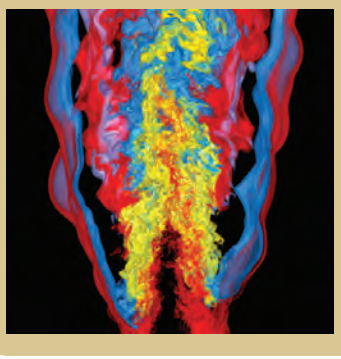
Artificial photosynthesis

Artificial photosynthesis is the generation of fuels directly from sunlight, water, and carbon dioxide by nonbiological, molecular-level energy conversion "machines." The realization of this process on an industrial scale will revolutionize our energy system. This is a very ambitious project that requires significant effort.

Converting Biomass to Fuels



Clean Combustion of Low-Carbon Fuels



Predictive capabilities for chemical design

Simulation and screening of photocatalysts for solar fuel production require the computational treatment of a large number of elementary processes covering a wide spectrum of timescales. Simulation of such processes requires methods to calculate the dynamics of charge pairs formation, separation, and mechanisms used to drive catalytic chemical reactions. Complete and accurate modeling of surface catalysis at the molecular level is required to predict reaction rates accurately. The tools of modern quantum chemistry and molecular dynamics form the basis for these needed new capabilities, but they must be extended, verified, and deployed on the most powerful available computing resources.

Large eddy simulation tools developed over the last decade will be required to simulate modern combustion engines and capture critical cycle-to-cycle variations in their performance. These tools bridge the gap between high-fidelity, first principles–based direct numerical simulation tools and Reynolds-averaged Navier-Stokes tools used in current industrial design. In addition, new methods are required to automatically generate high-accuracy reaction rate sets for arbitrary fuels.

For biomass conversion, efficient simulation methods are required to describe the multiscale dynamics and thermodynamics of solvated biopolymers. Quantum chemical simulation of biomass-catalyst interactions including the effects of solvent are also needed to help guide the selection of catalysts that will facilitate the conversion of sugars to suitable substitutes for gasoline and diesel.

All of these simulation capabilities will be developed in close collaboration with experiments conducted at the DOE Combustion Research Facility and national light source facilities at the Advanced Photon Source, Advanced Light Source, Linac Coherent Light Source, and in particular the ultrafast light sources being developed in the United States and abroad.

Decades of development provide a firm foundation for methods and algorithms of computational chemistry and molecular dynamics that support these three technologies. Timely deployment of these technologies in a software infrastructure that can be used in federally supported projects, like the Joint Center for Artificial Photosynthesis, and in industry is critical to capturing the benefits of predictive capability in chemical design.

Recent research has yielded enormous advances in our understanding of the subtle and complex photochemistry behind the natural photosynthetic system, and in the use of inorganic photocatalytic methods to split water or reduce carbon dioxide—key steps in photosynthesis.

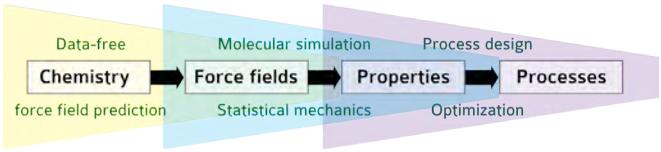
The components of an artificial photosynthesis device are shown. There are two photocatalysts (far left), one to perform the oxidation step that converts water into oxygen and hydrogen ions and the other for the reduction step that converts carbon dioxide into a usable carbon fuel. Also required are photoelectrochemical membrane layers that provide ionic pathways and good optical and light-scattering properties, while remaining impermeable to the product fuels and to oxygen. The DOE has recently announced the formation of the Joint Center for Artificial Photosynthesis (JCAP) at the California Institute of Technology and the Lawrence Berkeley National Laboratory to develop the components and assemble a working device and rapidly transfer research results to private industry for commercialization. The use and further development of predictive simulation, including quantum chemical and molecular level treatment of surface catalysis, are key to this project.

Courtesy of (clockwise from top) Nate Lewis (California Institute of Technology), Oak Ridge National Laboratory, J. Chen (Sandia National Laboratories), and (left) JCAP (Caltech and Lawrence Berkely National Laboratory)

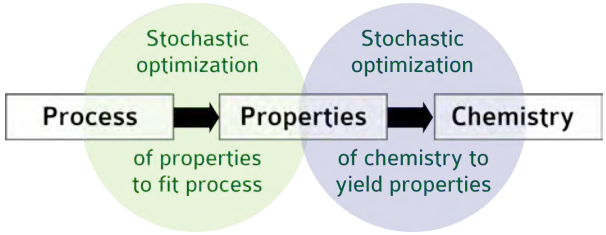
Designer fluids: Separations and carbon capture

Gases and liquids are collectively called fluids. Many of our most important global climate and energy challenges relate to fluids and separating them from other fluids or from solids. Examples include removing CO_2 from fossil power plant emissions; purifying water, since sufficient water supplies is one of the biggest challenges to ensure future global health and prosperity; and extracting high-energy-content liquid fuels for transportation applications from crude oil, or from the liquid mixtures obtained from biomass conversion.

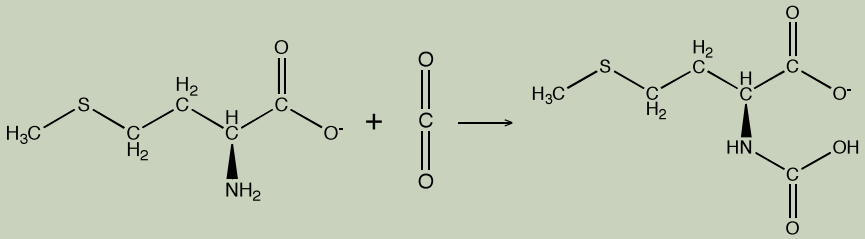
Today, the number of possible fluids and fluid mixtures that have the potential to revolutionize the world's energy and environmental future is virtually limitless. The discovery of new, large classes containing over a billion completely tailorable (i.e., designer) liquids, such as room-temperature ionic liquids, and new, equally large classes of tailorable solids that can be used in adsorption-based separation processes, such as metal-organic frameworks, has made the design space of possible fluids and separations processes essentially infinite. Thus, computational screening of these processes for energy and environmental applications is no longer simply desirable—it is *imperative*. However, the properties of fluids, which in turn determine the nature and efficiency of the processes used to separate them, depend, often very subtly, on the atomic- and molecular-level forces within and between molecules (known as force fields). Given accurate force fields, methods exist (molecular simulation, statistical mechanics) to computationally derive the properties needed to evaluate the potential applicability and separability of fluids. However, our current predictive capabilities are limited because we do not have robust methods for predicting force fields in an arbitrary fluid mixture. Specifically, we need to be able to predict force fields in the absence of experimental data (for systems not yet synthesized or characterized). Data-free force field prediction (DF^3P) must be achieved by using first-principles calculations (quantum chemistry, density functional theory, etc.) as input, but given the high computational costs of such methods, this is an enormous challenge. Success in DF^3P will enable true fluid properties prediction and revolutionize our ability to optimize and invent new energy and environmentally relevant systems. We can envision the flow of information beginning with the chemistry of a system (its chemical composition) and ending up with optimized processes.



As DF^3P is realized, we can invert the flow of information by the use of stochastic optimization (e.g., simulated annealing) at each step. For example, given a *desired* process, we can determine the properties needed to achieve that process; once the required properties are established, we can determine the optimal fluids for the process.

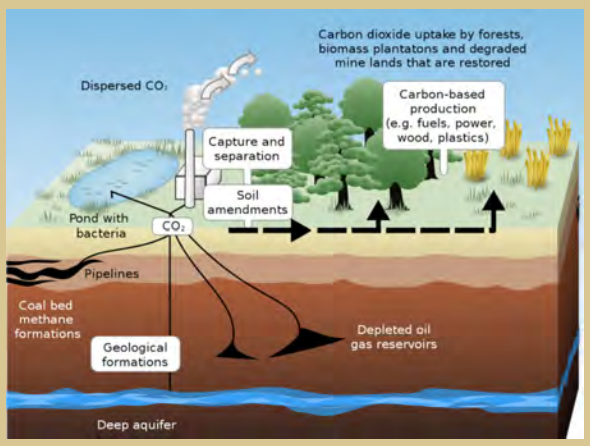


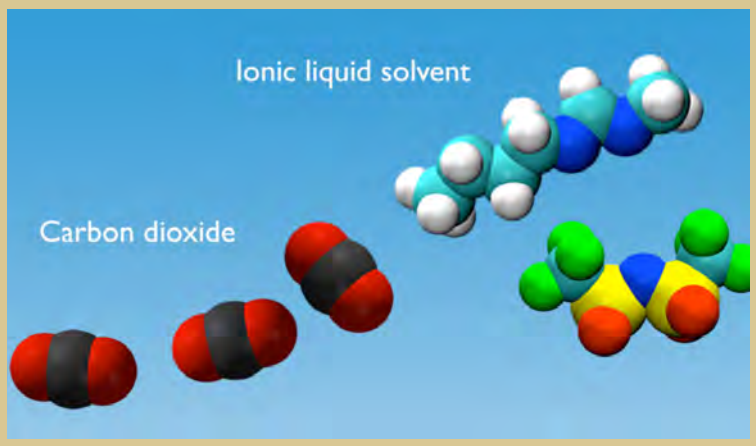
The result will be unlimited innovation in energy-relevant processes enabled by designer fluids.



Ionic liquids: Non-volatile, tailored solvents for CO_2 capture

To eliminate the single biggest source of greenhouse gases—CO_2 production from fossil-fuel-fired power plants— CO_2 must be captured (i.e., separated) from the flue gas that exits the plant's furnace and then buried underground (i.e., sequestered) or used as raw material for producing other chemicals (including liquid fuels). Liquid solvents for CO_2 capture selectively dissolve CO_2 out of the flue gas and then release it in another condition (e.g., different temperature); radically new solvents are needed if CO_2 capture is to be affordable (i.e., much less than the cost of producing the electricity itself). Among the most promising solvents are room-temperature ionic liquids (RTILs) that, unlike salts composed of simple ions (such as





Designer fluids and separations for a clean energy future

Data-free force field prediction (DF^3P) will enable the development of computational screening of solvents and adsorbents for carbon capture, leading to new, cost-efficient processes. The urgency of this effort is clear: As nations grapple with reducing greenhouse gas emissions, carbon capture is poised to become a multi-trillion-dollar industry in the next few decades. The time to examine alternatives to existing technologies is now and in the near future, before industry becomes committed to a specific technology, so that most effective carbon capture processes can be identified and implemented. Likewise, optimizing the extraction of liquid fuels from the mixtures resulting from biomass conversion and the purification and/or desalination of water are just two of many other profound energy/environmental challenges that can be addressed by computational modeling made quantitative by a robust DF^3P capability. DF^3P is also a key enabling technology across all of chemistry, geochemistry, biochemistry, and engineering: any field in which molecular interactions in fluids in bulk or at interfaces are important is currently limited by the availability of robust, accurate force fields.

Force field development today is an artisanal activity, practiced by many individual research groups with different goals, depending on their specific applications. For DF^3P to become a reality, force field development must become an automated workflow utilizing petascale and exascale computational resources. We are at the point where the confluence of past experience, computational resources, and national need make this an imperative. In the field of carbon capture alone, failure to do so will result in potentially trillions of dollars in infrastructure cost and loss of U.S. competitiveness that could have been avoided or dramatically reduced by having better alternatives early.

The outputs of a force field–based molecular simulation or statistical mechanical calculation of most interest to a process designer are thermophysical and themochemical properties; however, for experimental validation purposes, such methods also predict structures that are much more sensitive measures of force field accuracy. The DOE has an unequalled collection of experimental facilities for measuring structure at the molecular level, including the Spallation Neutron Source and the Advanced Light Source, that are the perfect tools for validation.

common table salt NaCl), are liquid in their pure state at or below room temperature. RTILs have many unique and highly desirable properties for CO_2 capture: high solubility for CO_2 that can be made even higher by adding functional groups such as amine (NH_2) that chemically react with CO_2, high thermal stability, and low vapor pressure (i.e., they will not evaporate during use and can be regenerated in novel ways). By adding cation, anion, and functional groups to RTILs, an almost limitless number of ionic liquids can be prepared.

In the future, high-throughput computational screening of possible RTILs must be developed, because to synthesize, characterize, and evaluate billions of possible RTILs is simply not feasible. Even today, computational approaches are leading the way in the search for new, more effective RTILs for CO_2 capture.

For example, using density functional theory, this year engineers predicted that the addition of an NH_2 functional group to the negative ion (e.g., see the ion on the left of the reaction shown opposite) resulted in CO_2 capture efficiency that is twice as high as when the same group is added to the positive ion, and thus twice the efficiency of current technology (amines dissolved in water). This prediction has now been confirmed by experiment.

Designer interfaces: From interfacial materials to advanced batteries

Fuel cells offer a way to extract twice the energy from hydrocarbons as internal combustion engines. Photovoltaics provide direct access to the most abundant energy source available on our planet. Fiber-reinforced polymer matrix composites achieve strength and stiffness characteristics paralleling those of steel at a fraction of the weight, thus providing for lighter, fuel-efficient vehicles. These are but a few examples of devices and structures in which functionality is achieved by deliberately juxtaposing disparate types of materials, and where the processes that are fundamental to the device performance occur at the interfaces between constituents. For example, fine-tuning the bonding interactions between fibers and matrix provides for simultaneous high strength and toughness of the composite. In solar cells and solid-state lighting, the separation and recombination of charge carriers at interfaces provide the basis for converting light into electricity, or vice versa, and the efficiency of these processes depends on the quality and perfection of the interfacial region. The long-term stability of the interfaces between electrodes and separator membranes is essential for sustaining the electrochemical processes responsible for the generation or storage of electric energy in fuel cells or batteries.

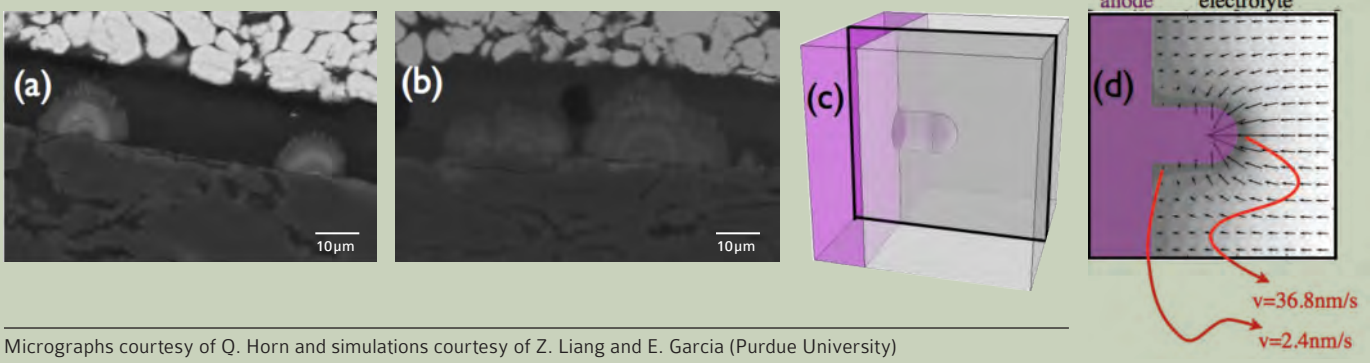
Today, we cannot achieve the highest energy conversion efficiencies or create the strongest composites because interfaces are imperfect and degrade with time. The key to producing materials systems with the desired performance characteristics is the ability to fabricate them consistently and with nanoscale precision to design specifications. This entails the realization of atomically sharp definition and long-term stability of interfaces. Hence, detailed knowledge about the structure of interfaces and the mechanisms of interfacial phenomena, both as they govern the functional response of a device and contribute to the deterioration of the interface, is essential for advancing many critical technologies.

Given their small extent in one dimension and because they are typically buried within bulk materials, interfaces are difficult to resolve or access by experimental means. Simulation and modeling is therefore ideally suited to complement experiments and supply the missing information. Computational science and its infrastructure will impact research and development with respect to interface science in two transformative ways: (1) we will be able to use modeling and simulation not simply to recreate experimental observations, and thereby provide for detailed interpretation, but to generate new information that is inaccessible by experiments; (2) through combinatorial and high throughput, rational exploration of interfacial phenomena, and modeling and simulation will yield the necessary fundamental insights to develop a predictive design toolset.

With the advancement of HPC, modeling and simulation can guide and accelerate materials development. We can conceive materials building blocks encoded to self-assemble into desired configurations, numerically test and optimize design criteria for specific interfacial functionality, and achieve high figures of merit for multiple performance criteria simultaneously, for example, electrolytes with high ionic mobility and stiffness, electrodes with high intercalation capacity and phase stability, and low-density composites with high strength and thermal conductivity.

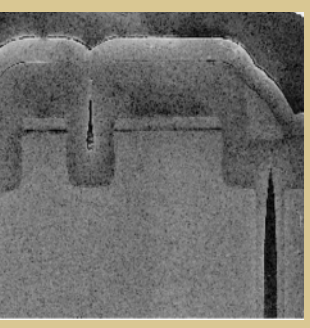
Predictive capabilities for the design of interfaces

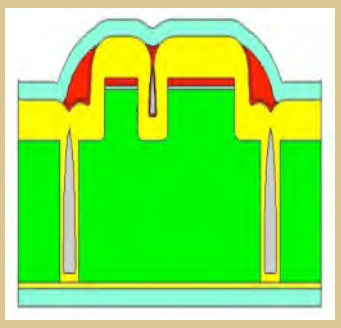
Unlike with new experimental probes, where breakthroughs occur somewhat sporadically, computational power



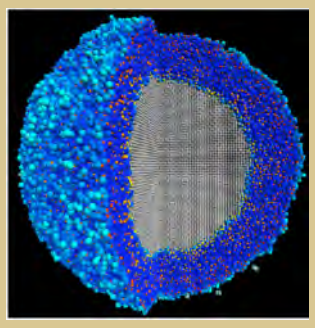
Micrographs courtesy of Q. Horn and simulations courtesy of Z. Liang and E. Garcia (Purdue University)

Growth structures in semiconductor devices

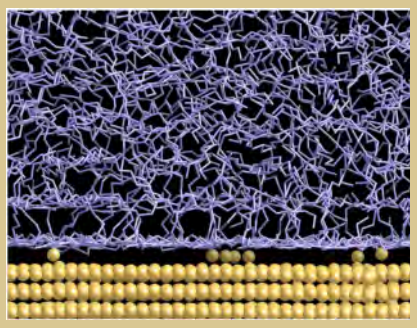




Oxidation of aluminum nanoparticle



Polymer–metal interface



increases at a predictable rate due to relatively steady progress in chip circuit density and computer architectures. Based on the projected performance growth, we can mobilize resources to harness this power and engage in the creative process that leads to establishing new theoretical frameworks, modeling approaches, algorithms, and codes for increasingly realistic and demanding simulations that allow us to predict interfacial phenomena. Without these advances in modeling and simulation, the crucial knowledge gap that prevents us from developing technological materials with precise control of those properties governed by interfaces will persist.

To account for the important phenomena occurring at interfaces, features such as the electron distributions within the irregular gaps between adjacent materials must be resolved, while interfacial reconstructions, defects, and roughness are described at scales encompassing millions to billions of atoms. To accurately predict the behavior and properties of interfaces, realistic structural models must first be generated. This requires specialized procedures, such as acceleration algorithms, heuristic schemes for advancing structural evolution, and statistical sampling techniques. Such an inherently multi-scale computational challenge must include electronic structure calculations, atomistic simulations, and continuum methods, and key improvements in the available computational infrastructure still need to be achieved. Simulation algorithms and statistical analysis formalisms must be adapted to account for lack of periodicity and symmetry of interfacial regions. Quantum mechanical, particle-based deterministic, statistical, and geometric simulation techniques must be effectively integrated or coupled through adaptable information conduits. Workflow integrators that autonomously balance multi-scale simulation tasks, better order-N methods for first-principles calculations, and more sophisticated reactive force fields will allow us to eliminate the trade-off between computational speed and accuracy. Validation of these simulation approaches will be possible with in situ experimental characterization of buried interfaces using powerful new neutron and synchrotron sources, Z-contrast high-resolution electron microscopy, and nano-probe transport measurements that have only recently become available.

Modeling and simulation will provide predictive capabilities for the design of interfaces in materials. As a result, we will improve the efficiency of solar panels, solid-state lighting, thermoelectric generators, and fuel cells; create high-capacity batteries; fabricate lightweight composites with increased strength, stiffness, and toughness; and extend the lifetime of materials systems, devices, and components.

Lithium batteries for high-power density

Lithium dendrite growth occurs in all currently used and emerging lithium-based rechargeable battery architectures as a result of the electrochemical field localization at high discharge rates, leading to battery failure. Simulations reveal for the first time why the dendrite tip grows fifteen times faster than the flat lithium substrate, short-circuiting the device. Understanding how to suppress dendrite growth will enable the development of reliable rechargeable batteries with the high-power densities needed for automotive applications.

Shown at left: (a and b) examples of dendrites in lithium batteries; (c) a simulation of a lithium dendrite in the presence of a 3 V potential difference; (d) the cross section of the electric fields and simulated dendrite growth profile.

Images (above) courtesy of J. Sethian (University of California-Berkeley); P. Vashista (University of Southern California); and C. Shao, K. Becher, and J. Kieffer (University of Michigan)

Controlling electronic structure: Modeling strongly correlated electrons

Strongly correlated materials, whose behavior is dominated by the Coulomb repulsion among electrons, are exceptionally rich in dramatic behavior and useful functionality. Magnets that enable digital memory, superconductors that carry electricity without loss above liquid nitrogen temperature, actinides that power nuclear reactors, and quantum dots that enable nanotechnology are all strongly correlated materials. These materials typically display a host of competing phases closely spaced in energy (see figure at lower left) leading to "colossal" response to small external stimuli, a feature with endless potential for technological exploitation.

Although we use some of these materials on an empirical basis, we cannot model, predict, or control their properties as we do for semiconductors like silicon. This lack of predictive capability is a severe bottleneck—strongly correlated materials are so common and their compositions and structures so complex that they simply overwhelm serendipity as a discovery and development tool. Reliable predictions of the behavior of strongly correlated materials are critical for designing the next generation of globally competitive information, communication, sensing, and clean energy technologies.

In the past decade, however, strongly correlated materials have begun to yield their secrets to a host of modeling approaches that go beyond existing density functional theory. The challenge set by strongly correlated electrons is to develop methods that can simultaneously describe the strong correlations that can lead to localization of electrons on atomic sites and the weak correlations that allow itinerant electrons to move freely throughout a material.

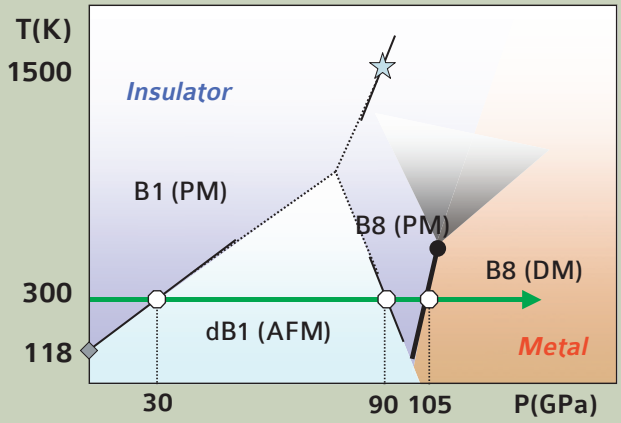
For 50 years this problem has evaded fundamental treatment; we are now on the verge of cracking this bottleneck to the understanding and use of strongly correlated materials.

The density functional approach excels where dynamical correlations are modest in size, which is in the weakly correlated materials. Static extensions of density functional theory have proven useful, but the real need for the future is to treat strong dynamic correlations directly. Impressive advances have recently been made in this area, with dynamical mean field implementations providing the solution to several long-standing, classic problems. Quantum Monte Carlo techniques promise essentially exact solutions that, due to technical challenges and issues of scaling with system size, will require a longer time frame for broad application. Low-dimensional correlated systems present additional challenges, and density matrix methods are most promising for this class.

Achieving predictive capability

The challenge and the opportunity are to take the treatment of strongly correlated materials to the same level of accuracy, accessibility, and confidence as we have achieved for weakly correlated electrons with density functional theory using the local density approximation. The opportunity has never been as clear in form or as ripe for harvest as it is now. The community is at a tipping point—a critical mass of ideas, researchers, and techniques is at hand.

Crucial extensions of density functional theory are required, with the dynamical treatment of intra-atomic



The pressure-temperature phase diagram of manganese oxide (MnO) illustrating the many competing phases that depend on the local/itinerant character of the strongly correlated 3*d* manganese electrons. Promising advances in treating the behavior of strongly correlated electrons by dynamical mean field theory, extended density functional theory, density matrix renormalization group, and quantum Monte Carlo techniques bring within reach the capability to predict the complex phase diagrams and materials properties of correlated electron materials for technological applications.

Courtesy of C. S. Yoo, B. Maddox, J.-H. P Klepeis, V. Iota, W. Evans, A. McMahan, M. Y. Hu, P. Chow, M. Somayazulu, D. Häusermann, R. T. Scalettar, and W. E. Pickett, *Physical Review Letters* **94**, 115502.

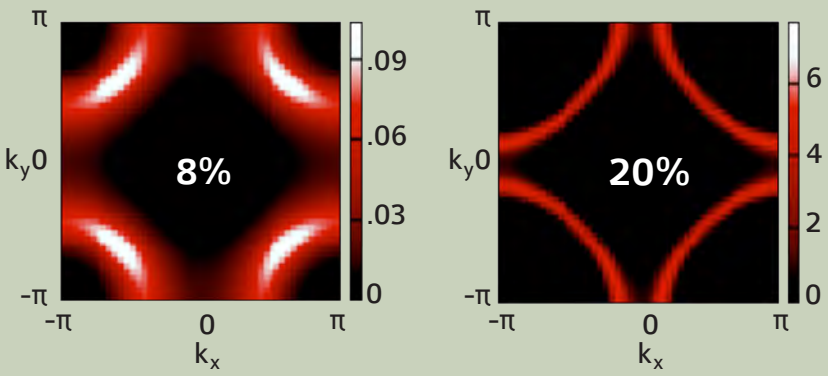
interactions and of interactions of localized and itinerant electrons comprising the minimum requirements. The energy resolution of correlated electron treatments needs to be increased in order to treat the low energy states, where electrons fluctuate on short timescales between local and itinerant character. This rapid fluctuation between dual existences lies at the very heart of strongly correlated behavior.

One fundamental barrier to modeling strongly correlated materials is the continuing lack of resources and mechanisms for development of robust, open-source computer codes in the United States, a trend dating from the 1980s. Europe has demonstrated the power of supporting code development; they are now dominant in the world in producing codes for materials science. East Asia and China are rapidly emerging leaders; by 2012 China will overtake the United States in publications based on first-principles density functional theory. The United States must develop policies and procedures that will nurture the collective effort of its scientists and engineers to establish the next generation of open-source materials simulation methods and community codes. The United States has the accumulated expertise and creative inspiration, but the mechanisms to develop robust, user-friendly open-source software are missing. In addition, full integration of software with the revolutionary advances occurring in hardware and computational paradigms is needed if we are to achieve predictive materials capability. An effective implementation strategy that capitalizes on existing theoretical and computational capabilities will increase the number of productive users and the frequency of potentially transformative advances.

Experimental validation is essential to developing predictive capabilities for strongly correlated electron materials. Many strongly correlated electron phenomena take place at ultrasmall spatial scales and ultrafast timescales. Continuing advances in experimental tools such as x-ray free electron lasers, aberration-corrected electron microcopy, high-resolution photoemission, diffuse neutron scattering, and scanning probe microscopy are critical to probe, verify, and refine the theory and modeling predictions.

The rewards of predicting the behavior and functionality of strongly correlated materials are enormous—next-generation magnetic memories, spintronic and metal-insulator ("Mott-tronic") digital logic, high-resolution sensors for electromagnetic radiation and environmental chemicals, and better performing high-temperature superconductors, among others. The competitive advantage to the institutions or countries that develop this new capability eminently justifies the effort.

Momentum dependence of strong correlation



The evolution of Fermi arcs in the pseudogap state of the high-temperature superconductors predicted by cluster extensions of dynamical mean field theory as hole doping increases from 8% to 20%. The Fermi arcs arise from the localization of some of the electronic states in momentum space, while others remain itinerant, one of the most startling and dramatic features of strong correlation in the high-temperature superconductors.

Courtesy of M. Ferrero, P. S. Cornaglia, L. De Leo, O. Parcollet, G. Kotliar, and Antoine Georges, *Physical Review B* **80**, 064501. Copyright (2009) by the American Physical Society.

Materials and chemistry by design: Creating an innovation ecosystem

Modeling and simulation is today a critical part of every discipline of science and engineering. However, while models and methods are well understood in areas such as structural engineering and modeling tools are embedded within several related industry sectors, simulation-based engineering and science capabilities for materials research are much less mature. Although scientific models and algorithms are in hand for many materials applications, critical information is missing for others, and there is only a handful of simulation-based materials design tools sufficiently predictive and robust for industrial use. As a result, despite many successful examples of the use of simulation-based engineering and science, we have only just begun to exploit its full capabilities and promise for discovery and innovation when it comes to the critical pacing technologies of new materials. Emerging capabilities in predictive modeling and simulation have the potential to revolutionize the development of new materials and chemical processes. Coupled with world-leading materials characterization and nanoscale science facilities, this predictive capability provides the foundation for an innovation ecosystem that can accelerate discovery and the development of new technologies, including advanced energy systems.

Achieving predictive capability

To lead in R&D for energy and other technologies, the United States must establish a predictive capability based on simulation-based engineering and science that is second to none. Developing and sustaining this capability requires a long-term commitment that is at the same time financial, intellectual, and programmatic. It requires ongoing investment in all aspects of computational science and engineering—from theory, models, and algorithms to languages and compilers, to faster computers, to software and open-source databases, to workforce. It requires close partnership between experiment, theory, and simulation to advance fundamental scientific understanding and to quantify the uncertainty inherent in any prediction, which is required for risk assessment and decision-making. It requires expediting and facilitating the transformation of scientific research codes to design tools suitable for the industrial laboratory setting and manufacturing floor, and the training of a future workforce sufficiently expert to both develop and use these tools. Together, these elements of computational science and engineering form the foundational infrastructure for the predictive capability afforded by simulation-based engineering and science.

Integration of synthesis, processing, characterization, theory, and modeling and simulation

Recent advances in high-performance computing have been nothing short of astounding. Over the past decade, computational power has increased by a factor of a million due to advances in hardware and software. Fast new chips developed primarily for the brilliant graphics needed by the billion-dollar video game industry and supported just in the last year or two for use by the scientific community are providing additional spectacular increases in speed for many codes, including those used by the materials and chemistry communities. Because of these advances we now have computer simulations capable of overnight results with unprecedented fidelity.

At the same time, the United States has developed over the past two decades the world's most powerful collection of research facilities for materials and chemical sciences. Our synthesis and characterization facilities enable unprecedented insight into, and manipulation at, the nanoscale, the length scale where properties are determined and chemical reactions

are controlled. For the first time in history, simulation and experiment now meet on common ground at this critical scale, providing an unparalleled opportunity for scientific insight and the parameterization and testing of theories and models central to predictive simulation for materials and chemical processes. Only through the integration of synthesis, characterization, and modeling and simulation of complex materials and chemical processes will we transform our ability to understand and design new materials and chemistries with predictive power. This integration requires investments in fundamental experiments and theory whose primary aim is to provide measurements or analytical values, respectively, as both inputs to and validation of materials and chemical models and codes. It also requires the development of open-source community databases and virtualization tools for the capture, sharing, and reuse of reference materials data, and a long-term commitment to the education and training of a new generation of data-centric and cyber-savvy scientists fluent in the "language" of both experiment and simulation, and capable of developing and using sophisticated software tools.

Simulation-based engineering and science (SBE&S) as a critical and sustainable national infrastructure

The United States gave birth to the modern field of electronic digital computing back in the early days of World War II. We have come far from the first digital predictions of ballistic firing trajectories, with simulations today yielding critical insights into the beginnings of disease, the atomistic mechanisms behind material failure, the development and likely path of hurricanes, and even impending crises in the stock market. The investments we have made as a nation in the field of computing and in computational science and engineering provide the foundation for the next essential step—the integration and full-scale deployment of computational methodologies as community tools for predictive simulation. This step requires investment in software as infrastructure, which in turn requires substantial investment in and long-term support and nurturing of software development communities and the codes they develop; in the development, validation, and verification of models, algorithms, and databases; in the preparation of a highly skilled SBE&S workforce; and in the continued development of both commodity and high-end computing technologies and the infrastructure to use them.

Critical elements of a national infrastructure for simulation-based engineering and science capable of transforming our predictive capability for materials and chemical processes include a capacity for the following:

- ongoing development of new theories of materials and chemical processes and their rapid integration into robust, validated software;
- ongoing development of new computational algorithms and methods, including multiscale methods, as well as new computing platforms;
- validation, verification, and uncertainty quantification, including "open-data" community databases of validation data from experiments, theory, and simulations;
- development, dissemination, and long-term support of materials models, codes, and simulation platforms, with particular attention to code maintenance, interoperability, sharing, and reuse;
- sustainable partnering among industry, government, and academia in the development, application, and use of SBE&S tools; and
- educating and training the next generation of computational scientists and engineers.

Benefits of predictive capability in science and engineering

Accelerating scientific discovery

The scientific discovery process is not linear—it follows an often chaotic path of intuition, trial and error, and serendipity. While we cannot schedule serendipity, we can strengthen intuition and optimize trial and error through improved predictive capability enabled by advances in modeling and simulation. This is essential if we are to explore the enormous phase space presented by the complex materials and processes that are key to achieving needed performance gains. Predictive capability accelerates discovery by guiding experiments in the most productive directions, by reducing the number of options or configurations that need to be tried, by suggesting specific breakthrough opportunities for experimental verification, and by providing powerful tests for theories that improve fundamental understanding. In many cases, progress demands predictive capability due to the complexity that must be navigated.

Predictive capability is transforming the discovery process, enabling rational discovery strategies for systems that were not tractable a few years ago.

The development and application of predictive modeling and simulation are transforming the discovery process. Rational discovery strategies can now be implemented for complex systems that were not tractable a few years ago. This greatly increases the parameter space that can be explored and significantly reduces the time required for this exploration. Due to advances in computing power, modeling and simulation have become powerful components of a tightly coupled discovery system dependent on the integration of experimental, theoretical, and computational capabilities. Building on recent advances in experimental and computational facilities, the United States is well positioned to lead this integration and the subsequent acceleration of scientific discovery.

Enabling new technologies

Predictive capability is also driving the transformation of technological innovation. New materials and chemical processes are needed to meet demanding performance requirements across the broad spectrum of advanced energy technologies. The development of new materials, from discovery to deployment, has typically required two decades. On the other hand, the product development and manufacturing cycle has been reduced by computer-aided design to as little as 3 years. This mismatch precludes incorporation of new materials in products in a timely manner, sacrificing both performance and competitiveness.

Integrated computational materials engineering has been shown to accelerate the introduction of new materials and processes into the product development cycle by minimizing testing requirements, reducing failures, and increasing quality. Early successes in several industry sectors have demonstrated significant return on investment and reduced development times. Combining integrated computational materials engineering with accelerated discovery of new materials and processes offers the opportunity to incorporate new materials earlier in the product design cycle, increasing performance and shortening the materials development cycle to better align with product development. The impact is a reduction in the development cycle with significant impacts on technology deployment and innovation.

Seizing the opportunity

Recent federal investments in world-leading materials characterization, nanoscale science, and computational facilities have prepared the foundation for an innovation ecosystem that can accelerate discovery in materials science and chemistry. Creating this ecosystem is pivotal in order to capture the benefits of these investments and secure the resulting competitive advantage. Delivering on the promise of this ecosystem is dependent on the following.

- **Integration of synthesis, processing, characterization, theory, and simulation and modeling.** Many of the newly established Energy Frontier Research Centers and Energy Hubs are exploiting this integration.
- **Achieving/strengthening predictive capability in foundational challenge areas.** Predictive capability in the seven foundational challenge areas described in this report is critical to the development of advanced energy technologies.
- **Developing validated computational approaches that span vast differences in time and length scales.** This fundamental computational challenge crosscuts all of the foundational challenge areas. Similarly challenging is coupling of analytical data from multiple instruments and techniques that are required to cross these length and time scales.
- **Experimental validation and quantification of uncertainty in simulation and modeling.** Uncertainty quantification becomes increasingly challenging as simulations become more complex.
- **Robust and sustainable computational infrastructure, including software and applications.** For modeling and simulation, software equals infrastructure. To validate the computational tools, software is critical infrastructure that effectively translates huge arrays of experimental data into useful scientific understanding. An integrated approach for managing this infrastructure is essential.
- **Efficient transfer and incorporation of simulation-based engineering and science in industry.** Strategies for bridging the gap between research industrial applications and for widespread industry adoption of integrated computational materials engineering are needed.

Achieving predictive capability in materials and chemistry is critical to accelerating discovery and the development of new technologies.

Advances in materials and chemistry are essential to leadership in virtually all technologies. The integration of simulation-based engineering and science into the discovery process provides a transformational opportunity to accelerate innovation and achieve unprecedented performance, with profound implications for the pace of discovery and the development of new technologies.

Workshop Agenda

DOE Workshop on Computational Materials Science and Chemistry for Innovation

Monday July 26

7:30–8:15 am	**Registration; Continental Breakfast**
8:15–8:30 am	**Welcome** Steve Koonin, Under Secretary for Science
8:30–8:45 am	**Workshop overview and goals** Jim Roberto, Oak Ridge National Laboratory
8:45–9:15 am	**Basic research for energy** Harriet Kung, Associate Director, Office of Basic Energy Sciences
9:15–9:30 am	**Computational materials science and chemistry for innovation** Michael Strayer, Associate Director, Office of Advanced Scientific Computing Research
9:30–10:00 am	**High performance computing: Opportunities and cross-cutting issues** Paul Messina, Argonne National Laboratory
10:00–10:30 am	**Opportunities and challenges in computational chemistry and materials science: Report from the BES Workshop on Extreme-scale Computing** Thom Dunning, University of Illinois
10:30–10:45 am	**Break**
10:45–11:15 am	**Simulation-based engineering and science for discovery and innovation** Chuck Romine, National Institute of Standards and Technology
11:15–11:45 am	**The Materials Genome Project: High-throughput ab-initio computing** Gerd Ceder, Massachusetts Institute of Technology
11:45 am–12:00 pm	**Charge to breakout groups** Sharon Glotzer, University of Michigan
12:00–1:15 pm	**Working lunch: Designing a national research initiative** Tom Kalil, Deputy Director for Policy, White House Office of Science and Technology Policy
1:15–5:30 pm	**Panel breakouts** **Panel 1:** Materials for extreme conditions **Panel 2:** Chemical reactions **Panel 3:** Thin films, surfaces, and interfaces **Panel 4:** Self-assembly and soft matter **Panel 5:** Strongly correlated electron systems and complex materials **Panel 6:** Electron dynamics, excited states, and light-harvesting materials and processes **Panel 7:** Separations and fluidic processes
5:30–6:30 pm	**Working dinner: Integrated computational materials** John Allison, Ford/University of Michigan

Tuesday July 27

7:30–8:15 am	**Breakfast**
8:15 am–12:00 pm	**Panel breakouts continue**
12:00–1:00 pm	**Working lunch**
1:00–4:00 pm	**Reports from each panel**
4:00–4:15 pm	**Closeout**

Participants

Registered participants for the DOE Workshop on Computational Materials Science and Chemistry for Innovation

Abild-Pedersen, Frank	SLAC National Accelerator Laboratory	Invited Observer
Allison, John	Ford Motor Company / University of Michigan	Plenary Speaker
Aronson, Igor	Argonne National Laboratory	Panel Co-Lead
Aspuru-Guzik, Alan	Harvard University	Panelist
Bair, Ray	Argonne National Laboratory	Panel Co-Lead
Baruah, Tunna	University of Texas at El Paso	Panelist
Bell, Alexis	University of California, Berkeley	Panel Co-Lead
Bell, John	Lawrence Berkeley National Laboratory	Panelist
Bishop, Alan	Los Alamos National Laboratory	Invited Observer
Biven, Laura	Department of Energy, Office of Science	Invited Observer
Blaisten-Barojas, Estela	National Science Foundation	Invited Observer
Brown, David	Lawrence Livermore National Laboratory	Panelist
Burke, Kieron	University of California, Irvine	Panelist
Carim, Altaf	Department of Energy, Basic Energy Sciences	Invited Observer
Carter, Emily	Princeton University	Panelist
Ceder, Gerbrand	Massachusetts Institute of Technology	Plenary Speaker
Chatterjee, Lali	Department of Energy, Office of Science	Invited Observer
Chen, Chau-Chyun	Aspen Technology, Inc.	Panelist
Chen, Gang	Massachusetts Institute of Technology	Panelist
Chipman, Daniel	University of Notre Dame, Radiation Laboratory	Panelist
Clark, Aurora	Washington State University,	Panelist
Colella, Phillip	Lawrence Berkeley National Laboratory	Panelist
Colina, Coray	Pennsylvania State University	Panelist
Cooper, Clark	National Science Foundation	Invited Observer
Corrales, Rene	The University of Arizona	Panelist
Cummings, Peter	Vanderbilt University / ORNL	Panel Co-Lead
D'Azevedo, Ed	Oak Ridge National Laboratory	Panelist
Davenport, James	Department of Energy, Basic Energy Sciences	Invited Observer
Dean, David	Department of Energy	Invited Observer
Dehmer, Patricia	Department of Energy, Office of Science	Invited Observer
Devanathan, Ram	Pacific Northwest National Laboratory	Panelist
Dunietz, Barry	University of Michigan	Panelist
Dunning, Thom	NCSA / University of Illinois	Plenary Speaker
Falk, Michael	Johns Hopkins University	Panelist
Farrell, Helen	Idaho National Laboratory	Invited Observer
Fennie, Craig	Cornell University	Panelist
Ferris, Kim	Department of Energy, Basic Energy Sciences	Invited Observer
Fichthorn, Kristen	Pennsylvania State University	Panelist
Foiles, Stephen	Sandia National Laboratories	Panelist
Fong, Dillon	Argonne National Laboratory	Panelist
Franceschetti, Alberto	National Renewable Energy Laboratory	Panelist
Fried, Laurence	Lawrence Livermore National Laboratory	Panelist
Galvin, Mary	Department of Energy, Basic Energy Sciences	Invited Observer
Ganesan, Venkat	The University of Texas at Austin	Panelist
Garcia, Edwin	Purdue University	Panelist
Garofalini, Stephen	Rutgers University	Panelist
Garrett, Bruce	Pacific Northwest National Laboratory	Panel Co-Lead
Garrison, Stephen	Savannah River National Laboratory	Invited Observer
Glotzer, Sharon	University of Michigan	Workshop Co-Chair
Glownia, Jim	Department of Energy, Office of Science	Invited Observer
Goldfield, Evelyn	National Science Foundation	Invited Observer
Gruzalski, Greg	Oak Ridge National Laboratory	Other
Harding, Lawrence	Argonne National Laboratory	Panelist
Harmon, Bruce	Ames Laboratory	Panelist
Harrison, Judith	U.S. Naval Academy	Panelist
Harrison, Robert	Oak Ridge National Laboratory	Panelist

Participants continued

Hase, Bill	Texas Tech University	Panelist
Hayes, Robin	Department of Energy, Basic Energy Sciences	Invited Observer
Helland, Barbara	Department of Energy, ASCR	Invited Observer
Hess, Daryl	National Science Foundation	Invited Observer
Ho, Kai Ming	Ames Laboratory / Iowa State University	Panelist
Horton, Linda	Department of Energy, Basic Energy Sciences	Invited Observer
Hrbek, Jan	Department of Energy, Basic Energy Sciences	Invited Observer
Hybertsen, Mark	Brookhaven National Laboratory	Panel Co-Lead
Iyengar, Srinivasan	Indiana University	Panelist
Jarrell, Mark	Louisiana State University	Panelist
Johannes, Michelle	Naval Research Laboratory	Panelist
Johnson, Duane	Ames Laboratory	Panelist
Kalil, Tom	White House OSTP	Plenary Speaker
Kamath, Chandrika	Lawrence Livermore National Laboratory	Panelist
Kao, Chi-Chang	National Synchrotron Light Source	Panelist
Keblinski, Pawel	Rensselaer Polytechnic Institute	Panelist
Kent, Paul	Oak Ridge National Laboratory	Panelist
Khaleel, Moe	Pacific Northwest National Laboratory	Invited Observer
Kieffer, John	University of Michigan	Panel Co-Lead
Klippenstein, Stephen	Argonne National Laboratory	Panelist
Koonin, Steve	Department of Energy	Plenary Speaker
Kozemchak, Paul	Department of Defense, DARPA	Invited Observer
Krause, Jeff	Department of Energy	Invited Observer
Kumar, Sanat	Columbia University	Panelist
Kung, Harriet	Department of Energy, Basic Energy Sciences	Plenary Speaker
Lahti, Paul	University of Massachusetts, Amherst	Panelist
Laird, Brian	University of Kansas	Panelist
Landsberg, Alexandra	Department of Energy, ASCR	Invited Observer
Lee, Steven	Department of Energy, ASCR	Invited Observer
LeSar, Richard	Iowa State University	Panel Co-Lead
Lewis, James	West Virginia University	Panelist
Li, Xiaosong	University of Washington	Panelist
Lipkowitz, Kenny	Office of Naval Research	Invited Observer
Liu, Ping	Brookhaven National Laboratory	Invited Observer
Lucchese, Robert	Texas A&M University	Panelist
Luijten, Erik	Northwestern University	Panelist
Lumsden, Mark	Oak Ridge National Laboratory	Invited Observer
Mailhiot, Christian	Lawrence Livermore National Laboratory	Panelist
Mandrus, David	University of Tennessee / ORNL	Panelist
Markowitz, Michael	Department of Energy, Basic Energy Sciences	Invited Observer
Marques, Osni	Department of Energy	Invited Observer
Martin, Richard	Los Alamos National Laboratory	Panelist
Maupin, Paul	Department of Energy, Basic Energy Sciences	Invited Observer
McCabe, Clare	Vanderbilt University	Panel Co-Lead
McIlroy, Andrew	Sandia National Laboratories	Panel Co-Lead
Messina, Paul	Argonne National Laboratory	Plenary Speaker
Metiu, Horia	University of California, Santa Barbara	Panelist
Miller, John	Department of Energy	Invited Observer
Miller, Thomas	California Institute of Technology	Panelist
Miranda, Raul	Department of Energy, Office of Science	Invited Observer
Mount, Richard	SLAC National Accelerator Laboratory	Panelist
Mryasov, Oleg	University of Alabama	Panelist
Muckerman, James	Brookhaven National Laboratory	Panelist
Najm, Habib	Sandia National Laboratories	Panelist
Neaton, Jeffrey	Lawrence Berkeley National Laboratory	Panelist
Nguyen, Van	Department of Energy, Basic Energy Sciences	Invited Observer
Ogut, Serdar	National Science Foundation	Invited Observer
Olvera de la Cruz, Monica	Northwestern University	Panelist
Ozolins, Vidvuds	University of California, Los Angeles	Panelist

Parkin, Stuart	IBM Research, Almaden	Panelist
Pederson, Mark	Department of Energy, Basic Energy Sciences	Invited Observer
Peralta, Juan	Central Michigan University	Panelist
Perine, Katie	Department of Energy	Other
Peterson, Brian	ExxonMobil Research & Engineering	Panelist
Pickett, Warren	University of California, Davis	Panel Co-Lead
Piecuch, Piotr	Michigan State University	Panelist
Polansky, Walt	Department of Energy, ASCR	Invited Observer
Powell, Cynthia	National Energy Technology Laboratory	Invited Observer
Pratt, Stephen	Argonne National Laboratory	Panelist
Rahn, Larry	Department of Energy, Basic Energy Sciences	Invited Observer
Rappe, Andy	University of Pennsylvania	Panelist
Redondo, Antonio	Los Alamos National Laboratory	Panelist
Roberto, James	Oak Ridge National Laboratory	Workshop Co-Chair
Rohlfing, Celeste	National Science Foundation	Invited Observer
Rohlfing, Eric	Department of Energy, Basic Energy Sciences	Invited Observer
Rollett, Anthony	Carnegie Mellon University	Panelist
Romine, Chuck	National Institute of Standards and Technology	Plenary Speaker
Russell, Thomas	University of Massachusetts	Panelist
Sarrao, John	Los Alamos National Laboratory	Panel Co-Lead
Schultz, David	Oak Ridge National Laboratory	Panelist
Schwartz, Andy	Department of Energy, Basic Energy Sciences	Invited Observer
Scuseria, Gustavo	Rice University	Panel Co-Lead
Sethian, James	University of California, Berkeley /LBNL	Panelist
Siepmann, Ilja	University of Minnesota	Panelist
Singer, Marvin	Department of Energy, Basic Energy Sciences	Invited Observer
Smith, Darryl	Los Alamos National Laboratory	Panelist
Stevens, Mark	Sandia National Laboratories	Panelist
Stocks, G. Malcolm	Oak Ridge National Laboratory	Panel Co-Lead
Stoller, Roger	Oak Ridge National Laboratory	Panelist
Strayer, Michael	Department of Energy, ASCR	Plenary Speaker
Studt, Felix	SLAC National Accelerator Laboratory	Invited Observer
Sumpter, Bobby	Oak Ridge National Laboratory	Panelist
Thornton, Katsuyo	University of Michigan	Panelist
Travesset, Alex	Ames Lab and Iowa State University	Panelist
van Schilfgaarde, Mark	Arizona State University	Panelist
Vashishta, Priya	University of Southern California	Panelist
Vetrano, John	Department of Energy, Basic Energy Sciences	Invited Observer
Violi, Angela	University of Michigan	Panelist
Wadia, Cyrus	White House OSTP	Invited Observer
Walker, Homer	Worcester Polytechnic Institute	Panelist
Wang, Cai-Zhuang	Ames Laboratory	Panelist
Woodward, Nick	Department of Energy, Basic Energy Sciences	Invited Observer
Xantheas, Sotiris	Pacific Northwest National Laboratory	Panelist
Yang, Chao	Lawrence Berkeley National Laboratory	Panelist
Zhu, Jane	Department of Energy, Basic Energy Sciences	Invited Observer

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