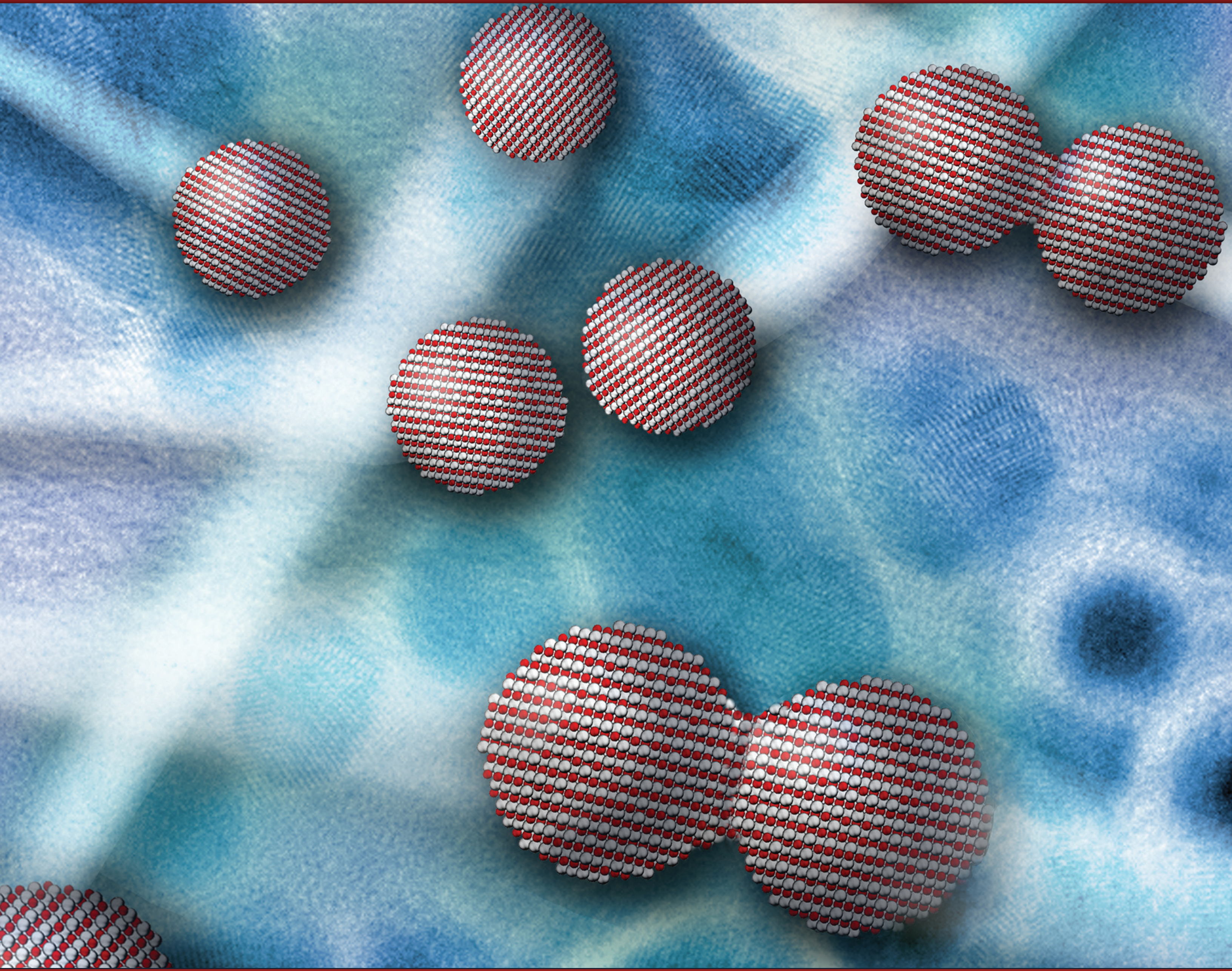
Basic Research Needs for

Synthesis Science



***Synthesis Science**—Research to Enable Transformative Discoveries and Innovation for Energy*

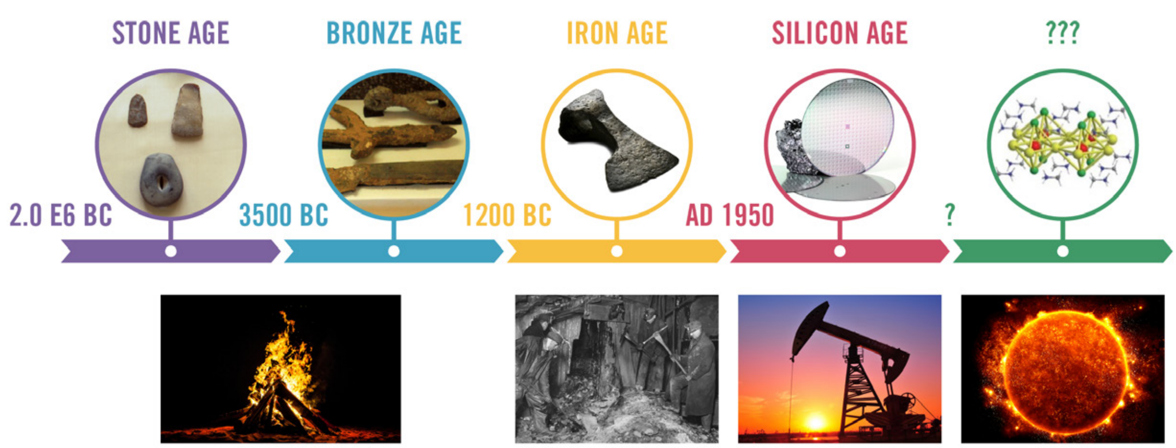
Synthesis Science—Understanding how to produce matter that does what we want it to do…

The technology at our fingertips becomes more powerful each day. Smartphones are handheld computers, cameras, music players, boarding passes, and sometimes phones. Cars are ever more fuel-efficient, safer and loaded with computing power. LED lighting and solar panels are becoming common worldwide. None of these advances would have been possible without the capability to discover, develop, and create new materials and chemical processes.

If the only limit to synthesizing new forms of matter were the imagination of scientists, then assemblies of atoms and molecules with unparalleled new architectures and capabilities would be possible—catalysts that turn garbage into fuels, solar cells to power buildings directly from sunlight, batteries with the energy density of gasoline, and materials that transport charge hundreds of times faster than silicon.

However, to bring about this future, advances in synthesis science are required in addition to imagination: researchers not only must know how to design new molecules and materials with desired functions and properties—they also must be able to make them. Doing so requires a sea change in thinking about the science of synthesis. Chemical and materials sciences have traditionally focused on predicting *where* atoms should be placed to achieve a targeted property or process. We need now a predictive science of synthesis—understanding *how* to get the atoms where they need to go to achieve desired structures.

A report from a Basic Research Needs workshop held in 2016 identifies four priority research directions for realizing this vision of predictive, science-directed synthesis. The full report can be downloaded from https://science.energy.gov/bes/community-resources/reports/.



The manipulation of materials has been the engine of human advancement. Stages along the march of civilization are named for the materials on which humans in succeeding eras depended: stone, bronze, iron, and on to silicon, which underlies the emergence of the Information Age. The ascent of civilization from one material to the next has been the result not of crisis but of opportunity. Humanity now has the opportunity to transition to a new energy economy as the synthesis of new materials enables new energy technologies.

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Priority Research Directions

- **Achieve mechanistic control of synthesis to access new states of matter**

  Key questions: *How can we develop a fundamental understanding of the processes by which reactants assemble into products and how they can be controlled? How can we use metastable ordered phases that are formed during synthesis but subsequently dissolve or transform before equilibrium is reached?*

  Opportunities for synthesizing new materials are almost limitless if prior experience and examples are combined with new theoretical, computational, and experimental tools to tease out specific molecular structures with targeted properties. Harnessing the rulebook that atoms and molecules use to self-assemble will accelerate the discovery and creation of new materials.

- **Accelerate materials discovery by exploiting extreme conditions, complex chemistries and molecules, and interfacial systems**

  Key questions: *Materials discovery is crucial for progress in science and technology, but how will the new materials of the future be created? And where should we look for them?*

  Many future discoveries will come from extreme conditions of high fluxes, fields, and forces; complex chemistries and heterogeneous structures; and the high-information content made possible by sequence-defined macromolecules such as DNA to create complex forms of matter.

- **Harness the complex functionality of hierarchical matter**

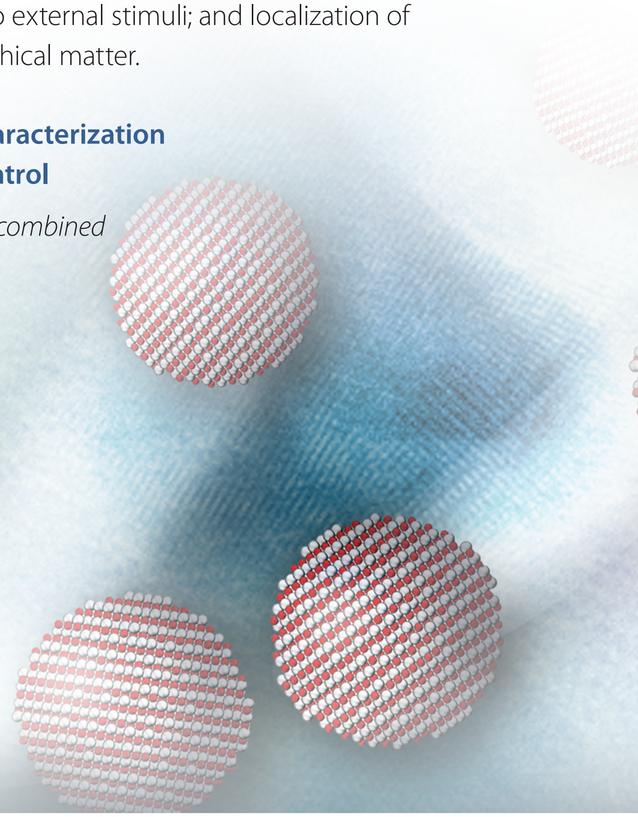
  Key question: *How can synthesis access multiscale structures to produce desired novel functionality?*

  Hierarchical matter exploits the coupling among different types of atomic assemblies across multiple length scales. These interactions lead to emergent properties not possible in homogeneous materials. Dramatic advances in energy production, storage, and use will result from control over the transport of charge, mass, and spin; assembly and reconfiguration in response to external stimuli; and localization of sequential and parallel chemical reactions made possible by hierarchical matter.

- **Integrate emerging theoretical, computational, and in situ characterization tools to achieve directed synthesis with real time adaptive control**

  Key question: *How can characterization, theory, and computation be combined to make the leap from predictive understanding of existing materials to predictive control enabling radically new molecules and materials?*

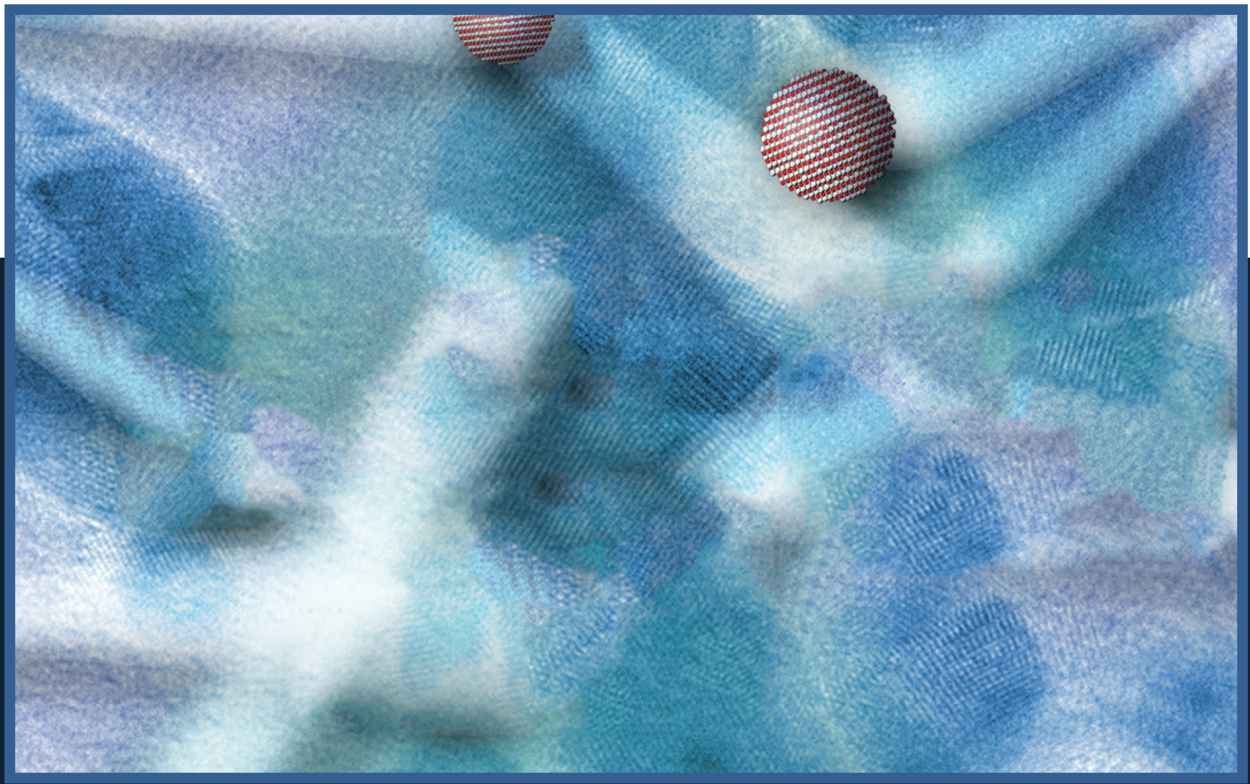
  Theory, computation, and characterization are critical components of the discovery and design of new molecules and materials. It is essential to know and predict how materials assemble, and how the assembly affects final material properties. Combining in situ probes with theory and modeling to guide synthesis in real time, and then directing synthesis through adaptive control to accommodate system variations, will dramatically reduce time and energy requirements for materials development.



Summary

Future energy technologies depend upon advances in the science of synthesis. The historical impact of chemistry and materials sciences on society makes the case for developing an approach to materials design and creation that can quickly predict and discover new molecules and materials and master their synthesis to rapidly deploy new technologies. Future energy technologies depend upon advances in the science of synthesis. Conversion of sunlight to fuel, energy storage breakthroughs, low-temperature catalysis, efficient separation of rare-earth and precious metals, water purification, superconducting materials for the smart electric grid, lightweight vehicles—all of these require new high-performance materials. To make those materials a reality we must develop synthesis processes that build on our knowledge of physical and chemical principles and our ability to establish conceptual designs.

The priority research directions identified hold the promise of enabling discovery and synthesis of these new molecules and materials on demand by realizing the ability to link *predictive design* to *predictive synthesis*—coupling the ability to define where the atoms need to be placed *to achieve the desired function* with the capability to get them where they need to go *to achieve the targeted structure*.



Images courtesy of Pacific Northwest National Laboratory; Artwork by Zina Deretsky (http://www.zina-studio.com).

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