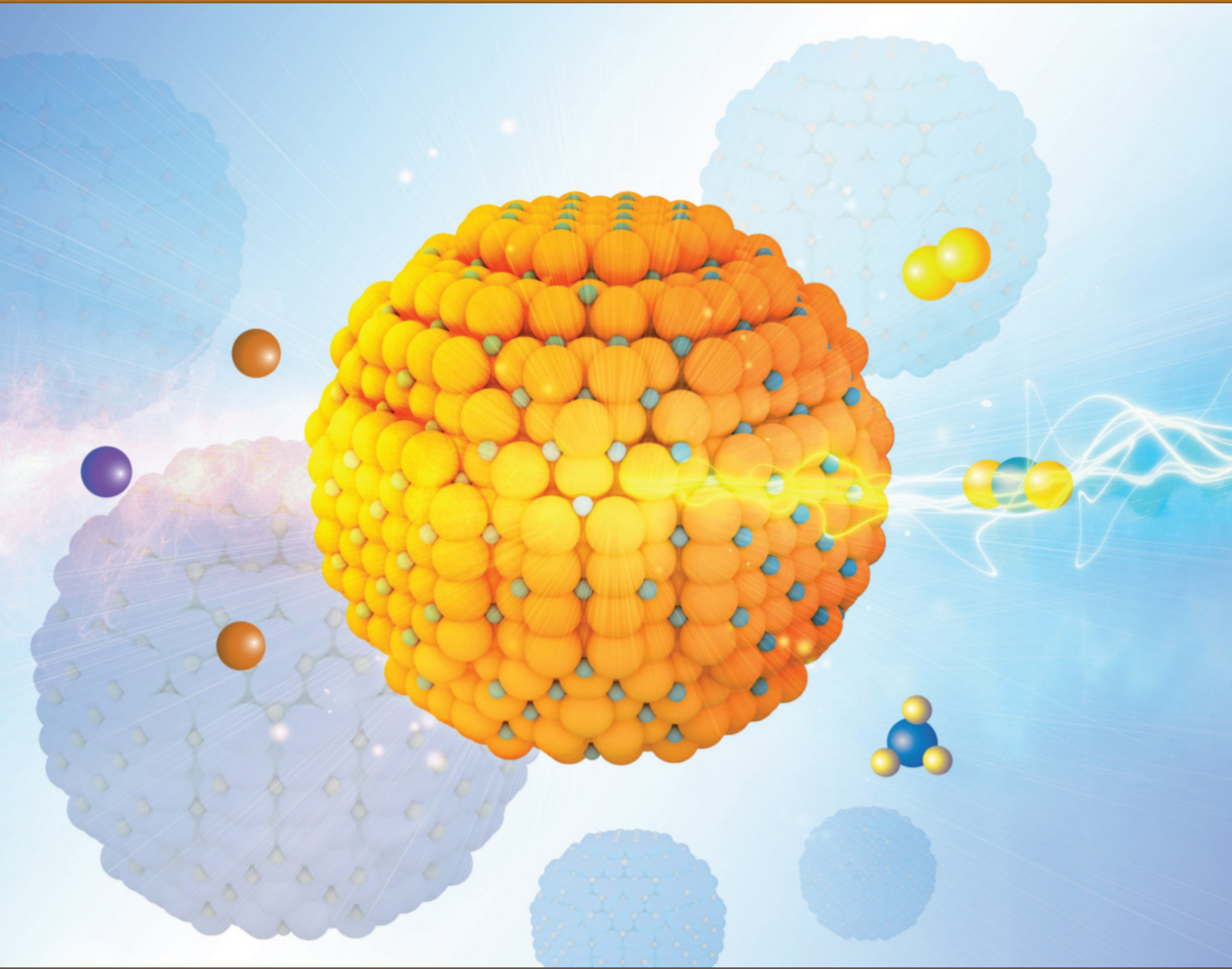
Basic Research Needs for

Transformative Experimental Tools



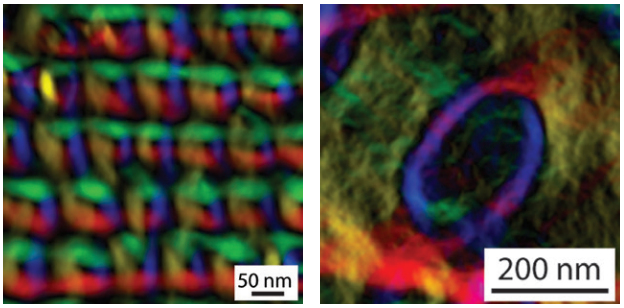
Instrumentation Science*—Driving the Invention of Novel Experimental Tools to Accelerate Scientific Discovery*

Transformative Experimental Tools—Developing new instruments to observe and manipulate matter

Scientific discoveries that expand the frontiers of human understanding and lead to technological innovation require experimental tools and methods that enable ever finer observation and manipulation of matter. The quest for deeper insight and the drive to control matter and energy at the atomic and molecular levels require increasingly powerful and sophisticated scientific instruments.

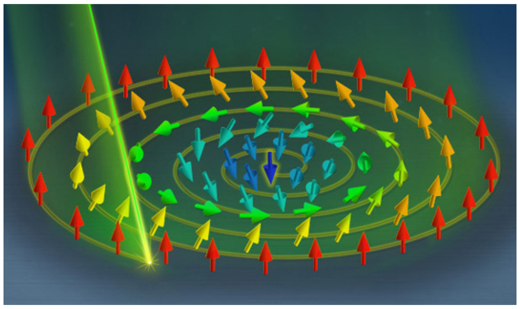
The scientific challenges ahead all point to the need for basic research involving complex materials and chemical systems, energy systems in realistic environments, and systems that are dynamic and extremely heterogeneous. Basic research provides critical insight into the fundamental processes that drive the functionality of key chemical, material, and biological systems—chemical reactions in liquids and at interfaces; correlation of charge in materials; molecular assembly and nucleation; electron solvation; ion transport; lattice, orbital, and spin dynamics; and the interactions of these processes on a variety of length scales. Typically, these processes occur far from equilibrium, meaning that the state of the system changes over time. In contrast to conventional approaches to discovery in which each experiment measures a single property of an idealized system—often near equilibrium—the new frontier in instrumentation for energy sciences is defined by innovative tools that can observe, clarify, and control complex, disordered, and hierarchical chemical and materials processes across multiple length, time, and energy scales.

A report from a Basic Research Needs workshop held in 2016 identifies four priority research directions for realizing innovative experimental capabilities needed to accelerate scientific discovery. The full report will be available at https://science.energy.gov/bes/community-resources/reports/.



Specialized transmission electron microscopy of magnetism, in combination with simulations, allows observation of skyrmion formation, behavior, and stability..

Quantum materials research is one scientific area where instrumentation breakthroughs could significantly advance the field. Harnessing the fundamental physics of emergent phenomena in quantum materials such as skyrmions requires new tools that operate over a wide range of spatial and temporal resolutions to determine how properties at near atomic scales can affect mesoscale characteristics, to understand the effects of disorder and heterogeneity, and to access and control order that emerges on different length and time scales.



A skyrmion is a topological magnetic structure with spin directions (imagine tiny North-South magnetic poles) that are twisted in an axially symmetric vortex-like geometry such that the spin arrangement is not easily perturbed. Skyrmions have potential uses in transporting information because they are tiny, stable, and easily controlled with very low electric currents.

Images courtesy of Argonne National Laboratory.

Priority Research Directions

- **Establish new frontiers in time, space, and energy resolution for characterization and control**

  Key question: *How can instrumentation break through current resolution barriers to characterize and control chemical and material systems at the finest time, length, and energy scales?*

  To examine the complexity of matter and chemical transformations, it is necessary to invent new instruments and methods that break through the resolution limits of the current state of the art. There is a need for probes with high discrimination to precisely target local phenomena occurring within complex environments, and for noninvasive, nondestructive methods. These capabilities will enable detailed characterization, ultimately leading to exquisite control of processes with unprecedented spatial and temporal precision.

- **Create innovative experimental methods for investigating "real-world" systems**

  Key question: *What revolutionary new approaches are needed to provide insights into materials synthesis and complex chemical transformations of functioning systems in real-world environments that go beyond the use of model systems in idealized environments?*

  Novel methods and instruments are needed to advance our knowledge of fundamental processes in real-world systems. These tools, operating at conditions as close as possible to those of functioning materials and chemical systems—e.g., extreme pressures, temperatures, and chemical environments—will provide fundamental insight into the processes that control synthesis and the complex chemical transformations found in real systems.

- **Simultaneously interrogate form and function, bridging time, length, and energy scales**

  Key question: *How can methods be integrated to simultaneously interrogate a material or chemical system to understand, control, and correlate collective behavior and properties across the relevant time, length, and energy scales?*

  Full understanding and control of complex heterogeneous materials and chemical systems requires experimental approaches that combine and integrate complementary tools to simultaneously characterize the most critical properties. Multiple tools must be integrated into multimodal platforms that bridge spatial and temporal scales to reveal how underlying atomic, molecular, and nanoscale processes of a functioning system collectively control its macroscopic behavior.

- **Drive a new paradigm for instrumentation design through integration of experiment, theory, and computation**

  Key question: *How can computational modeling/theory be integrated in the design of an experiment or new instrument to optimize measurements and enable physical insights not previously attainable?*

  Integrating experimentation with computational modeling and theory at the outset of the design of an experiment or the development of a new instrument will provide entirely new platforms that enable researchers to extract salient physical insights not previously attainable. Such an approach has the potential to greatly accelerate materials and chemical discovery, paving the way to next-generation energy technologies that exploit new understanding of fundamental materials and chemical processes.

Summary

A secure energy future requires technologies that use existing resources more efficiently, harness renewable resources, and efficiently store energy. The urgent demand for new energy technologies makes it essential to decipher the complexity found at the core of chemical and materials processes. Historically, novel experimental tools and methods have been foundational in scientific and technological advances—ranging from high-resolution microscopes that "see" atomic structures, to lithography that has enabled advances in semiconductors and computing. Expanding the frontiers of basic research requires new generations of instrumentation to reveal the intricacies of complex materials and chemical systems; energy systems in realistic working environments; and systems that are dynamic, far from equilibrium, and extremely heterogeneous.

The identified priority research directions aim to drive innovation in instrumentation science that will provide cutting-edge capabilities necessary for new insights into complex energy systems and control of matter and energy at the atomic and molecular levels. The availability of these tools will be a game changer across many fields of energy-related scientific research, enabling new scientific breakthroughs and transformative technologies to address the energy challenges of the 21st century.

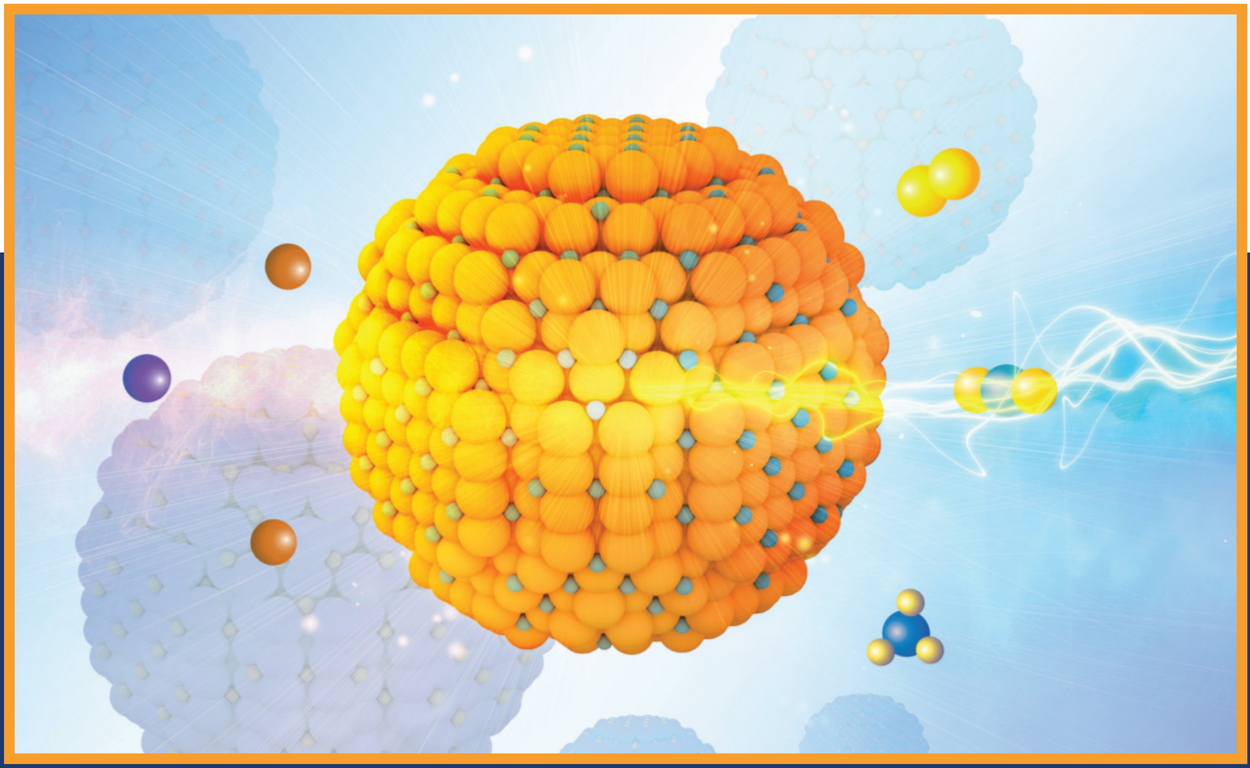


Image courtesy of Lawrence Berkeley National Laboratory.

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