LEWIS–BURKE ASSOCIATES LLC

Agency Update: Outlook on Major Department of Energy Research and Funding Initiatives

Lewis-Burke Associates LLC – March 2, 2020

The Department of Energy (DOE) Office of Science is making major investments in new research initiatives. Some of these research initiatives are tied to the Trump Administration's research and development priorities in the Industries of the Future, such as Artificial Intelligence and Quantum Information Science, while others are unique to meeting DOE missions, such as critical materials for energy applications and revolutionizing polymer upcycling. This analysis provides advance intelligence on future funding and research priorities for each major research initiative in the Office of Science.

The Office of Science currently has 13 major research initiatives. Seven were launched several years ago while six are proposed as new initiatives for fiscal year (FY) 2021. While Congress will ultimately decide final funding levels for these major initiatives through the FY 2021 appropriations process, which recently started in February 2020, the table below lists the major initiatives, proposed funding levels in FY 2021, and a comparison to prior years.

DOE Office of Science FY 2021 Research Priorities
(funding in millions)

	FY 2019 Enacted	FY 2020 Enacted	FY 2021 Request	FY 2021 Request vs. FY 2020 Enacted
Ongoing Research Initiatives				
Artificial Intelligence and Machine Learning	22	71	125	+54 (76%)
Quantum Information Science	125	197	237	+40 (20%)
Next-Generation Microelectronics	4	5	45	+40 (800%)
Exascale Computing Initiative	514	505	475	-30 (6%)
Biosecurity	4	20	25	+5 (25%)
DOE Isotope Science and Production		3	17	+14 (467%)
U.S. Fusion Program Acceleration	2	4	5	+1 (25%)
New Research Initiatives				
Next Generation Biology Initiative			9	--
Rare Earth/Separations Science			25	--
Revolutionizing Polymer Upcycling			14	--
Strategic Accelerator Technology			13	--
Integrated Computational and Data Infrastructure for Scientific Discovery			12	--
Data and Computational Collaboration with NIH			1	--
Total	**667**	**832**	**1,003**	**+171 (21%)**

In FY 2020, the Office of Science dedicated 12 percent of its total budget and 33 percent of its research budget to these initiatives. In FY 2021, these research initiatives are expected to make up 14 percent of the Office of Science's total budget and approximately 40 percent of its research budget. Below is more detailed information on each major research initiative.

Artificial Intelligence and Machine Learning (AI/ML)

The Office of Science plans to grow AI and ML research across all six major programs. Investments will range from applied mathematics to understand the robustness and reliability of AI and ML systems, to automating the data collection and control of large-scale user facilities. Some major new investments are likely to include:

- $24 million in applied mathematics and computer science to expand scientific AI/ML techniques and better leverage data intensive science. Many current machine learning methods lack mathematical approaches to provide robustness, reliability, and transparency and require better domain knowledge to be effectively applied. In addition, better AI/ML applications and tools are needed to extract insights from massive scientific datasets across the Office of Science programs. To address these challenges, the Office of Science will focus investments in areas unique to science such as the transparency and interpretability of AI/ML, uncertainty quantification, and the computer science and software infrastructure for AI/ML applications, including tools for data management.
- $10 million to support additional AI methods and ML tools to accelerate the discovery of new materials and chemistries with unique properties and functions for energy applications.
- $13 million to support additional AI/ML efforts in high energy physics to help manage increasingly high volumes and complexity of experimental and simulated data across experimental frontiers.
- $10 million to help improve the efficiency and operations of scientific user facilities, such as light sources and neutron sources, using AI/ML tools.

Quantum Information Science

Close to $200 million in funding is dedicated to continue funding prior awards in fundamental research in quantum information science across the six major programs as well as new National Quantum Centers, which will be awarded in Summer 2020. The only major new investment of about $30 million will be in supporting early stage research associated with establishing the nation's first dedicated Quantum Network which would link together the DOE national laboratories. Specifically, basic research would focus on quantum information networks and the opportunities and challenges of transporting and storing quantum information over interconnects and networks.

Next Generation Microelectronics

The Office of Science plans to launch a new multi-disciplinary microelectronics research effort. Based on feedback from the Microelectronics Research Request for Information and the research priorities in the Basic Research Needs for Microelectronics report, the Office of Science plans to invest an additional $40 million in FY 2021 in several key areas: materials, chemistry, and device physics; component integration, architecture, and algorithms; and next-generation tools for synthesis, fabrication, and characterization of devices and systems. The Office of Science is considering center-level mechanisms to develop co-

design opportunities in which materials, chemistries, devices, systems, architectures, algorithms, and software are developed in a closely integrated fashion. A major motivation in new microelectronics technologies is the looming end of Moore's Law and the ability to drive major new innovations in microchip design and functionality. New architectures and designs are needed to maintain U.S. leadership in strategic computing.

Exascale Computing Initiative

This is the only major research initiative which would see a decrease in funding in FY 2021 but is consistent with prior plans. Funding for this initiative is tied to the development and deployment of the first exascale computing systems which will come online starting in 2021. Funding for this initiative is shifting primarily to new investments in AI/ML. The only major funding call under this initiative in FY 2021 will be to recompete computational chemical sciences research centers. The goal is to establish publicly accessible databases and open source computational codes to improve the predictive capability of chemical systems and accelerate chemical research in the U.S.

Biosecurity

This initiative is currently focused at the national laboratories. The goal is to use secure gene-editing techniques while advancing the redesign and optimization of plant and microbial pathways to produce fuels and higher value chemicals and bioproducts. In FY 2021, DOE plans to expand efforts such as developing fail-safe genome engineering, genome remodeling to control the persistence of engineered functions in soil microbes, and securing genomes against the CRISPR/CAS9 gene-editing tool.

DOE Isotope Science and Production

The goal of this initiative is to expand isotope production and processing sites to meet U.S. demand for isotopes in short supply. Specifically, increased funding in this initiative is to grow capabilities in stable isotope enrichment technologies beyond the current electromagnetic ion separation and gas centrifuge technologies to improve efficiencies in isotope production. Funding would also be directed at competitive research and development grants at research universities and national laboratories to support efforts to make novel and critical isotopes to support research and other applications, as well as expand the University Isotope Network to support research and development to enable routine production of needed isotopes.

U.S Fusion Program Acceleration

The main focus of this initiative is to support a newly established Innovation Network for Fusion Energy Program (INFUSE). This program provides private-sector fusion companies with access to the expertise and facilities of DOE's national laboratories to overcome critical scientific and technological hurdles in pursuing development of fusion energy systems. Initiated in FY 2019, this private-public research partnership program, the first of its kind for the Office of Science, is modeled after the Gateway for Accelerated Innovation in Nuclear (GAIN) Nuclear Energy Voucher program. The INFUSE program does not provide funding directly to private companies, but instead provides support to the national laboratories to help them collaborate and work with industrial partners. INFUSE's primary areas of support include the development of fusion technologies, such as new and improved magnets; materials science, including engineered materials, testing and qualification; plasma diagnostic development; modeling and simulation; and access to magnetic fusion experimental capabilities. In FY 2021, DOE also

is requesting $1 million to begin a study on the design and requirements of a future fusion facility in the U.S.

Next Generation Biology Initiative

The goal of this initiative is to leverage discoveries and approaches across the biological, physical, and computational sciences to develop bio-inspired, biohybrid, and biomimetic systems. Areas of focus are likely to include neuromorphic computing, programmable biomaterials and biocatalysts, and next-generation tools for characterization of chemical, biological, biomaterial, and biohybrid systems. About $5 million will be available in FY 2021 to support research in the biosciences to design bio-inspired, biohybrid, and biomimetic energy systems with desired functions and properties. For example, research may target the molecular-level mechanisms nature uses to control complex chemical conversions, including error-correcting and defect-managing mechanisms.

Rare Earth and Separations Science

This research initiative is tied to a broader cross-agency Critical Minerals research and development effort. Critical materials, including rare earth elements, are essential to advance energy technologies, but the U.S. does not have an abundant domestic supply and is reliant on imports from foreign countries. The Office of Science is focused on understanding fundamental properties of critical materials, identifying methodologies to reduce their use and find substitutes, and enhancing chemical processing and separation science for rare earths. In FY 2021, $20 million will be available to fund research that advances the discovery, design, and synthesis of new materials and processes that limit the use of rare earths, and separation science to enhance recovery of rare earth elements from both minerals and recycled materials. This may include advancing the predictive design of controlled molecular and material structures; understanding the interactions of solutions with interfaces, including mineral interfaces, to improve separations of rare earth elements from critical minerals and recycled materials; and designing new catalysts that limit the use of rare earths and noble metals.

Revolutionizing Polymer Upcycling

The goal of this research initiative is to increase foundational knowledge of polymer upcycling; that is, the selective deconstruction of the polymers that constitute plastics, followed by reassembly into high-value chemicals, fuels, or materials in a repeating cycle. In FY 2021, $10 million will be available to support research in chemistry and biology for chemical conversion and upcycling of polymers, design of next generation polymers and polymeric materials, and next generation tools for determining chemical and biochemical mechanisms with potential benefit for polymer upcycling.

Strategic Accelerator Technology

The goal of this initiative is to improve coordination across the Office of Science programs to allow the U.S. to develop the world's most advanced accelerator-based facilities for scientific research, and to continue to attract and train the workforce needed to design and operate these facilities. As competing accelerator-based facilities are built abroad, DOE is concerned that they are beginning to draw away scientific and technical talent. DOE is launching this new initiative to grow investments in high-risk, high-reward accelerator research and development to stay at the global forefront, and develop a world-leading workforce to build and operate future generations of facilities. There won't be a dedicated funding call, but rather investments through existing accelerator research and development programs

across the six major Office of Science programs. The areas of interest include superconducting magnet development, ultrafast laser research and development, upgrades to superconducting radiofrequency facilities, and potentially co-funding a multi-program research and development initiative in superconducting materials.

Integrated Computational and Data Infrastructure for Scientific Discovery

DOE plans to grow core investments in computer science to develop software that improves the utility of high-performance computing and advanced networks for science, and integrates these capabilities with new AI techniques, workflows, data management, analytics and visualization tools. The goal is to improve the effectiveness and efficiency of existing capabilities and near-term capabilities coming online such as exascale computers, as well as to prepare for emerging technologies such as quantum networking, specialized and heterogeneous hardware and accelerators, and quantum and neuromorphic computing.

Data and Computational Collaboration with NIH

DOE has a partnership with NIH's National Cancer Institute to make available its computational capabilities and big data analytics for precision medicine applications. In FY 2021, DOE is requesting dedicated funding to partner with NIH to expand DOE's tools and capabilities to address NIH's rapidly growing data and computational challenges. In particular, DOE would invest in data analytics and AI tools for NIH's connectome project, which is an effort to map the neural pathways that underlie human brain function.