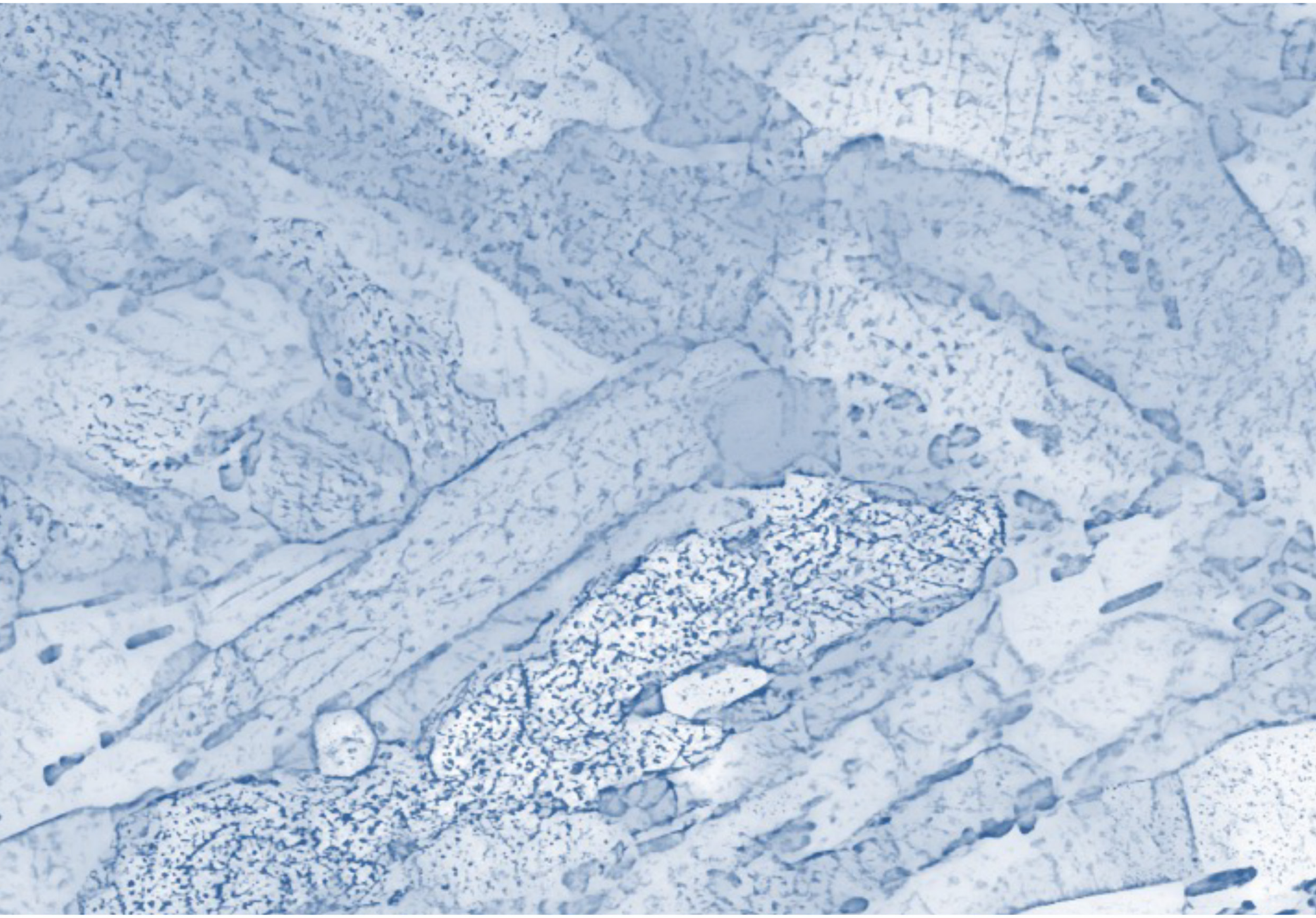
Basic Energy Sciences Roundtable

Foundational Science to Accelerate Nuclear Energy Innovation



Scientific Breakthroughs to Realize the Full Potential of Nuclear Energy

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Energy security, availability, and reliability are among the greatest challenges facing the nation and the planet. An abundant potential source of energy resides in the fundamental atomic building blocks of the universe in the form of the nuclear reactions of fission and fusion. In fact, energy from nuclear fission currently provides the majority of the world's zero-carbon electricity, and future fusion energy systems offer great promise; carbon-free nuclear energy technologies can be key to the world's decarbonized energy future. While contemporary fission systems use well-established technologies to supply safe and efficient baseload power, they could be more fuel efficient and less costly. Moving beyond massive light-water fission reactors to a variety of advanced nuclear systems, varying in size and operating in extremes of temperature, corrosivity, and other parameters, will place stringent conditions on materials and chemical systems. New demands will be made of the coolants and solvents, the materials, and the monitoring tools used in these reactors. Fusion-based nuclear energy will require superior materials to withstand extremely high temperatures, plasma exposure, radiation damage, and implanted gases. The advantages associated with these new fission and fusion technologies will only be realized through continued advancements in the fundamental science underpinning our knowledge of the physics and chemistry of nuclear systems through improved experimental and computational methods.

In July 2022, the U.S. Department of Energy's (DOE) Office of Basic Energy Sciences (BES)—in coordination with DOE's Offices of Nuclear Energy, Fusion Energy Sciences, and Advanced Scientific Computing Research—held a virtual roundtable titled "Foundational Science to Accelerate Nuclear Energy Innovation" to discuss the scientific and technical barriers for advanced nuclear energy systems. Five priority research opportunities were identified to address these scientific and technical challenges and to accelerate progress toward the realization of next-generation fusion and fission energy systems.

This brochure, a technology status document developed for the roundtable, and the full report will be posted at: https://science.osti.gov/bes/Community-Resources/Reports.

Priority Research Opportunities

- **Master complex electronic structures to tailor thermochemical reactivity, transport, and microstructural evolution**

  Key question: *How do we elucidate, predict, and harness coupled electron-ion dynamics to enable discovery and deployment of novel materials, coolants, and solvents for future fission and fusion energy?*

  Chemical and materials phenomena in nuclear systems have historically been described through atomic and molecular interactions, with limited consideration of sub-atomic electron structures. However, electronic interactions fundamentally govern the nature and energy of bonding, transport, defect energies, and phase stability of solids and liquids. Bridging quantum physical considerations from electron-ion and electron-electron interactions to bulk phenomena like mass transport and mesoscale restructuring is necessary to understand evolution of matter in nuclear environments and to predict phase dynamics and thermophysical properties of liquids and solids in nuclear systems. Harnessing these interactions will subsequently enable tuning of materials and chemical performance under coupled extremes.

- **Interrogate and direct the physics and chemistry underpinning next-generation coolants and solvents**

  Key question: *How can we probe and control the physics and chemistry of coolants, solvents, and their solutions in the harsh environments associated with nuclear energy?*

Advanced nuclear technologies will require the deployment of next-generation coolants and solvents. Ionic and organic liquids, molten metals and salts, and gases display fundamentally divergent properties from aqueous solutions, challenging currently established paradigms in actinide and radiation chemistry. It is critical to understand how differences in the fundamental physical and chemical properties of these coolants and solvents influence their behavior under extreme conditions. Mastering these behaviors also requires the ability to dynamically characterize and manipulate the chemistry of solutes, including actinides, fission and corrosion products, and process molecules.

- **Elucidate and control the underlying physics and chemistry of interfaces in complex nuclear environments**

  Key question: *How do we harness dynamic interfaces to tailor robust materials and processes for next-generation nuclear reactors?*

  Interfaces play a fundamental role in many innovative energy technologies. However, for nuclear energy applications, long-standing research challenges remain and must be overcome to harness the power of interfacial processes. Understanding interfacial properties associated with radiation effects in materials, radiolytic effects in coolants and solvents, plasma-materials interfaces in fusion reactors, and liquid-liquid interfaces in molten salts or liquid metals is essential to predict and mitigate degradation of materials for fission and fusion reactors. Ultimately, the design of new types of compositionally diverse and dynamically evolving interfaces is needed to enable and control the processes occurring in extreme environments.

- **Bridge multi-fidelity multi-resolution experiments, computational modeling, and data science to control dynamic behavior**

  Key question: *Which novel techniques can be coupled to provide operando and in situ measurements to better understand and control dynamical properties, behaviors, and processes for extreme nuclear energy environments?*

  The dynamic evolution of nuclear material systems is intrinsically multiscale. While the creation of radiation damage occurs over picoseconds, subsequent interactions occur over much longer times and lead to microstructural changes over multiple length scales. Similarly, the chemistry of molten salts, solvents, and coolants evolves following complex reaction networks whose elementary steps are realized over vastly different time scales. Clearly, the overall dynamical evolution of complex nuclear systems cannot be captured by isolated experimental probes and modeling approaches that only capture narrow time- and length-scales. Instead, a complete picture can only be painted by correlating and fusing multiple sources of operando experimental and modeling data, simultaneously characterizing the real-time evolution of a target system.

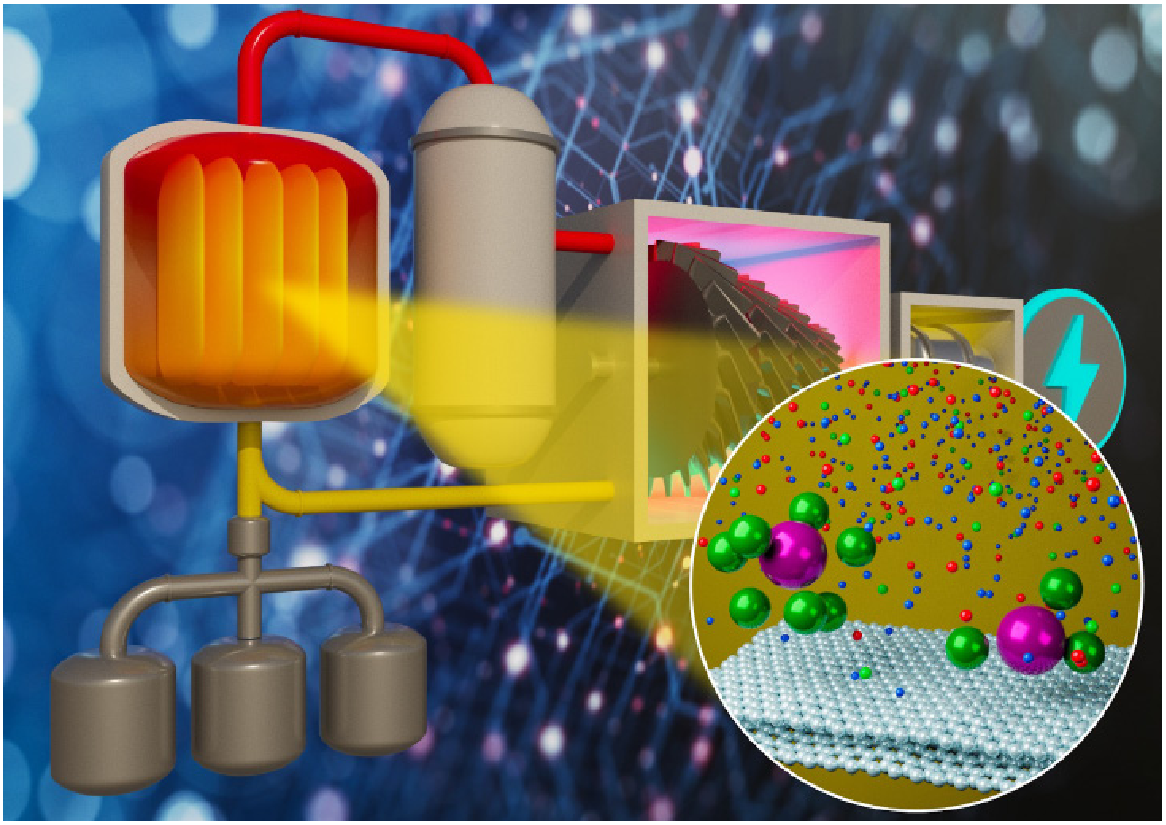
- **Harness artificial intelligence to design inherently resilient condensed phases**

  Key question: *What defines self-resilient mechanisms and how can they be discovered in nuclear materials and chemical systems in coupled extreme environments?*

  A critical factor in the deployment of advanced nuclear reactors is the development of materials and coolants that are resilient against aggressive environments. However, the discovery, improvement, and assessment of materials resistant to extreme environments is complex and costly. Bottom-up multiscale modeling frameworks offer the promise to aid experimental exploration of new materials. Unfortunately, such scale-bridging is plagued by uncertainty propagation across scales and can only incorporate known physics, preventing the effective use of computational approaches for the discovery of novel materials. Breaking this conundrum necessitates the development and use of pioneering predictive methods enabled by data from high-throughput experiments coupled with machine learning and artificial intelligence.

Summary

The foundational science gaps inhibiting the advancement of nuclear energy technologies are identified and tackled in five priority research opportunities. These opportunities pave the way to accelerate the development and ultimately the adoption of new nuclear energy systems. They include the fundamental aspects of ion-electron interactions; novel properties of next-generation coolants and solvents; interfacial dynamics, not only in solids, but in other aspects of nuclear reactors; novel operando and in situ monitoring and sensing; and artificial intelligence to accelerate condensed phases discovery. Building on the foundation established by previous BES workshops, these opportunities encompass recent advances in fundamental knowledge and focus on the experimental and computational methods needed to resolve major technical challenges for nuclear energy technologies. Through developing fundamental scientific insight as well as pushing the frontiers of modeling complex systems and probing the operation of materials and chemical systems in extreme environments, research motivated by the priorities identified here will further develop the promise, potential, and utilization of nuclear energy for a clean energy future.



Nuclear energy systems, which harness the enormous energy stored in atomic nuclei, host complex, extreme environments resulting in significant changes in chemical and material components. Intense cascades of events at the atomic scale in solids, liquids, and gases are manifested on macroscopic time and length scales and impact their performance.

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