

MAJOR INITIATIVE DESCRIPTIONS

▪ **Artificial intelligence (AI) for science**

Topics include deep learning and scalable data analytics for scientific workflows, algorithms, software, and applications for the beyond-Moore era (quantum and neuromorphic), and integration of advanced computing across Argonne. This area also focuses on the opportunity to apply AI methods to both fundamental and applied problems. Emphasis is placed on the combination of high-throughput experimental and computational methods with new computational architectures to enhance the potential for AI-guided science breakthroughs using massive data sets.

▪ **Autonomous discovery**

This area focuses on scientific problems that can be solved by accelerating discovery through the application of AI models to drive the design of experiments. This area is seeking to answer fundamental problems through successive iterations of experimental data generation and AI model improvement. Emphasis is placed on laboratory automation, programming abstractions for laboratory protocol development, and AI methods that crosscut scientific domains, including those associated with active learning.

▪ **Circular economy**

Topics addressed in this focus area include autonomous design of recyclable polymers; development of pathways for waste management and recovery of critical materials from battery, e-waste, and permanent magnets; advance supply chain research and life-cycle analysis; and establishment of design principles for carbon management with a focus on new materials and processes for carbon capture, conversion, and temporal sequestration.

▪ **Climate action**

This area has a two-part focus: AI to advance predictive understanding of climate risks impacts and decision science to help to empower communities and businesses to build long-term resilience to local impacts. Topics include development of AI and machine learning (ML) methods for high-resolution, built-for-purpose climate models, scale- and process-relevant observation, and AI/ML-driven translation of local climate predictions into actionable adaptations.

▪ **Coherent X-ray science**

- **Accelerator research and development**

This area supports seed research for future accelerator-based X-ray source concepts and enabling accelerator technology that can expand the scientific capabilities of existing and future sources. This includes concepts for compact hard X-ray free electron lasers, high-gradient acceleration, novel permanent magnet and superconducting undulators, and ultralow-emittance electron sources.

- **Hard X-ray sciences**

Topics in this focus area address development of innovative X-ray techniques and approaches to transform our understanding of material, chemical, and biological processes. The focus includes application of high-performance computing and AI/ML approaches to data analysis and experiment control, enabling new science at the APS and novel X-ray techniques that will translate the promise of the upgraded APS into some of

the first scientific results on the future beamlines. Research and development of new beamline enhancements will also be supported.

- ***Deep decarbonization***

This area addresses two broad topics. The first is low- or zero-carbon energy carriers, with a focus on developing capabilities to characterize the use of such energy carriers and advancing technologies for manufacturing them. The second is identification and advancement of new routes for decarbonized production of metals and chemicals, with a focus on developing new chemistries, identifying process conditions that can tolerate intermittent energy supplies, identifying methods for integrating decarbonized energy sources, developing materials that can withstand the high temperatures and corrosive environments required for generating process heat from low-carbon sources, and developing materials for thermal energy storage.

- ***Imaging and detection of signatures***

This area focuses on advancing the science of sensing, detection, and imaging of signatures to enable scientific discoveries and translate those discoveries to benefit U.S. national security. Topics include expanding the portfolio of detectors and sensors for nuclear and particle physics research; supporting fundamental research in quantum sensing and imaging and translating those discoveries into sensors and detectors for national security missions; establishing “end-to-end” capabilities to accelerate the development of sensors and detectors for multiple missions; and AI/ML-driven prediction, development, and analysis of novel chemical, biological, and nuclear signatures and advanced detection methods and technologies. For the national security portion of this initiative only, the selected candidate will be required to obtain and maintain a clearance and must be a U.S. citizen. Please see <http://www.state.gov/m/ds/clearances/c10978.htm> for more information about requirements for obtaining a security clearance process.

- ***Radioisotope discovery***

This area focuses on novel methods to enable production of isotopes that are presently in short supply but needed for a variety of research and applications. The emphasis is on radioisotopes useful for nuclear medicine. This includes development of new approaches for challenging aspects of radioisotope production, advanced targetry to compensate for high-power-density deposition in targets, radiochemical separation and purification, and generation and analysis of nuclear data. Also of interest are concepts that incorporate AI/ML and robotic technologies.