# FINANCIAL ASSISTANCE NOTICE OF FUNDING OPPORTUNITY





# ADVANCED RESEARCH PROJECTS AGENCY – ENERGY (ARPA-E) U.S. DEPARTMENT OF ENERGY

# QUANTUM COMPUTING FOR COMPUTATIONAL CHEMISTRY (QC³)

Announcement Type: Initial Announcement
Notice of Funding Opportunity No. DE-FOA-0003482
Assistance Listing Number 81.135

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#### **BASIC INFORMATION**

KEY DATES:	
Notice of Funding Opportunity (NOFO) Issue Date:	October 24, 2024
Deadline for Concept Paper Questions to <a href="mailto:ARPA-E-CO@hq.doe.gov">ARPA-E-CO@hq.doe.gov</a> :	5 PM ET, November 11, 2024
Submission Deadline for Concept Papers:	9:30 AM ET, November 21, 2024
Anticipated Timeframe for Encourage/Discourage Notifications:	January 2025
Deadline for Full Application Questions to <a href="mailto:ARPA-E-CO@hq.doe.gov">ARPA-E-CO@hq.doe.gov</a> :	5 PM ET, TBD
Submission Deadline for Full Applications:	9:30 AM ET, TBD
Expected Reviewer Comment Release Date:	5 PM ET, TBD
Submission Deadline for Replies to Reviewer Comments:	5 PM ET, TBD
Anticipated Timeframe for Selection Notifications:	May 2025
Anticipated Timeframe for Award:	August 2025
Anticipated Period of Performance:	August 2025 – August 2028

BASIC INFORMATION:		
Total Amount to Be Awarded	Approximately \$30 million, subject to the availability of appropriated funds to be shared between NOFOs DE-FOA-0003482 and DE-FOA-0003483.	
Anticipated Number and Value of Awards	ARPA-E anticipates making approximately 5–10 awards between NOFOs DE-FOA-0003482 and DE-FOA-0003483. ARPA-E may, at its discretion, issue one, multiple, or no awards. The Federal share of awards under this NOFO may vary between \$250,000 and \$10 million.	
Agency Contact Information	<ul> <li>Questions and answers (Q&amp;As) about ARPA-E and this specific NOFO:         <a href="http://arpa-e.energy.gov/faq">http://arpa-e.energy.gov/faq</a>.</li> <li>Send other questions about the NOFO to: <a href="https://arpa-e.energy.gov/faq">ARPA-E-CO@hq.doe.gov</a>.</li> <li>Send questions about use of ARPA-E eXCHANGE to:         <a href="mailto:ExchangeHelp@hq.doe.gov">ExchangeHelp@hq.doe.gov</a>.</li> <li>Upon the issuance of a NOFO, only the Grants Officer via <a href="mailto:ARPA-E-CO@hq.doe.gov">ARPA-E-CO@hq.doe.gov</a> may communicate with Applicants. This "quiet period" remains in effect until ARPA-E's public announcement of project selections. Emails sent to other email addresses will be disregarded.</li> </ul>	

The objective of the Quantum Computing for Computational Chemistry program (QC³) is to accelerate development of algorithms for quantum computers to advance energy applications of computational chemistry and materials science. Computer simulations of chemistry and materials have been driving the cutting edge of discovery for decades. Despite massive advancements in both computer hardware and algorithms, important classes of problems remain effectively impossible to solve with conventional (classical) computers. Quantum computers offer a fundamentally new form of computing that leverages the quantum nature of matter to solve certain problems exponentially faster than classical computers. Quantum computing hardware is advancing rapidly but has yet to reach the scale where it can outperform classical computers for problems of practical value. The QC³ program seeks to apply quantum computers to high-impact problems in energy by developing new algorithms and software that achieve a scalable quantum advantage on near-term quantum hardware. Applicants to QC³ will identify a specific energy-relevant problem, develop quantum algorithms,

and run them on real quantum hardware, with the goal of improving the speed, accuracy, or some other relevant parameter by 100 times compared with the classical state-of-the-art approach. The problems chosen will have the potential to result in a cumulative energy impact of 1 quadrillion British thermal units, or a reduction of roughly 1 gigaton of carbon dioxide equivalent emissions from energy-related activities.

Questions about this NOFO? Check the Frequently Asked Questions available at <a href="https://arpa-e.energy.gov/fags">https://arpa-e.energy.gov/fags</a>. For questions that have not already been answered, email <a href="https://arpa-e.energy.gov/fags">ARPA-E exchanged</a>, email <a href="https://arpa-e.energy.gov/fags">Exchanged</a>, email <a href="https://arpa-e.energy.gov/fags">Ex

#### I. FUNDING OPPORTUNITY DESCRIPTION

# A. AGENCY OVERVIEW

The Advanced Research Projects Agency – Energy (ARPA-E), an organization within the Department of Energy (DOE), is chartered by Congress in the America COMPETES Act of 2007 (P.L. 110-69), as amended by the America COMPETES Reauthorization Act of 2010 (P.L. 111-358), as further amended by the Energy Act of 2020 (P.L. 116-260):

- "(A) to enhance the economic and energy security of the United States through the development of energy technologies that—
  - (i) reduce imports of energy from foreign sources;
  - (ii) reduce energy-related emissions, including greenhouse gases;
  - (iii) improve the energy efficiency of all economic sectors;
  - (iv) provide transformative solutions to improve the management, clean-up, and disposal of radioactive waste and spent nuclear fuel; and
  - (v) improve the resilience, reliability, and security of infrastructure to produce, deliver, and store energy; and
- (B) to ensure that the United States maintains a technological lead in developing and deploying advanced energy technologies."

ARPA-E issues this Notice of Funding Opportunity (NOFO) under its authorizing statute codified at 42 U.S.C. § 16538. The NOFO and any cooperative agreements or grants made under this NOFO are subject to 2 C.F.R. Part 200 as supplemented by 2 C.F.R. Part 910.

ARPA-E funds research on, and the development of, transformative science and technology solutions to address the energy and environmental missions of the Department. The agency focuses on technologies that can be meaningfully advanced with a modest investment over a defined period of time in order to catalyze the translation from scientific discovery to early-stage technology. For the latest news and information about ARPA-E, its programs and the research projects currently supported, see: <a href="http://arpa-e.energy.gov/">http://arpa-e.energy.gov/</a>.

ARPA-E funds transformational research. Existing energy technologies generally progress on established "learning curves" where refinements to a technology and the economies of scale that accrue as manufacturing and distribution develop drive improvements to the cost/performance metric in a gradual fashion. This continual improvement of a technology is important to its increased commercial deployment and is appropriately the focus of the private sector or the applied technology offices within DOE. In contrast, ARPA-E supports transformative research that has the potential to create fundamentally new learning curves. ARPA-E technology projects typically start with cost/performance estimates well above the level of an incumbent technology. Given the high risk inherent in these projects, many will fail to progress, but some may succeed in generating a new learning curve with a projected cost/performance metric that is significantly better than that of the incumbent technology. ARPA-E will provide support at the highest funding level only for submissions with significant

technology risk, aggressive timetables, and careful management and mitigation of the associated risks.

ARPA-E funds technology with the potential to be disruptive in the marketplace. The mere creation of a new learning curve does not ensure market penetration. Rather, the ultimate value of a technology is determined by the marketplace, and impactful technologies ultimately become disruptive – that is, they are widely adopted and displace existing technologies from the marketplace or create entirely new markets. ARPA-E understands that definitive proof of market disruption takes time, particularly for energy technologies. Therefore, ARPA-E funds the development of technologies that, if technically successful, have clear disruptive potential, e.g., by demonstrating capability for manufacturing at competitive cost and deployment at scale.

ARPA-E funds applied research and development (R&D). The Office of Management and Budget defines "applied research" as an "original investigation undertaken in order to acquire new knowledge...directed primarily towards a specific practical aim or objective" and defines "experimental development" as "creative and systematic work, drawing on knowledge gained from research and practical experience, which is directed at producing new products or processes or improving existing products or processes." Applicants interested in receiving financial assistance for basic research (defined by the Office of Management and Budget as "experimental or theoretical work undertaken primarily to acquire new knowledge of the underlying foundations of phenomena and observable facts")1 should contact the DOE's Office of Science (http://science.energy.gov/). Office of Science national scientific user facilities (http://science.energy.gov/user-facilities/) are open to all researchers, including ARPA-E Applicants and awardees. These facilities provide advanced tools of modern science including accelerators, colliders, supercomputers, light sources and neutron sources, as well as facilities for studying the nanoworld, the environment, and the atmosphere. Projects focused on earlystage R&D for the improvement of technology along defined roadmaps may be more appropriate for support through the DOE applied energy offices including: the Office of Energy Efficiency and Renewable Energy (<a href="http://www.eere.energy.gov/">http://www.eere.energy.gov/</a>), the Office of Fossil Energy and Carbon Management (https://www.energy.gov/fecm/office-fossil-energy-and-carbonmanagement), the Office of Nuclear Energy (http://www.energy.gov/ne/office-nuclear-energy), and the Office of Electricity (<a href="https://www.energy.gov/oe/office-electricity">https://www.energy.gov/oe/office-electricity</a>).

ARPA-E encourages submissions stemming from ideas that still require proof-of-concept R&D efforts as well as those for which some proof-of-concept demonstration already exists. Submissions can propose a project with the end deliverable being an extremely creative, but partial solution.

Questions about this NOFO? Check the Frequently Asked Questions available at <a href="https://arpa-e.energy.gov/faqs">https://arpa-e.energy.gov/faqs</a>. For questions that have not already been answered, email <a href="https://arpa-e.energy.gov/faqs">ARPA-E exchange email area and all area

<sup>&</sup>lt;sup>1</sup> OMB Circular A-11 (https://www.whitehouse.gov/wp-content/uploads/2018/06/a11\_web\_toc.pdf), Section 84, pg. 3.

#### B. Program Overview

The Quantum Computing for Computational Chemistry program (QC³) aims to harness the transformative power of quantum computing to accelerate energy innovation. Computation plays an essential role in modern R&D, but classical computers struggle to simulate quantum systems with the speed, scale, and accuracy necessary to advance many commercial energy applications. This program will support the R&D of scalable, generalizable quantum computing approaches to computational chemistry and materials science. These approaches will be exponentially faster than the classical computing state-of-the-art (SoA), improving speed, accuracy, or problem size by 100 times (100x). This could result in a cumulative energy impact of 1 quadrillion British thermal units (1 quad), which is equal to a reduction of roughly 1 gigaton of carbon dioxide equivalent ( $CO_2e$ ) emissions from energy-related activities.

The development of electronic digital computers sparked revolutionary advances in science. Not only did computers accelerate hand calculations, but they also created entirely new modes of computation from the Monte Carlo methods developed at Los Alamos National Lab, to computational chemistry simulations, to artificial intelligence.

Despite the power of classical (i.e., nonquantum) computational methods, many important problems—especially in chemistry and materials science—remain frustratingly out of reach. The first quantum revolution resulted in the fundamental laws that determine the behavior of atoms and molecules, but exact solutions of these laws are staggeringly difficult to calculate. As R. B. Laughlin and David Pines wrote, "[the Schrödinger Equation] cannot be solved accurately when the number of particles exceeds about 10. No [classical] computer existing, or that will ever exist, can break this barrier because it is a catastrophe of dimension."

The computational cost of exact solutions grows exponentially with the number of particles. It is precisely this difficulty that led Richard Feynman to first propose the idea of a quantum computer: If nature is fundamentally quantum, our simulations of nature should be quantum as well.<sup>3</sup>

The QC<sup>3</sup> program focuses on developing and applying quantum algorithms in key energy research areas where classical methods are insufficient. This includes the development of quantum chemistry algorithms, their translation into quantum circuits or analog programs, and rigorous validation against classical benchmarks and experiments. The goal is to validate these algorithms on a quantum computer with approximately 100 logical qubits to show scalability and practical advantages over classical computation for energy applications.<sup>4</sup>

<sup>&</sup>lt;sup>2</sup> R.B. Laughlin and David Pines, "The Theory of Everything," *Proceedings of the National Academy of Sciences* 91, no. 1 (2001): 28–31, doi.org/10.1073/pnas.97.1.28.

<sup>&</sup>lt;sup>3</sup> Richard Feynman, *The Quotable Feynman* (Princeton University Press, 2015), 76.

<sup>&</sup>lt;sup>4</sup> This program defines a logical qubit as a virtual qubit composed of many physical qubits in combination with an error correction scheme to produce an error rate lower than that of the underlying physical qubits.

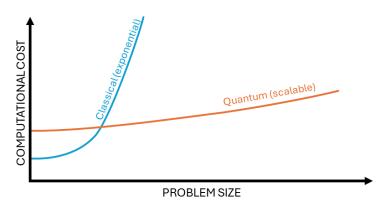
#### **Limitations of Classical Computational Chemistry Simulations**

Classical simulations generally fall into two categories: exact or scalable. Exact methods capture the complete quantum physics of nature. These methods are accurate, but their computational complexity grows exponentially with system size, giving rise to the so-called "catastrophe of dimension" (Figure 1).<sup>3</sup>

Several families of scalable methods, such as quantum Monte Carlo and Density Functional Theory (DFT) have enabled scientists to make significant strides in understanding chemical behavior and material characteristics. The scalability comes at the expense of uncontrolled approximations or limitations on types of systems that can be studied. DFT, for instance, is a powerful method that can simulate hundreds or even thousands of atoms, but the exact functional encoding electron-electron correlations is unknown. There are many materials for which DFT is simply not able to produce accurate results. Scalable classical methods are especially limited with regard to simulations of dynamics and simulations of materials with strongly correlated electrons.<sup>5</sup>

Classical methods remain powerful tools, but they are fundamentally limited, regardless of future advances in classical computing hardware. These limitations affect a wide range of problems with important energy applications central to ARPA-E's mission, including heterogeneous catalysis, photoexcitation, and high-temperature superconductivity.

#### **Potential of Quantum Computing**



**Figure 1.** Qualitative comparison of the computational cost of simulating a quantum system with a classical computer vs. a quantum computer.

Quantum computing presents a promising solution to these challenges by operating within an inherently quantum mechanical framework. Quantum algorithms offer the potential for massive improvements in performance over classical methods, providing both greater accuracy and scalability (Figure 1). In contrast to the "catastrophe of dimension" suffered by classical

<sup>&</sup>lt;sup>5</sup> Philipp Schleich et al., "Chemically Motivated Simulation Problems are Efficiently Solvable by a Quantum Computer," [preprint] *arXiv*:2401.09268 (2024), <u>arxiv.org/abs/2401.09268</u>

computers, the cost of simulating a quantum system on a quantum computer is often polynomial in problem size (Table 1).

**Table 1.** Quantum algorithms are highly scalable compared to the exponential or high-degree polynomial scaling of classical methods.

Task	Scaling of logical qubits $(N_q)$	Gate scaling
Ground state energy estimation for a molecule (Ru-CO <sub>2</sub> complexes). <sup>6</sup>	Linear in number of orbitals $(N_o)$	Toffoli gates $\sim N_o^{3.5}$
Ground state energy estimation for a material (Hubbard Model). <sup>7</sup>	Linear in number of sites $(N_s)$	Constant gate depth
First-quantized, grid-based time evolution <sup>5</sup>	For $N_p$ number of particles, $N_q{\sim}N_p\log N_p$	Linear in simulation time

A combination of developments in hardware and error correction algorithms has recently led to the first logical qubits, a critical step on the path to achieving fault-tolerant quantum computing.<sup>8</sup> In the past year, multiple quantum hardware vendors have announced roadmaps to quantum computers with more than 100 logical qubits by 2030.<sup>9</sup> These devices have the potential to unlock the first transformative energy applications of quantum computers, but the potential may not be realized without focused development of quantum algorithms for energy applications.<sup>10</sup>

#### **Optimizing the Full Quantum Computational Stack**

A key part of QC<sup>3</sup> will be optimizing the entire computational stack, which encompasses all software and hardware layers involved in quantum computing (see Figure 2 in Section I.D). Optimizing through the stack includes:

- 1. Applications: Identifying a problem important in the energy sector;
- 2. Algorithms/Software: Refining quantum algorithms and workflows, co-optimized with quantum error correction; and
- 3. Hardware: Optimizing for specific hardware.

Finally, all recipients must run their solution on real quantum hardware. The QC<sup>3</sup> program strives to push forward ARPA-E's mission by advancing, optimizing, and co-designing each of these interconnected levels in the context of some of the most urgent challenges in energy.

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<sup>&</sup>lt;sup>6</sup> Vera von Burg et al., "Quantum computing enhanced computational catalysis," *Physical Review Research* 3, no. 3 (2021): 033055, doi.org/10.1103/PhysRevResearch.3.033055

<sup>&</sup>lt;sup>7</sup> Earl T. Campbell, "Early fault-tolerant simulations of the Hubbard model," *Quantum Science and Technology* 7, no. 1 (2021): 015007, doi.org/10.1088/2058-9565/ac3110

<sup>&</sup>lt;sup>8</sup> 'Fault tolerant' here means quantum computers capable of suppressing error to arbitrarily low levels and performing long error-free calculations.

<sup>&</sup>lt;sup>9</sup> Jean-Francois Bobier et al., "The Long-Term Forecast for Quantum Computing Still Looks Bright," (Boston Consulting Group, 2024). <a href="https://docs.precedings.org/looks-bright">bcg.com/publications/2024/long-term-forecast-for-quantum-computing-still-looks-bright</a>
<sup>10</sup> Yash Sherry and Neil C. Thompson, "How Fast Do Algorithms Improve? [Point of View]," *Proceedings of the IEEE* 109, no. 11 (2021): 1768, <a href="https://doi.org/10.1109/JPROC.2021.3107219">doi.org/10.1109/JPROC.2021.3107219</a>

#### **Illustrative Application Areas**

The following use cases represent illustrative examples of key opportunity spaces where quantum computing can significantly advance ARPA-E's mission. While these areas are highlighted as examples, applicants are also encouraged to propose other innovative applications of quantum computing that align with the program's overarching goals.

- Catalysts: Catalysts are central to various industrial processes, including chemical synthesis, fuel production, and emissions reduction. By improving the understanding of reaction mechanisms and networks, new catalysts can be designed that will require less energy and produce fewer emissions.<sup>6,11,12</sup> In addition, there is a great opportunity to discover and design new catalytically active surfaces while reducing the experimental validation parameter space.
- X-ray absorption spectroscopy (XAS) for materials diagnostics: XAS can reveal details of atomic structure deep inside materials. This can lead to a better understanding of phenomena like lithiation states in battery degradation and oxidation states in fuels for advanced nuclear reactors. <sup>13, 14, 15</sup> However, classical computers struggle to generate accurate spectra for comparison to experimental data. Quantum algorithms for the analysis of XAS would enable rapid progress in the development of new energy materials. <sup>13</sup>
- Superconductors: Understanding and optimizing the properties of superconductors
  through quantum simulation could lead to the discovery of materials with higher critical
  superconductor temperatures.<sup>7</sup> Advances in this area could revolutionize transmission,
  making the power grid more efficient and significantly reducing overall energy
  consumption.
- Battery Chemistry: Quantum computing can model the complex chemical interactions in battery materials more accurately, leading to the design of batteries with longer lifespans and higher energy densities. <sup>16</sup> Quantum simulations could also accelerate the development of next-generation batteries, such as solid-state batteries, which promise to outperform current lithium-ion technology and contribute to the decarbonization of the transportation and energy sectors.

<sup>&</sup>lt;sup>11</sup> Nicole Bellonzi et al., "Feasibility of accelerating homogeneous catalyst discovery with fault-tolerant quantum computers," [preprint] *arXiv*:2406.06335 (2024) <a href="https://arxiv.org/abs/2406.06335">https://arxiv.org/abs/2406.06335</a>

<sup>&</sup>lt;sup>12</sup> Aleksei V. Ivanov et al., "Quantum computation for periodic solids in second quantization," Physical Review Research 5, no. 1 (2023): 013200, <a href="doi:oir:do

<sup>&</sup>lt;sup>13</sup> Stepan Fomichev et al., "Simulating x-ray absorption spectroscopy of battery materials on a quantum computer," [preprint] *arXiv*:2405.11015 (2024) <a href="mailto:arxiv.org/abs/2405.11015"><u>arxiv.org/abs/2405.11015</u></a>

<sup>&</sup>lt;sup>14</sup> David L. Clark, "SSRL Studies Aid Environmental Cleanup at Rocky Flats," SLAC. Los Alamos National Laboratory, May 29, 2002. <a href="www-ssrl.slac.stanford.edu/research/highlights\_archive/rockyflats.html">www-ssrl.slac.stanford.edu/research/highlights\_archive/rockyflats.html</a>

<sup>&</sup>lt;sup>15</sup> Stephen K. Wilke, et al. "Plutonium oxide melt structure and covalency." *Nature Materials* (2024): 1–6.

<sup>&</sup>lt;sup>16</sup> Isaac H. Kim et al., "Fault-tolerant resource estimate for quantum chemical simulations: Case study on Li-ion battery electrolyte molecules," *Physical Review Research* 4, no. 2 (2022): 023019, <a href="https://doi.org/10.1103/PhysRevResearch.4.023019">doi.org/10.1103/PhysRevResearch.4.023019</a>

Earth-abundant magnetic materials: Strong magnets made of rare-earth elements are
essential for efficiently transforming between electrical and mechanical energy in
applications ranging from wind turbines to electric motors..<sup>17</sup> However, these materials
are heavy, expensive, and vulnerable to supply chain risks. Quantum computers could
help design new permanent magnets made of earth-abundant materials.

# C. PROGRAM OBJECTIVES

The QC³ program aims to support the R&D of scalable quantum algorithms for chemistry and materials simulations for energy applications. The performance period will culminate in quantum simulations running on available quantum hardware showing dramatic (100x) improvement in speed or accuracy compared to the classical SoA, and a clear path to transformative impact on the energy application area of the simulation. In the event available quantum hardware is not able to outperform the classical SoA, recipients must run a quantum calculation for a smaller problem and establish that the method can scale to solve the problem of interest on quantum hardware that will be available in the near-term.

Multiple vendors have released public hardware roadmaps planning for quantum computers with 100 logical qubits coming online by 2030. However, published quantum algorithms for energy-relevant systems require hundreds to thousands of logical qubits.<sup>13</sup> This program aims to close that gap with a full-stack co-design approach, producing optimized or novel algorithms and workflows that bring energy innovation within the reach of near-term quantum hardware.

Projects under this program must complete the following program objectives:

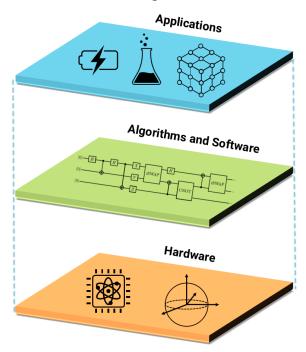
- 1. Identify a specific problem in chemistry or materials science where a quantum solution, if scalable and generalizable, can lead to cumulative quad-scale energy impact or gigaton-scale reduction in energy-related CO₂e emissions.
- 2. Develop solutions which are optimized through the full quantum computational stack (applications, software/algorithms, and hardware). The solution must have a provable ability to scale effectively as quantum hardware improves.
- 3. Have access to and validate on quantum hardware.
- 4. Complete one of the following:
  - Achieve a scalable 100x improvement over the classical SoA in speed, accuracy, problem size, or some other relevant capability on the identified energyrelevant problem; or
  - b. Prove scalability using hardware resource estimation and running smaller dimensional problems on available quantum hardware if 100x improvement cannot be realized on the identified energy-relevant problem by the end of the performance period.

Questions about this NOFO? Check the Frequently Asked Questions available at <a href="https://arpa-e.energy.gov/faqs">https://arpa-e.energy.gov/faqs</a>. For questions that have not already been answered, email <a href="https://arpa-e.energy.gov/faqs">ARPA-E.ENERGY (WITH NOFO NOTE) (WITH NOTE) (WITH NOFO NOTE) (WITH NOFO NOTE) (WITH NOFO NOTE) (WITH NOTE) (WITH NOFO NOTE) (WITH NOTE) (WI

<sup>&</sup>lt;sup>17</sup> U.S. Department of Energy, "Achieving American Leadership in the Rare Earth Magnets Supply Chain," Advanced Manufacturing Office (2022). <a href="www.energy.gov/sites/default/files/2022-02/Neodymium Magnets Supply Chain Fact Sheet Final.pdf">www.energy.gov/sites/default/files/2022-02/Neodymium Magnets Supply Chain Fact Sheet Final.pdf</a>

# D. TECHNICAL CATEGORIES OF INTEREST

It is anticipated that the program metrics will be achieved through projects that span the quantum computational stack, illustrated in Figure 2.



**Figure 2**. The quantum computational stack spans applications, algorithms/software, and hardware. Near-term quantum advantage will require optimizing through the full stack.

The stack can be divided into three general layers: applications, algorithms/software, and hardware. In the applications layer, applicants will identify problems impactful to ARPA-E's statutory goals where a new quantum computational capability would unlock progress. In the algorithms/software layer, applicants will design quantum algorithms and workflows optimized for both the specific application needs (up through the stack) and for the specific quantum hardware on which the workflow will be run (down through the stack). In the hardware layer, applicants will provide insights into the strengths and limitations of their particular hardware to enable software and hardware co-design. All recipients must execute their algorithms on real quantum hardware.

These layers are provided as a framing tool, and there will be tasks and recipients that do not map neatly onto them. For example, designing a hybrid quantum-classical workflow would fall between applications and algorithms/software. Integrating the layers is expected to be necessary for success. For example, it was recently shown that an algorithmic approach tailored to periodic materials could reduce the logical qubit cost by 2–3x and the Toffoli gate cost by 10,000x. 18 Meanwhile, many algorithms have a trade-off between circuit width (number of

<sup>&</sup>lt;sup>18</sup> Modjtaba Shokrian Zini et al., "Quantum simulation of battery materials using ionic pseudopotentials," *Quantum* 7, (2023): 1049, <a href="doi:org/10.22331/q-2023-07-10-1049">doi:org/10.22331/q-2023-07-10-1049</a>

logical qubits) and circuit depth (number of gates); the optimal balance will depend upon the capabilities of the available hardware.<sup>6</sup> A full-stack approach that finds a 2–3x improvement in each layer will plausibly realize the 10x reduction in quantum hardware resources necessary to achieve quantum advantage on near-term hardware with roughly 100 logical qubits.

The layers of the stack are described, and layer-specific objectives are defined, in more detail below. The following example deliverables are representative examples for selected QC<sup>3</sup> projects. Project-specific milestones and deliverables will be negotiated prior to award. Successful teams will need to have expertise at each layer of the stack:

1. **Application Definition:** Identify an energy application where quantum computing can have a transformational impact. Define the classical SoA and its limitations and specify how the quantum calculation fits into a broader R&D workflow.

<u>Example Deliverable</u>: An energy application, with a detailed explanation of how the specific calculations chosen will enable transformational impact over SoA.

#### 2. Algorithms and Software:

- a. Algorithm Development: Develop and optimize quantum algorithms tailored to specific energy-related applications, ensuring their scalability and efficiency. <u>Example Deliverable</u>: A set of optimized quantum algorithms, proven to be scalable, with performance metrics establishing their applicability to energy-related challenges as defined in Section I.E, such as catalysis design, battery chemistry, or carbon capture.
- b. **Quantum Circuit Implementation**: Convert high-level quantum algorithms into quantum circuits or analog programs optimized for execution on specific quantum hardware. <sup>19</sup> This includes considering the performance and error-correction capabilities of the available quantum systems.

<u>Example Deliverable</u>: Fully functional quantum circuits ready for deployment on quantum hardware, with detailed documentation on their performance, error rates, and implementation efficiency.

3. **Hardware Embedding and Optimization**: Adapt algorithms for specific quantum hardware, incorporating error correction and noise mitigation strategies to maximize performance and reliability.

<u>Example Deliverable</u>: Optimizations and co-design for specific hardware platforms, including error correction techniques and their effectiveness in achieving reliable computation on near-term quantum computers.

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<sup>&</sup>lt;sup>19</sup> A quantum circuit is a sequence of logic gates and measurements which executes a quantum algorithm. It does not include the hardware.

In addition to innovating through the quantum computational stack, recipients will pursue the following cross-cutting objectives:

 Scalability and Performance Analysis: Analyze the scalability and performance of quantum algorithms, projecting resource needs for future quantum systems. This involves establishing the scalability of quantum solutions from small-scale implementations to larger systems.

<u>Example Deliverable</u>: Detailed scalability analysis results, including resource estimates (qubit counts, gate operations, etc.) for future quantum hardware and an extrapolated performance summary for larger-scale quantum systems.

2. **Validation**: Validate quantum results against classical simulations and experimental data.

<u>Example Deliverable</u>: Validation and benchmarking results comparing quantum results with classical benchmarks, establishing the reliability of the quantum results that are beyond the limit of classical simulations.

3. Technology-to-Market (T2M) Analysis: Establish the energy and emissions impacts for various adoption scenarios compared to the SoA in the application area, considering efficiency gains and impacts from accelerated deployment of cost-effective solutions. Establish the market requirements for successfully leveraging quantum simulations. Develop and compare business models that could lead to a successful market impact for both the quantum technology and the application of its outputs.

<u>Example Deliverable</u>: A comprehensive T2M analysis, outlining the potential market adoption pathways, economic impact, energy savings, and CO<sub>2</sub>e reductions achievable through the implementation of the developed quantum solutions.

If a project is selected, Recipients will be required to: 1) prepare a Commercialization Plan for the targeted software as a milestone during performance and 2) agree to special provisions that require the reporting of the targeted software and its utilization. This special approach to projects that target software mirrors the requirements for reporting that attach to new inventions made in performance of an award. In addition, to facilitate the commercialization of the targeted software, ARPA-E is prepared to consider modifications to the standard data provisions that provide for government rights in the targeted software.

# E. TECHNICAL PERFORMANCE TARGETS

Projects under the QC<sup>3</sup> program must have the potential to both enable the objectives listed in Section I.C. and meet the targets described in Table 2 and in more detail below.

**Table 2.** Summary of program metrics and targets.

	Metric	Target
1.	Energy and Mission Impact	Identify a specific application where a scalable, generalizable solution can lead to the cumulative impact of 1 quad of energy or emissions reductions of 1 gigaton CO <sub>2</sub> e.
2.	Computational Performance	A transformational new capability that enables Metric 1: A scalable 100x improvement over the classical SoA in speed, accuracy, problem size, or some other relevant capability on the identified energy-relevant problem.
3.	T2M Impact	Path for the application of Metric 1 to be economically transformed through the improved computational speed and scaling of Metric 2 and reduced computational costs.

#### **Target 1: Energy and Mission Impact**

The project must aim to use quantum computing to solve a specific problem with energy applications where a scalable, generalizable solution has the clear potential for quad-scale energy impact or gigaton-scale CO<sub>2</sub>e emissions reductions. Energy impacts should be understood through a careful system-level accounting of energy consumption and greenhouse gas emissions for new technology that is enabled by quantum simulation.

The following should be considered when estimating the impact:

- The basis and methodology by which energy and emissions impacts were determined and the comparison to current incumbent technologies;
- How the quantum simulation enables the impact, including how a quantum calculation fits into the broader R&D workflow in an industrially relevant setting; and
- How the quantum simulation compares to SoA classical computational methods, including machine learning/artificial intelligence, and experimental methods.

#### **Target 2: Computational Performance**

The project must achieve a scalable 100x improvement in speed, accuracy, problem size, or some other relevant capability over classical SoA, either during the period of performance or through a scalable pathway on quantum hardware available in the short- to medium-term.

The following should be considered when evaluating the computational performance:

- As a baseline: The strengths and limitations of classical computational solutions to this
  problem, how those approaches scale, and whether the quantum solution outperforms
  the best available classical approach (not merely brute force approaches);
- The scale of the improvement: If the calculation has no classical computation analog, how classical methods would attempt to obtain the same information and how can the proposed improvement be quantified;

- Validation of beyond-classical results: How reliability of the quantum method can be established (e.g., comparison to experimental data or classical results for a smaller problem);
- Scalability: How scalability (defined as whether computational cost scales favorably with problem size and whether utility scales with hardware advancements) is proven within the period of performance, and how the approach will scale as hardware improves in the short-to medium-term (by 2030); and
- Running on real hardware: Creating a feasible plan to run on a quantum computer that supports meeting program targets.

#### Target 3: T2M Impact

To realize energy and emissions impacts from quantum simulation, the implementation of the technology insights must be cost effective and must successfully compete with mature incumbent solutions. The potential economic value afforded by future fully fault-tolerant quantum simulation in materials and chemistry is predicted to be over \$100 billion annually. It is likely that the full economic value of quantum computing will not be realized with near-term hardware. If this is the case, recipients must show an understanding of costs for the technology advances suggested by the simulation results, as well as key cost drivers that could be addressed through further simulation progress, increased production scale, or other advancement.

The following should be considered when estimating the economic viability and impact:

- Potential application market size and the existing market's cost, manufacturing viability, and supply chain drivers;
- Cost of running quantum simulation and how it scales with problem size and ongoing hardware and software developments;
- Financial impact of the developed quantum solutions, including savings from efficiency improvements and changes to manufacturing and maintenance costs over the useful lifetime of the new technology;
- Impact on total available market and timescale to introduce a quantum solution; and
- Anticipated barriers to adopting the materials and energy solutions developed with quantum technologies.

# F. OTHER PROJECT REQUIREMENTS

**Running on quantum hardware:** All teams are required to perform calculations on quantum hardware. Teams must submit a letter of intent from a provider or host of quantum hardware, which may be a participant on the submission or a third-party, to provide adequate access to quantum computational resources to meet program technical performance targets. This letter will be a component of the Concept Paper application.

**Recommended team member expertise:** Experts in all of the following areas are highly recommended for each team. Individual team members can assume more than one role.

- 1. **Materials Science and Chemistry**: Domain experts who can identify and guide relevant energy-related applications and interpret quantum simulation results;
- 2. **Classical Computational Science**: Experts in classical high-performance computing to ensure accurate benchmarking and hybrid quantum-classical simulations;
- 3. **Quantum Algorithms and Software**: Expert engineers in quantum algorithm design, particularly for chemistry and materials science applications;
- 4. **Quantum Compiling and Embedding**: Specialists in optimizing gate structures for each algorithm including error correction and fault tolerance;
- 5. **Quantum Hardware**: Engineers knowledgeable in quantum computing hardware who can help optimize algorithm compatibility with existing quantum devices; and
- 6. **Market Strategy:** Professionals with experience in the application market or similar markets who can understand the impacts of the mature quantum technology deployed at scale and can also identify barriers and drivers in the application market.

# G. STATEMENT OF SUBSTANTIAL INVOLVEMENT

Congress directed ARPA-E to "establish and monitor project milestones, initiate research projects quickly, and just as quickly terminate or restructure projects if such milestones are not achieved." Accordingly, ARPA-E is substantially involved in the direction of projects from inception to completion. For the purposes of an ARPA-E project, substantial involvement means:

- Project Teams must adhere to ARPA-E's agency-specific and programmatic requirements.
- ARPA-E may intervene at any time in the conduct or performance of work under an award.
- ARPA-E does not limit its involvement to the administrative requirements of an award.
   Instead, ARPA-E has substantial involvement in the direction and redirection of the technical aspects of the project as a whole.
- ARPA-E may, at its sole discretion, modify or terminate projects that fail to achieve predetermined Go/No Go decision points or technical milestones and deliverables.
- During award negotiations, ARPA-E Program Directors and Recipients mutually establish
  an aggressive schedule of quantitative milestones and deliverables that must be met
  every quarter. In addition, ARPA-E will negotiate and establish "Go/No-Go" milestones
  for each project. If the Recipient fails to achieve any of the "Go/No-Go" milestones or
  technical milestones and deliverables as determined by the ARPA-E Grants Officer,
  ARPA-E may at its discretion renegotiate the statement of project objectives or
  schedule of technical milestones and deliverables for the project. In the alternative,

<sup>&</sup>lt;sup>20</sup> U.S. Congress, Conference Report to accompany the 21<sup>st</sup> Century Competitiveness Act of 2007, H. Rpt. 110-289 at 171-172 (Aug. 1, 2007).

- ARPA-E may suspend or terminate the award in accordance with 2 C.F.R. §§ 200.339 200.343.
- ARPA-E may provide guidance and/or assistance to the Recipient to accelerate the
  commercialization of ARPA-E-funded technologies. Guidance and assistance provided by
  ARPA-E may include coordination with other Government agencies and nonprofits.<sup>21</sup> to
  provide mentoring and networking opportunities for Recipients. ARPA-E may also
  organize and sponsor events to educate Recipients about key barriers to the
  commercialization of their ARPA-E-funded technologies. In addition, ARPA-E may
  establish collaborations with private and public entities to provide continued support
  for the development and commercialization of ARPA-E-funded technologies.

# H. FUNDING RESTRICTIONS

#### 1. ALLOWABLE COSTS

All expenditures must be allowable, allocable, and reasonable in accordance with the applicable Federal cost principles. Pursuant to 2 C.F.R. § 910.352, the cost principles in the Federal Acquisition Regulations (48 C.F.R. Part 31.2) apply to for-profit entities. The cost principles contained in 2 C.F.R. Part 200; Subpart E apply to all entities other than for-profits.

#### 2. PRE-AWARD COSTS

ARPA-E will not reimburse any pre-award costs incurred by Applicants before they are selected for award negotiations. Please refer to Section VI.A of the NOFO for guidance on award notices.

Upon selection for award negotiations, Applicants may incur pre-award costs at their own risk, consistent with the requirements in 2 C.F.R. Part 200, as modified by 2 C.F.R. Part 910, and other Federal laws and regulations. All submitted budgets are subject to change and are typically reworked during award negotiations. ARPA-E is under no obligation to reimburse preaward costs if, for any reason, the Applicant does not receive an award or the award is made for a lesser amount than the Applicant expected, or if the costs incurred are not allowable, allocable, or reasonable.

#### 3. PATENT COSTS

For Subject Inventions disclosed to DOE under an award, ARPA-E will reimburse the Recipient – in addition to allowable costs associated with Subject Invention disclosures - up to \$30,000 of expenditures for filing and prosecution of United States patent applications, including international applications (PCT application) submitted to the United States Patent and Trademark Office (USPTO).

have not already been answered, email <u>ARPA-E-CO@hq.doe.gov</u> (with NOFO name and number in subject line). Problems with ARPA-E eXCHANGE? Email <u>ExchangeHelp@hq.doe.gov</u> (with NOFO name and number in subject line).

Questions about this NOFO? Check the Frequently Asked Questions available at <a href="https://arpa-e.energy.gov/fags">https://arpa-e.energy.gov/fags</a>. For questions that

<sup>&</sup>lt;sup>21</sup> "Nonprofits" or "nonprofit organizations" has the meaning set forth at 2 C.F.R. § 200.70.

The Recipient may request a waiver of the \$30,000 cap. Note that patent costs are considered to be Technology Transfer & Outreach (TT&O) costs (see Section I.H.8 of the NOFO below) and should be requested as such.

#### 4. CONSTRUCTION

ARPA-E generally does not fund projects that involve major construction. Recipients are required to obtain written authorization from the Grants Officer before incurring any major construction costs.

#### 5. FOREIGN TRAVEL

ARPA-E generally does not fund projects that involve foreign travel. Recipients are required to obtain written authorization from the ARPA-E Program Director before incurring any foreign travel costs and provide trip reports with their reimbursement requests.

#### 6. Performance of Work in the United States

ARPA-E requires all work under ARPA-E funding agreements to be performed in the United States. However, Applicants may request a waiver of this requirement where their project would materially benefit from, or otherwise requires, certain work to be performed overseas.

Applicants seeking this waiver must include an explicit request in the Business Assurances & Disclosures Form. Such waivers are granted where ARPA-E determines there is a demonstrated need.

#### 7. Purchase of New Equipment

All equipment purchased under ARPA-E funding agreements must be made or manufactured in the United States, to the maximum extent practicable. This requirement does not apply to used or leased equipment. The Recipients are required to notify the ARPA-E Grants Officer reasonably in advance of purchasing any equipment that is not made or manufactured in the United States with a total acquisition cost of \$250,000 or more. Purchases of foreign equipment with a total acquisition cost of \$1,000,000 or more require the approval of the Head of Contracting Activity (HCA). The ARPA-E Grants Officer will provide consent to purchase or reject within 30 calendar days of receipt of the Recipient's notification.

#### 8. TECHNOLOGY TRANSFER AND OUTREACH

ARPA-E is required to contribute a percentage of appropriated funds to Technology Transfer and Outreach (TT&O) activities. In order to meet this mandate, every Project Team must spend at least 5% of the Federal funding (i.e., the portion of the award that does not include the recipient's cost share) provided by ARPA-E on TT&O activities to promote and further the

development and eventual deployment of ARPA-E-funded technologies. Project Teams must seek a waiver from ARPA-E, located in the Business Assurances & Disclosures Form, to spend less than the minimum 5% TT&O expenditure requirement.

All TT&O expenditures are subject to the applicable Federal cost principles (i.e., 2 C.F.R. 200 Subpart E and 48 C.F.R. Subpart 31). Examples of TT&O expenditures are as follows:

- Documented travel and registration for the ARPA-E Energy Innovation Summit and other energy-related conferences and events;
- Documented travel to meet with potential suppliers, partners, or customers;
- Documented work by salaried or contract personnel to develop technology-to-market models or plans;
- Documented costs of acquiring industry-accepted market research reports; and
- Approved patent costs.

#### 9. LOBBYING

Recipients and Subrecipients may not use any Federal funds, directly or indirectly, to influence or attempt to influence, directly or indirectly, congressional action on any legislative or appropriation matters pending before Congress, other than to communicate to Members of Congress as described in 18 U.S.C. § 1913. This restriction is in addition to those prescribed elsewhere in statute and regulation.

Recipients and Subrecipients are required to complete and submit SF-LLL, "Disclosure of Lobbying Activities" (<a href="https://www.gsa.gov/forms-library/disclosure-lobbying-activities">https://www.gsa.gov/forms-library/disclosure-lobbying-activities</a>) if any non-Federal funds have been paid or will be paid to any person for influencing or attempting to influence any of the following in connection with your application:

- An officer or employee of any Federal agency,
- A Member of Congress,
- An officer or employee of Congress, or
- An employee of a Member of Congress.

#### **10.** Conference Spending

Recipients and Subrecipients may not use any Federal funds to:

- Defray the cost to the United States Government of a conference held by any Executive branch department, agency, board, commission, or office which is not directly and programmatically related to the purpose for which their ARPA-E award is made and for which the cost to the United States Government is more than \$20,000; or
- To circumvent the required notification by the head of any such Executive Branch department, agency, board, commission, or office to the Inspector General (or senior

ethics official for any entity without an Inspector General), of the date, location, and number of employees attending such a conference.

#### 11. INDEPENDENT RESEARCH AND DEVELOPMENT COSTS

ARPA-E does not fund Independent Research and Development (IR&D) as part of an indirect cost rate under its Grants and Cooperative Agreements. IR&D, as defined at FAR 31.205-18(a), includes cost of effort that is not sponsored by an assistance agreement or required in performance of a contract, and that consists of projects falling within the four following areas: (i) basic research, (ii) applied research, (iii) development, and (iv) systems and other concept formulation studies.

ARPA-E's goals are to enhance the economic and energy security of the United States through the development of energy technologies and ensure that the United States maintains a technological lead in developing and deploying advanced energy technologies. ARPA-E accomplishes these goals by providing financial assistance for energy technology projects and has well recognized and established procedures for supporting research through competitive financial assistance awards based on merit review of proposed projects. Reimbursement for independent research and development costs through the indirect cost mechanism could circumvent this competitive process.

To ensure that all projects receive similar and equal consideration, eligible organizations may compete for direct funding of independent research projects they consider worthy of support by submitting proposals for those projects to ARPA-E. Since proposals for these projects may be submitted for direct funding, costs for independent research and development projects are not allowable as indirect costs under ARPA-E awards. IR&D costs, however, would still be included in the direct cost base that is used to calculate the indirect rate so as to ensure an appropriate allocation of indirect costs to the organization's direct cost centers.

#### 12. Buy America Requirement for Public Infrastructure Projects

Projects funded through this NOFO that are for, or contain, construction, alteration, maintenance, or repair of public infrastructure in the United States undertaken by applicable recipient types, require that:

- All iron, steel, and manufactured products used in the infrastructure project are produced in the United States; and
- All construction materials used in the infrastructure project are manufactured in the United States.

However, ARPA-E does not anticipate soliciting for or selecting projects that propose project tasks that are for, or contain, construction, alteration, maintenance, or repair of public infrastructure. If a project selected for award negotiations includes project tasks that may be

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subject to the Buy America Requirement, those project tasks will be removed from the project before any award is issued – i.e., no federal funding or Recipient cost share will be available for covered project tasks.

This "Buy America" requirement does not apply to an award where the Recipient is a for-profit entity.

#### **13.** REQUIREMENT FOR FINANCIAL PERSONNEL

ARPA-E requires Small Business or Nonprofit applicants to identify a finance/budget professional (employee or contracted support) with an understanding of Federal contracting and/or financial assistance and cost accounting (including indirect costs, invoicing, and financial management systems) that will support the team in complying with all applicable requirements.

#### 14. PARTICIPANTS, COLLABORATING ORGANIZATIONS, AND CURRENT AND **PENDING SUPPORT**

If selected for award negotiations the selected applicant must submit, before the award is issued, an updated list of Covered Individuals.<sup>22</sup> who are proposed to work on the project, both at the Recipient and subrecipient level, and a list of all participating.<sup>23</sup> organizations. Further, the selectee must submit 1) current and pending support disclosures and resumes for any new Covered Individuals, and 2) updated disclosures if there have been any changes to the current and pending support submitted with the application.

Throughout the life of the award, recipients have an ongoing responsibility to notify DOE of changes to the Covered Individuals and collaborating organizations, within 30 days of such change, and to submit 1) current and pending support disclosure statements and resumes for any Covered Individuals; and 2) updated disclosures if there are changes to the current and pending support previously submitted to ARPA-E. Recipients must certify on an annual basis that no such changes have occurred since their most recent certification.

Note that foreign participation is treated separately and may require a Foreign Entity Waiver, per Section II.A.5.

<sup>&</sup>lt;sup>22</sup> See Section IX, Glossary, for the definition of Covered Individual.

<sup>&</sup>lt;sup>23</sup> For a definition of "participation" please see footnote 32.

#### II. **ELIGIBILITY INFORMATION**

# A. **ELIGIBLE APPLICANTS**

This NOFO is open to U.S. Institutions of Higher Education, national laboratories, industry and individuals.

#### 1. INDIVIDUALS

U.S. citizens or permanent residents may apply for funding in their individual capacity as a Standalone Applicant, <sup>24</sup> as the lead for a Project Team, <sup>25</sup> or as a member of a Project Team. However, ARPA-E will only award funding to an entity formed by the Applicant.

#### 2. DOMESTIC ENTITIES

For-profit entities (which includes large businesses and small businesses), educational institutions.<sup>26</sup>, and nonprofits.<sup>27</sup> that (A) are organized, chartered, or incorporated (or otherwise formed) under the laws of a particular state or territory of the United States; (B) have majority domestic ownership and control; and (C) have a physical place of business in the United States, including U.S. territories, are eligible to apply for funding as a Standalone Applicant, as the lead organization for a Project Team, or as a member of a Project Team.

Entities that do not meet the above criteria may still be eligible to apply as a Standalone Applicant, lead organization or member of a Project Team, but must either (1) designate in the Full Application a subsidiary or affiliate that meets the above criteria to receive funding (the Full Application must state the nature of the corporate relationship between the foreign entity and domestic subsidiary or affiliate); or (2) request a Foreign Entity Waiver via the Business Assurances & Disclosures Form.

• If a Foreign Country of Concern.<sup>28</sup> or individual citizen(s) of a Foreign Country of Concern has any ownership interest in any of the entities included in a proposal, then the Full Application must include a Foreign Entity Waiver request for each such entity in order for ARPA-E to consider the participation of such entities.<sup>29</sup>

<sup>&</sup>lt;sup>24</sup> A Standalone Applicant is an Applicant that applies for funding on its own, not as part of a Project Team.

<sup>&</sup>lt;sup>25</sup> A Project Team consists of the Project Team Lead, Subrecipients, and others performing or otherwise supporting work under an ARPA-E funding agreement.

<sup>&</sup>lt;sup>26</sup> Institutions of Higher Education (or educational institutions): Has the meaning set forth at 20 U.S.C. 1001.

<sup>&</sup>lt;sup>27</sup>Nonprofit organizations described in section 501(c)(4) of the Internal Revenue Code of 1986 that engaged in lobbying activities after December 31, 1995 are not eligible to apply for funding as a Recipient or Subrecipient.

<sup>&</sup>lt;sup>28</sup> "Foreign Countries of Concern", <u>as defined by the State Department</u>, include (as of December 29, 2023) Burma, People's Republic of China, Cuba, Eritrea, Iran, the Democratic People's Republic of Korea, Nicaragua, Pakistan, Russia, Saudi Arabia, Tajikistan, and Turkmenistan.

<sup>&</sup>lt;sup>29</sup> The contents of a Foreign Entity Waiver request can be found in the Business Assurances & Disclosures Form.

 All work under the ARPA-E award must be performed in the United States unless a separate Foreign Work Waiver request is granted.<sup>30</sup>

FFRDCs/DOE Labs are eligible to apply for funding as the lead organization for a Project Team or as a member of a Project Team that includes Institutions of Higher Education, companies, research foundations, or trade and industry research collaborations, but not as a Standalone Applicant.

State, local, and tribal government entities are eligible to apply for funding as a member of a Project Team, but not as a Standalone Applicant or as the lead organization for a Project Team.

Federal agencies and instrumentalities (other than DOE) are eligible to apply for funding as a member of a Project Team, but not as a Standalone Applicant or as the lead organization for a Project Team.

#### 3. Consortia

Consortia, which may include domestic and foreign entities, must designate one member of the consortium as the consortium representative to the Project Team. The consortium representative must be incorporated in the United States. The eligibility of the consortium will be determined by reference to the eligibility of the consortium representative under Section II.A of the NOFO. Each consortium must have an internal governance structure and a written set of internal rules. Upon request, the consortium entity must provide a written description of its internal governance structure and its internal rules to the Grants Officer (ARPA-E-CO@hq.doe.gov).

Unincorporated consortia must provide the Grants Officer with a collaboration agreement, commonly referred to as the articles of collaboration, which sets out the rights and responsibilities of each consortium member. This collaboration agreement binds the individual consortium members together and shall include the consortium's:

- Management structure;
- Method of making payments to consortium members;
- Means of ensuring and overseeing members' efforts on the project;
- Provisions for members' cost sharing contributions; and
- Provisions for ownership and rights in intellectual property developed previously or under the agreement.

# 4. Foreign National Participation From Countries of Concern

All applicants selected for an award under this NOFO and project participants (including subrecipients and contractors) who anticipate involving foreign nationals from Foreign

<sup>&</sup>lt;sup>30</sup> The contents of a Foreign Work Waiver can also be found in the Business Assurances & Disclosures Form.

Countries of Concern.<sup>31</sup> in the performance of an award may be required to provide ARPA-E with specific information about each foreign national to satisfy requirements for foreign national participation. A "foreign national" is defined as any person who is not a United States citizen by birth or naturalization. The volume and type of information collected may depend on various factors associated with the award. ARPA-E approval is required before a foreign national can participate in the performance of any work under an award.

ARPA-E may elect to deny a foreign national's participation in the award. Likewise, ARPA-E may elect to deny a foreign national's access to ARPA-E site, information, technologies, equipment, programs or personnel.

#### 5. FOREIGN PARTICIPATION CONSIDERATIONS

Foreign participation.<sup>32</sup> in a project requires a Foreign Entity Waiver (see Waiver Request – Foreign Entity Participation in the Business Assurances & Disclosure Form). Awardees have an ongoing obligation to report new foreign participation in a project and may be required to obtain a waiver before new foreign participation can occur. A Foreign Work Waiver may also be required (see Section I.H.6 and the Business Assurances & Disclosures Form).

# B. COMPLIANCE AND RESPONSIVENESS

Submissions that are noncompliant or nonresponsive to the NOFO as described in Sections IV.D and V.A are not eligible.

# C. LIMITATION ON NUMBER OF SUBMISSIONS

ARPA-E is not limiting the number of submissions from Applicants. Applicants may submit more than one application to this NOFO, provided that each application is scientifically distinct.

Small business Applicants that qualify as a "Small Business Concern".<sup>33</sup> may apply to only one of the two ARPA-E QC³ NOFOs: DE-FOA-0003483 (QC³ SBIR/STTR), or DE-FOA-0003482 (QC³). Small businesses that qualify as "Small Business Concerns" are strongly encouraged to apply under

<sup>&</sup>lt;sup>31</sup> Please see footnote 28 for list of Foreign Countries of Concern.

<sup>&</sup>lt;sup>32</sup> "Participation" includes any activities performed under an ARPA-E award, including, but not limited to, all work described in the milestone schedule of an award (commonly referred to as "Attachment 3" or the "Statement of Project Objectives (SOPO)") and any services that include testing, including services performed by vendors or consultants. Participation also includes activities that involve the procurement of foreign equipment or supplies.

<sup>33</sup> Please refer to the U.S. Small Business Administration (SBA) website. A Small Business Concern is a for-profit entity that: (1) maintains a place of business located in the United States; (2) operates primarily within the United States or makes a significant contribution to the United States economy through payment of taxes or use of American products, materials or labor; (3) is an individual proprietorship, partnership, corporation, limited liability company, joint venture, association, trust, or cooperative; and (4) meets the size eligibility requirements set forth in 13 C.F.R. § 121.702. Where the entity is formed as a joint venture, there can be no more than 49% participation by foreign business entities in the joint venture.

the former (SBIR/STTR NOFO). To determine eligibility as a "Small Business Concern" under DE-FOA-0003483 (QC<sup>3</sup> SBIR/STTR), please review the eligibility requirements in Sections II.A – II.D of that NOFO.

ARPA-E will accept only new submissions under this NOFO. Applicants may not seek renewal or supplementation of their existing awards through this NOFO.

# D. Cost Sharing

Applicants are bound by the cost share proposed in their Full Applications.

#### 1. Base Cost Share Requirement

ARPA-E generally uses Cooperative Agreements to provide financial and other support to Recipients (see Section VI.D.1 of the NOFO). Under a Cooperative Agreement or Grant, the Recipient must provide at least 20% of the Total Project Cost.<sup>34</sup> as cost share, except as provided in Sections II.D.2 or II.D.3.<sup>35</sup>

#### 2. INCREASED COST SHARE REQUIREMENT

Large businesses.<sup>36</sup> are strongly encouraged to provide more than 20% of the Total Project Cost as cost share.

Under an "other transaction" agreement, the Recipient is normally expected to provide at least 50% of the Total Project Cost as cost share. ARPA-E may reduce this cost share requirement, as appropriate.

#### 3. REDUCED COST SHARE REQUIREMENT

ARPA-E has reduced the base cost share requirement for the following types of projects:

- A domestic educational institution or domestic nonprofit applying as a Standalone Applicant is required to provide at least 5% of the Total Project Cost as cost share.
- Project Teams composed <u>exclusively</u> of domestic educational institutions, domestic nonprofits, and/or FFRDCs/DOE Labs/Federal agencies and instrumentalities (other than DOE) are required to provide at least 5% of the Total Project Cost as cost share. Small businesses – or consortia of small businesses – may provide 0% cost share from the outset of the project through the first 12 months of the project

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<sup>&</sup>lt;sup>34</sup> The Total Project Cost is the sum of the Applicant's share and the Federal Government share of total allowable costs. The Federal Government share generally includes costs incurred by GOGOs and FFRDCs.

<sup>&</sup>lt;sup>35</sup> Energy Policy Act of 2005, Pub.L. 109-58, sec. 988(c)

<sup>&</sup>lt;sup>36</sup> See Section IX.

(hereinafter the "Cost Share Grace Period"). <sup>37</sup> If the project is continued beyond the Cost Share Grace Period, then at least 10% of the Total Project Cost (including the costs incurred during the Cost Share Grace Period) will be required as cost share over the remaining period of performance.

- Project Teams where a small business is the lead organization and small businesses
  perform greater than or equal to 80% of the total work under the funding
  agreement (as measured by the Total Project Cost) are entitled to the same cost
  share reduction and Cost Share Grace Period as provided above to Standalone small
  businesses or consortia of small businesses.
- Project Teams where domestic educational institutions, domestic nonprofits, small businesses, and/or FFRDCs perform greater than or equal to 80% of the total work under the funding agreement (as measured by the Total Project Cost) are required to provide at least 10% of the Total Project Cost as cost share. However, any entity (such as a large business) receiving patent rights under a class waiver, or other patent waiver, that is part of a Project Team receiving this reduction must continue to meet the statutory minimum cost share requirement (20%) for its portion of the Total Project Cost.
- Projects that do not meet any of the above criteria are subject to the base cost share requirements described in Sections II.D.1 and II.D.2 of the NOFO.

#### 4. LEGAL RESPONSIBILITY

Although the cost share requirement applies to the Project Team as a whole, the funding agreement makes the Recipient legally responsible for paying or ensuring payment of the entire cost share. The Recipient's cost share obligation is expressed in the funding agreement as a static amount in U.S. dollars (cost share amount) and as a percentage of the Total Project Cost (cost share percentage). If the funding agreement is terminated prior to the end of the period of performance, the Recipient is required to contribute at least the cost share percentage of total expenditures incurred through the date of termination.

The Recipient is solely responsible for managing cost share contributions by the Project Team and enforcing cost share obligations assumed by Project Team members in subawards or related agreements.

#### 5. Cost Share Allocation

Each Project Team is free to determine how much each Project Team member will contribute towards the cost share requirement. The amount contributed by individual Project Team members may vary, as long as the cost share requirement for the project as a whole is met.

<sup>&</sup>lt;sup>37</sup> The term "small business" is defined in Section IX.

#### 6. COST SHARE TYPES AND ALLOWABILITY

Every cost share contribution must be allowable under the applicable Federal cost principles, as described in Section I.H of the NOFO. Upon selection for award negotiations, the Recipient must confirm in writing that the proposed cost share contribution is allowable in accordance with applicable Federal cost principles.

Project Teams may provide cost share in the form of cash or in-kind contributions. Cash contributions may be provided by the Recipient or Subrecipients. Allowable in-kind contributions include but are not limited to personnel costs, indirect costs, facilities and administrative costs, rental value of buildings or equipment, and the value of a service, other resource, or third-party in-kind contribution. Project Teams may use funding or property received from state or local governments to meet the cost share requirement, so long as the funding or property was not provided to the state or local government by the Federal Government.

The Recipient may <u>not</u> use the following sources to meet its cost share obligations:

- Revenues or royalties from the prospective operation of an activity beyond the period of performance;
- Proceeds from the prospective sale of an asset of an activity;
- Appropriated Federal funding or property (e.g., Federal grants, equipment owned by the Federal Government); or
- Expenditures that were reimbursed under a separate Federal program.

In addition, Project Teams may not use independent research and development (IR&D) funds.<sup>38</sup> to meet their cost share obligations under Cooperative Agreements. However, Project Teams may use IR&D funds to meet their cost share obligations under "other transaction" agreements.

Project Teams may not use the same cash or in-kind contributions to meet cost share requirements for more than one project or program.

Cost share contributions must be specified in the project budget, verifiable from the Recipient's records, and necessary and reasonable for proper and efficient accomplishment of the project. Every cost share contribution must be reviewed and approved in advance by the Grants Officer and incorporated into the project budget before the expenditures are incurred.

Applicants may wish to refer to 2 C.F.R. Parts 200 and 910, and 10 C.F.R Part 603.<sup>39</sup> for additional guidance on cost sharing, specifically 2 C.F.R. §§ 200.306 and 910.130, and 10 C.F.R. §§ 603.525-555.

<sup>&</sup>lt;sup>38</sup> As defined in Federal Acquisition Regulation Subsection 31.205-18.

<sup>&</sup>lt;sup>39 39</sup> In the case of Technology Investment Agreements under 42 USC §7256(g).

#### 7. Cost Share Contributions by FFRDCs and GOGOs

Because FFRDCs are funded by the Federal Government, costs incurred by FFRDCs generally may not be used to meet the cost share requirement. FFRDCs may contribute cost share only if the contributions are paid directly from the contractor's Management Fee or a non-Federal source.

Because GOGOs/Federal Agencies are funded by the Federal Government, GOGOs/Federal Agencies may not provide cost share for the proposed project. However, the GOGO/Agency costs would be included in Total Project Costs for purposes of calculating the cost-sharing requirements of the applicant.

#### 8. Cost Share Verification

The Recipient is required to provide cost share commitment letters from Subrecipients or third parties that are providing cost share, whether cash or in-kind, in their Full Application. Each Subrecipient or third party that is contributing cost share must provide a letter on appropriate letterhead that is signed by an authorized corporate representative.

Upon selection for award negotiations, Applicants are required to provide information and documentation regarding their cost share contributions. Please refer to Section II.D of the NOFO for guidance on the requisite cost share information and documentation.

#### III. APPLICATION CONTENTS AND FORMAT

### A. GENERAL APPLICATION CONTENT REQUIREMENTS

#### 1. Marking of Confidential Information

ARPA-E will use data and other information contained in Concept Papers, Full Applications, and Replies to Reviewer Comments strictly for evaluation purposes.

Concept Papers, Full Applications, Replies to Reviewer Comments, and other submissions containing confidential, proprietary, or privileged information should be marked as described below. Failure to comply with these marking requirements may result in the disclosure of the unmarked information under the Freedom of Information Act or otherwise. The U.S. Government is not liable for the disclosure or use of unmarked information and may use or disclose such information for any purpose.

The cover sheet of the Concept Paper, Full Application, Reply to Reviewer Comments, or other submission must be marked as follows and identify the specific pages containing confidential, proprietary, or privileged information:

Notice of Restriction on Disclosure and Use of Data:

Pages [\_\_\_] of this document may contain confidential, proprietary, or privileged information that is exempt from public disclosure. Such information shall be used or disclosed only for evaluation purposes or in accordance with a financial assistance or loan agreement between the submitter and the Government. The Government may use or disclose any information that is not appropriately marked or otherwise restricted, regardless of source.

The header and footer of every page that contains confidential, proprietary, or privileged information must be marked as follows: "Contains Confidential, Proprietary, or Privileged Information Exempt from Public Disclosure." In addition, every line and paragraph containing proprietary, privileged, or trade secret information must be clearly marked with double brackets or highlighting.

#### 2. EXPORT CONTROL INFORMATION

Do not include information subject to export controls in any submissions, including Concept Papers, Full Applications, and Replies to Reviewer Comments — whether marked as subject to US export control laws/regulations or otherwise. Such information may not be accepted by ARPA-E and may result in a determination that the application is non-compliant, and therefore not eligible for selection. This prohibition includes any submission containing a general, non-determinative statement such as "The information on this page [or pages \_ to\_\_] may be subject to US export control laws/regulations", or similar. Under the terms of their award, awardees shall be responsible for compliance with all export control laws/regulations.

# B. **CONCEPT PAPERS**

#### 1. FIRST COMPONENT: CONCEPT PAPER

<u>The Concept Paper is mandatory</u> (i.e., in order to submit a Full Application, a compliant and responsive Concept Paper must have been submitted) and must conform to the following formatting requirements:

- The Concept Paper must not exceed 4 pages in length including graphics, figures, and/or tables.
- The Concept Paper must be submitted in Adobe PDF format.
- The Concept Paper must be written in English.
- All pages must be formatted to fit on 8-1/2 by 11-inch paper with margins not less than one inch on every side. Single space all text and use Times New Roman typeface, a black font color, and a font size of 12 point or larger (except in figures and tables).
- The ARPA-E assigned Control Number, the Lead Organization Name, and the Principal Investigator's Last Name must be prominently displayed on the upper right corner of the header of every page. Page numbers must be included in the footer of every page.
- The first paragraph must include the Lead Organization's Name and Location, Principal Investigator's Name, Technical Category, Proposed Funding Requested (Federal and Cost Share), and Project Duration.

A fillable Concept Paper template is available on ARPA-E eXCHANGE at <a href="https://arpa-e-foa.energy.gov">https://arpa-e-foa.energy.gov</a>. Concept Papers must conform to the content requirements described in the template.

Each Concept Paper must be limited to a single concept or technology. Unrelated concepts and technologies must not be consolidated into a single Concept Paper.

Concept Papers found to be noncompliant or nonresponsive may not be merit reviewed or considered for award (see Section II.B of the NOFO).

#### 2. Second Component: Letter of Intent for Quantum Hardware

All teams must submit a letter of intent from a provider or host of quantum hardware, which may be a participant on the submission or a third-party, to provide adequate access to quantum computational resources to meet program technical performance targets.

The letter must be uploaded to ARPA-E eXCHANGE along with the Concept Paper in Adobe PDF format. If a Concept Paper application does not have an associated Letter of Intent for Quantum Hardware, it may be found noncompliant or nonresponsive.

#### 3. THIRD COMPONENT: SUMMARY SLIDE

Applicants are required to provide a single PowerPoint slide summarizing the proposed project. The slide must be submitted in Microsoft PowerPoint format. This slide will be used during ARPA-E's evaluation of Concept Papers. A summary slide template is available on ARPA-E eXCHANGE.

#### C. FULL APPLICATIONS

Full Applications must conform to the following formatting requirements:

- Each document must be submitted in the file format prescribed below and/or written in the document template at <a href="https://arpa-e-foa.energy.gov">https://arpa-e-foa.energy.gov</a>.
- The Full Application must be written in English.
- All pages must be formatted to fit on 8-1/2 by 11-inch paper with margins not less than
  one inch on every side. Single space all text and use Times New Roman typeface, a black
  font color, and a font size of 12 point or larger (except in figures and tables).
- The ARPA-E assigned Control Number, the Lead Organization Name, and the Principal Investigator's Last Name must be prominently displayed on the upper right corner of the header of every page. Page numbers must be included in the footer of every page.

Fillable Full Application template documents are available on ARPA-E eXCHANGE at <a href="https://arpa-e-foa.energy.gov">https://arpa-e-foa.energy.gov</a>.

Full Applications found in any component to be noncompliant or nonresponsive may not be merit reviewed or considered for award (see Section III.B of the NOFO).

ARPA-E provides detailed guidance on the content and form of each component below.

#### 1. FIRST COMPONENT: TECHNICAL VOLUME

The Technical Volume is the centerpiece of the Full Application. The Technical Volume must be submitted in Adobe PDF format. The Technical Volume must conform to the content and form requirements included within the template, including maximum page lengths. If Applicants exceed the maximum page lengths specified for each section, or add any additional sections not requested, ARPA-E may review only the authorized number of pages and disregard any additional pages or sections.

Applicants must provide sufficient citations and references to the primary research literature to justify the claims and approaches made in the Technical Volume. ARPA-E and reviewers may review primary research literature in order to evaluate applications. <u>However, all relevant technical information should be included in the body of the Technical Volume.</u>

#### 2. SECOND COMPONENT: SF-424

The SF-424 must be submitted in Adobe PDF format using the available template. An instructional document is also available on ARPA-E eXCHANGE. Applicants must complete all required fields in accordance with the instructions. Applicants may identify and include in Block 14 the entities, their addresses, and corresponding census tract numbers for any project activities that will occur within any designated Qualified Opportunity Zone (QOZ). To locate QOZ, go to: <a href="https://www.cdfifund.gov/opportunity-zones.">https://www.cdfifund.gov/opportunity-zones.</a>

Recipients and Subrecipients are required to complete SF-LLL (Disclosure of Lobbying Activities), also available on ARPA-E eXCHANGE, if any non-Federal funds have been paid or will be paid to any person for influencing or attempting to influence an officer or employee of any Federal agency, a Member of Congress, an officer or employee of Congress, or an employee of a Member of Congress in connection with your application or funding agreement. The completed SF-LLL must be appended to the SF-424.

ARPA-E provides the following supplemental guidance on completing the SF-424:

- Each Project Team should submit only one SF-424 (i.e., a Subrecipient should not submit a separate SF-424).
- The list of certifications and assurances in Block 21 can be found at <a href="https://www.energy.gov/management/articles/certifications-and-assurances-use-sf-424">https://www.energy.gov/management/articles/certifications-and-assurances-use-sf-424</a>.
- The dates and dollar amounts on the SF-424 are for the <u>entire period of performance</u>, not a portion thereof.
- Applicants are responsible for ensuring that the proposed costs listed in eXCHANGE match those listed on forms SF-424 and the Budget Justification Workbook/SF-424A.
   Inconsistent submissions may impact ARPA-E's final award determination.

# 3. THIRD COMPONENT: BUDGET JUSTIFICATION WORKBOOK/SF-424A

Applicants are required to complete the Budget Justification Workbook/SF-424A Excel spreadsheet using the available template. Recipients must complete each tab of the Budget Justification Workbook for the project as a whole, including all work to be performed by the Recipient and its Subrecipients and Contractors. The SF-424A form included with the Budget Justification Workbook will "auto-populate" as the Applicant enters information into the Workbook. Applicants should carefully read the "Instructions and Summary" tab provided within the Budget Justification Workbook, and all instructions at the top of each category tab. For more information, an ARPA-E Budget Justification Guidance document is also available on ARPA-E eXCHANGE.

Questions about this NOFO? Check the Frequently Asked Questions available at <a href="https://arpa-e.energy.gov/fags">https://arpa-e.energy.gov/fags</a>. For questions that have not already been answered, email <a href="https://arpa-e.energy.gov/fags">ARPA-E exchange email area and all area

Subrecipient information must be submitted as follows:

- Each Subrecipient incurring greater than or equal to 10% of the Total Project Cost must complete a separate Budget Justification workbook to justify its proposed budget. These worksheets must be inserted as additional sheets within in the Recipient's Budget Justification.
- Subrecipients incurring less than 10% of the Total Project Cost are <u>not</u> required to complete a separate Budget Justification workbook. However, such Subrecipients are required to provide supporting documentation to justify their proposed budgets. At a minimum, the supporting documentation must show which tasks/subtasks are being performed, the purpose/need for the effort, and a sufficient basis for the estimated costs.

#### 4. FOURTH COMPONENT: SUMMARY FOR PUBLIC RELEASE

Applicants are required to provide a 250-word maximum Summary for Public Release following the instructions in the available template. The Summary for Public Release must be submitted in Adobe PDF format. For applications selected for award negotiations, the Summary may be used as the basis for a public announcement by ARPA-E; therefore, this summary should not include any confidential, proprietary, or privileged information. This summary may not include any graphics, figures, or tables. The summary should be written for a lay audience (e.g., general public, media, Congress) using plain English.

#### 5. FIFTH COMPONENT: SUMMARY SLIDE

Applicants are required to provide a single PowerPoint slide summarizing the proposed project. The slide must be submitted in Microsoft PowerPoint format. This slide will be used during ARPA-E's evaluation of Full Applications. Summary Slides must conform to the content requirements described in the template.

#### 6. SIXTH COMPONENT: BUSINESS ASSURANCES & DISCLOSURES FORM

Applicants are required to provide the information requested in the Business Assurances & Disclosures Form. The information must be submitted in Adobe PDF format and digitally signed by all required parties. The fillable Business Assurances & Disclosures Form template on ARPA-E eXCHANGE includes instructions for items the Applicant is required to disclose, describe, or request a waiver for.

#### D. REPLIES TO REVIEWER COMMENTS

Written feedback on Full Applications is made available to Applicants before the submission deadline for Replies to Reviewer Comments. Applicants have a brief opportunity to prepare a short Reply to Reviewer Comments responding to one or more comments or supplementing

their Full Application. A fillable Reply to Reviewer Comments template is available on ARPA-E eXCHANGE (https://arpa-e-foa.energy.gov).

Replies to Reviewer Comments must conform to the following requirements:

- The Reply to Reviewer Comments must be submitted in Adobe PDF format.
- The Reply to Reviewer Comments must be written in English.
- All pages must be formatted to fit on 8-1/2 by 11-inch paper with margins not less than one inch on every side. Use Times New Roman typeface, a black font color, and a font size of 12 points or larger (except in figures and tables).
- The Reply to Reviewer Comments must be a maximum of 3 pages 2 pages maximum for text, and 1 page maximum for images (e.g., graphics, charts, or other data).
- The Control Number must be prominently displayed on the upper right corner of the header of every page. Page numbers must be included in the footer of every page.

#### IV. SUBMISSION REQUIREMENTS AND DEADLINES

All documents, templates, and instructions required to apply to this NOFO are either linked in this document or available on ARPA-E eXCHANGE at <a href="https://arpa-e-foa.energy.gov">https://arpa-e-foa.energy.gov</a>.

Concept Papers, Full Applications, and Replies to Reviewer Comments must be submitted through ARPA-E eXCHANGE. ARPA-E will <u>not review or consider applications submitted through other means</u> (e.g., fax, hand delivery, email, postal mail).

ARPA-E expects to retain copies of all Concept Papers, Full Applications, Replies to Reviewer Comments, and other submissions. No submissions will be returned. By applying to ARPA-E for funding, Applicants consent to ARPA-E's retention of their submissions.

## A. UNIQUE ENTITY IDENTIFIER AND SAM REGISTRATION

Applicants must register with the System for Award Management (SAM) at <a href="www.sam.gov/SAM">www.sam.gov/SAM</a> prior to submitting an application, at which time the system will assign (if newly registered) a Unique Entity Identifier (UEI). Applicants should commence this process as soon as possible. Registering with SAM and obtaining the UEI could take several weeks.

## Recipients must:

- Maintain a current and active registration in SAM.gov at all times during which it has an
  active Federal award or an application or plan under consideration by a Federal
  awarding agency, including (if applicable) information on its immediate and highestlevel owner and subsidiaries and on all predecessors that have been awarded a Federal
  contract or financial assistance award within the last three years.;
- Remain registered in SAM.gov after the initial registration;
- Update its information in SAM.gov as soon as it changes;
- Review its information in SAM.gov annually from the date of initial registration or subsequent updates to ensure it is current, accurate and complete;
- Include its UEI in each application it submits; and
- Not make a subaward to any entity unless the entity has provided its UEI.

Subrecipients are not required to complete a full registration in SAM.gov but must obtain a UEI.

ARPA-E may not execute a funding agreement with the Recipient until it has obtained a UEI and completed its SAM registration.

## B. Use of ARPA-E eXCHANGE

To apply to this NOFO, Applicants must register with ARPA-E eXCHANGE (<a href="https://arpa-e-foa.energy.gov/Registration.aspx">https://arpa-e-foa.energy.gov/Registration.aspx</a>). For detailed guidance on using ARPA-E eXCHANGE, please

refer to the "ARPA-E eXCHANGE Applicant Guide" (<a href="https://arpa-e-foa.energy.gov/Manuals.aspx">https://arpa-e-foa.energy.gov/Manuals.aspx</a>).

Upon creating an application submission in ARPA-E eXCHANGE, Applicants will be assigned a Control Number. If the Applicant creates more than one application submission, a different Control Number will be assigned for each application.

Once logged in to ARPA-E eXCHANGE (<a href="https://arpa-e-foa.energy.gov/login.aspx">https://arpa-e-foa.energy.gov/login.aspx</a>), Applicants may access their submissions by clicking the "Submissions" and then "My Submissions" links in the navigation on the left side of the page. Every application that the Applicant has submitted to ARPA-E and the corresponding Control Number is displayed on that page. If the Applicant submits more than one application to a particular NOFO, a different Control Number is shown for each application.

Applicants are responsible for meeting each submission deadline in ARPA-E eXCHANGE.

Applicants are strongly encouraged to submit their applications at least 48 hours in advance of the submission deadline. Under normal conditions (i.e., at least 48 hours in advance of the submission deadline), Applicants should allow at least 1 hour to submit a Concept Paper or Full Application. In addition, Applicants should allow at least 15 minutes to submit a Reply to Reviewer Comments. Once the application is submitted in ARPA-E eXCHANGE, Applicants may revise or update their application until the expiration of the applicable deadline.

Applicants should not wait until the last minute to begin the submission process. During the final hours before the submission deadline, Applicants may experience server/connection congestion that prevents them from completing the necessary steps in ARPA-E eXCHANGE to submit their applications. ARPA-E will not extend the submission deadline for Applicants that fail to submit required information and documents due to server/connection congestion.

## C. REQUIRED DOCUMENTS CHECKLIST AND DEADLINES

The following table outlines the required documents and their submission deadlines.

SUBMISSION	COMPONENTS	OPTIONAL/ MANDATORY	NOFO SECTION	DEADLINES
Concept Paper	<ul> <li>Concept Paper (Adobe PDF format)         <ul> <li>Sections 1-4 (4 pages max.)</li> <li>Bibliographic References (no page limit)</li> </ul> </li> <li>Letter of Intent for Quantum Hardware (no page limit, Adobe PDF format)</li> <li>Summary Slide (1 page limit, Microsoft PowerPoint format)</li> </ul>	Mandatory	III.B	9:30 AM ET, November 21, 2024
Full Application	<ul> <li>Technical Volume (Adobe PDF format):         <ul> <li>Cover Page (1 page max.)</li> <li>Executive Summary (1 page max.)</li> <li>Sections 1-5 (20 pages max.)</li> <li>Bibliographic References (no page limit)</li> <li>Personal Qualification Summaries (each summary limited to 5 pages in length, no cumulative page limit)</li> </ul> </li> <li>Signed SF-424 (Adobe PDF format);</li> <li>Budget Justification Workbook/SF-424A (Microsoft Excel format);</li> <li>Summary for Public Release (250 words max., Adobe PDF format);</li> <li>Summary Slide (1 slide limit, Microsoft PowerPoint format); and</li> <li>Signed Business Assurances &amp; Disclosures Form(s) (no page limit, Adobe PDF format).</li> </ul>	Mandatory	III.C	TBD
Reply to Reviewer Comments	Reply to Reviewer Comments (3 page max., Adobe PDF format)	Optional	III.D	TBD

## D. COMPLIANCE

ARPA-E may not review or consider incomplete applications and applications received after the deadline stated in the NOFO. Such applications may be deemed noncompliant (see Section II.B of the NOFO). The following errors could cause an application to be deemed "incomplete" and thus noncompliant:

- Failing to comply with the form and content requirements in Section III of the NOFO;
- Failing to enter required information in ARPA-E eXCHANGE;
- Failing to upload required document(s) to ARPA-E eXCHANGE;

- Failing to click the "Submit" button in ARPA-E eXCHANGE by the deadline stated in the NOFO;
- Uploading the wrong document(s) or application(s) to ARPA-E eXCHANGE; and
- Uploading the same document twice but labeling it as different documents. (In the latter scenario, the Applicant failed to submit a required document.)

ARPA-E urges Applicants to carefully review their applications and to allow sufficient time for the submission of required information and documents.

# E. INTERGOVERNMENTAL REVIEW

This program is not subject to Executive Order 12372 (Intergovernmental Review of Federal Programs).

## V. APPLICATION REVIEW INFORMATION

## A. RESPONSIVENESS

## 1. TECHNICAL RESPONSIVENESS REVIEW

ARPA-E performs a preliminary technical review of Concept Papers and Full Applications. The following types of submissions may be deemed nonresponsive and may not be reviewed or considered:

- Submissions that fall outside the technical parameters specified in this NOFO.
- Submissions that have been submitted in response to currently issued ARPA-E NOFOs.
- Submissions that are not scientifically distinct from applications submitted in response to currently issued ARPA-E NOFOs.
- Submissions for basic research aimed solely at discovery and/or fundamental knowledge generation.
- Submissions for large-scale demonstration projects of existing technologies.
- Submissions for proposed technologies that represent incremental improvements to existing technologies.
- Submissions for proposed technologies that are not based on sound scientific principles (e.g., violates a law of thermodynamics).
- Submissions for proposed technologies that are not transformational, as described in Section I.A of the NOFO.
- Submissions for proposed technologies that do not have the potential to become
  disruptive in nature, as described in Section I.A of the NOFO. Technologies must be
  scalable such that they could be disruptive with sufficient technical progress.
- Submissions that are not distinct in scientific approach or objective from activities currently supported by or actively under consideration for funding by any other office within Department of Energy.
- Submissions that are not distinct in scientific approach or objective from activities currently supported by or actively under consideration for funding by other government agencies or the private sector.
- Submissions that do not propose a R&D plan that allows ARPA-E to evaluate the submission under the applicable merit review criteria provided in Section V.B of the NOFO.

#### 2. SUBMISSIONS SPECIFICALLY NOT OF INTEREST

Submissions that propose the following will be deemed nonresponsive and will not be merit reviewed or considered:

- Hardware development;
- Quantum-enhanced optimization;
- Quantum machine learning;
- Quantum simulations of toy models or models for which the connection to energy impacts is merely incidental; and
- Quantum optimization for finance in the energy market, including arbitrage.

## B. REVIEW CRITERIA

ARPA-E considers a mix of quantitative and qualitative criteria in determining whether to encourage the submission of a Full Application and whether to select a Full Application for award negotiations.

#### 1. Criteria for Concept Papers

- (1) Impact of the Proposed Technology Relative to NOFO Targets (50%) This criterion involves consideration of the following:
  - The potential for a transformational and disruptive (not incremental) advancement compared to existing or emerging technologies;
  - Achievement of the technical performance targets defined in Section I.E of the NOFO;
  - Identification of techno-economic challenges that must be overcome for the proposed technology to be commercially relevant; and
  - Demonstration of awareness of competing commercial and emerging technologies and identifies how the proposed concept/technology provides significant improvement over existing solutions.
- (2) Overall Scientific and Technical Merit (50%) This criterion involves consideration of the following:
  - The feasibility of the proposed work, as justified by appropriate background, theory, simulation, modeling, experimental data, or other sound scientific and engineering practices;
  - Sufficiency of technical approach to accomplish the proposed R&D objectives, including
    why the proposed concept is more appropriate than alternative approaches and how
    technical risk will be mitigated;
  - Clearly defined project outcomes and final deliverables; and

 The demonstrated capabilities of the individuals performing the project, the key capabilities of the organizations comprising the Project Team, the roles and responsibilities of each organization and (if applicable) previous collaborations among team members supporting the proposed project.

Submissions will not be evaluated against each other since they are not submitted in accordance with a common work statement.

#### 2. CRITERIA FOR FULL APPLICATIONS

Full Applications are evaluated based on the following criteria:

- (1) *Impact of the Proposed Technology* (30%) This criterion involves consideration of the following:
  - The potential for a transformational and disruptive (not incremental) advancement in one or more energy-related fields;
  - Thorough understanding of the current state-of-the-art and presentation of an innovative technical approach to significantly improve performance over the current state-of-the-art;
  - Awareness of competing commercial and emerging technologies and identification of how the proposed concept/technology provides significant improvement over these other solutions; and
  - A reasonable and effective strategy for transitioning the proposed technology from the laboratory to commercial deployment.
- (2) Overall Scientific and Technical Merit (30%) This criterion involves consideration of the following:
  - Whether the proposed work is unique and innovative;
  - Clearly defined project outcomes and final deliverables;
  - Substantiation that the proposed project is likely to meet or exceed the technical performance targets identified in this NOFO;
  - Feasibility of the proposed work based upon preliminary data or other background information and sound scientific and engineering practices and principles;
  - A sound technical approach, including appropriately defined technical tasks, to accomplish the proposed R&D objectives; and
  - Management of risk, to include identifying major technical R&D risks and feasible, effective mitigation strategies.

- (3) *Qualifications, Experience, and Capabilities of the Proposed Project Team* (30%) This criterion involves consideration of the following:
  - The PI and Project Team have the skill and expertise needed to successfully execute the project plan, evidenced by prior experience that demonstrates an ability to perform R&D of similar risk and complexity; and
  - Access to the equipment and facilities necessary to accomplish the proposed R&D effort and/or a clear plan to obtain access to necessary equipment and facilities.
- (4) Soundness of Management Plan (10%) This criterion involves consideration of the following:
  - Plausibility of plan to manage people and resources;
  - Allocation of appropriate levels of effort and resources to proposed tasks;
  - Reasonableness of the proposed project schedule, including major milestones; and
  - Reasonableness of the proposed budget to accomplish the proposed project.

Submissions will not be evaluated against each other since they are not submitted in accordance with a common work statement.

#### 3. CRITERIA FOR REPLIES TO REVIEWER COMMENTS

ARPA-E has not established separate criteria to evaluate Replies to Reviewer Comments. Instead, Replies to Reviewer Comments are evaluated as an extension of the Full Application.

## C. PROGRAM POLICY FACTORS

In addition to the above criteria, ARPA-E may consider the following program policy factors in determining which Concept Papers to encourage to submit a Full Application and which Full Applications to select for award negotiations:

- I. **ARPA-E Portfolio Balance**. Project balances ARPA-E portfolio in one or more of the following areas:
  - a. Diversity of technical personnel in the proposed Project Team;
  - b. Technological diversity;
  - c. Organizational diversity;
  - d. Geographic diversity;
  - e. Technical or commercialization risk; or
  - f. Stage of technology development.
- II. **Relevance to ARPA-E Mission Advancement.** Project contributes to one or more of ARPA-E's key statutory goals:
  - a. Reduction of U.S. dependence on foreign energy sources;

- b. Stimulation of U.S. manufacturing and/or software development
- c. Reduction of energy-related emissions;
- d. Increase in U.S. energy efficiency;
- e. Enhancement of U.S. economic and energy security; or
- f. Promotion of U.S. advanced energy technologies competitiveness.

## III. Synergy of Public and Private Efforts.

- a. Avoids duplication and overlap with other publicly or privately funded projects;
- Promotes increased coordination with nongovernmental entities for demonstration of technologies and research applications to facilitate technology transfer; or
- c. Increases unique research collaborations.
- IV. **Low likelihood of other sources of funding.** High technical and/or financial uncertainty that results in the non-availability of other public, private or internal funding or resources to support the project.
- V. High Project Impact Relative to Project Cost.
- VI. **Qualified Opportunity Zone (QOZ).** Whether the entity is located in an urban and economically distressed area including a Qualified Opportunity Zone (QOZ) or the proposed project will occur in a QOZ or otherwise advance the goals of QOZ. The goals include spurring economic development and job creation in distressed communities throughout the United States. For a list or map of QOZs go to: <a href="https://www.cdfifund.gov/opportunity-zones">https://www.cdfifund.gov/opportunity-zones</a>.

## D. REVIEW AND SELECTION PROCESS

#### 1. CONCEPT PAPERS

ARPA-E performs a preliminary review of Concept Papers to determine whether they are compliant and responsive. ARPA-E makes an independent assessment of each compliant and responsive Concept Paper based on the criteria and program policy factors in Sections V.B.1 and V.C of the NOFO. ARPA-E considers a mix of quantitative and qualitative criteria in determining whether to encourage the submission of a Full Application.

#### 2. FULL APPLICATIONS

ARPA-E performs a preliminary review of Full Applications to determine whether they are compliant and responsive. Full Applications found to be noncompliant or nonresponsive may not be merit reviewed or considered for award. ARPA-E makes an independent assessment of each compliant and responsive Full Application based on the criteria and program policy factors in Sections V.B.2 and V.C of the NOFO.

#### 3. REPLY TO REVIEWER COMMENTS

Once ARPA-E has completed its review of Full Applications, reviewer comments on compliant and responsive Full Applications are made available to Applicants via ARPA-E eXCHANGE. ARPA-E may also provide more direct feedback at this time. Applicants may submit an optional Reply to Reviewer Comments, which must be submitted by the deadline stated in the NOFO.

ARPA-E performs a preliminary review of Replies to determine whether they are compliant, as described in Section III.D of the NOFO. ARPA-E will review and consider compliant Replies only.

#### 4. Pre-Selection Clarifications and "Down-Select" Process

Once ARPA-E completes its review of Full Applications and Replies to Reviewer Comments, it may, at the Grants Officer's discretion, conduct a pre-selection clarification process and/or perform a "down-select" of Full Applications. Through the pre-selection clarification process or down-select process, ARPA-E may obtain additional information from select Applicants through pre-selection meetings, webinars, videoconferences, conference calls, written correspondence, or site visits that can be used to make a final selection determination. ARPA-E will not reimburse Applicants for travel and other expenses relating to pre-selection meetings or site visits, nor will these costs be eligible for reimbursement as pre-award costs.

ARPA-E may select applications for award negotiations and make awards without pre-selection meetings and site visits. Participation in a pre-selection meeting or site visit with ARPA-E does not signify that Applicants have been selected for award negotiations.

#### 5. SELECTION FOR AWARD NEGOTIATIONS

ARPA-E carefully considers all of the information obtained through the application process and makes an independent assessment of each compliant and responsive Full Application based on the criteria, risk reviews, and program policy factors in Sections V.B, V.G, and V.C of the NOFO. ARPA-E considers a mix of quantitative and qualitative criteria in determining whether to select an application for award negotiation.

The Selection Official may select all or part of a Full Application for award negotiations. The Selection Official may also postpone a final selection determination on one or more Full Applications until a later date, subject to availability of funds and other factors. ARPA-E will enter into award negotiations only with selected Applicants.

ARPA-E expects to announce selections for negotiations in approximately May 2025 and to execute funding agreements in approximately August 2025.

#### E. ARPA-E REVIEWERS

By submitting an application to ARPA-E, Applicants consent to ARPA-E's use of Federal employees, contractors, and experts from educational institutions, nonprofits, industry, and governmental and intergovernmental entities as reviewers. ARPA-E selects reviewers based on their knowledge and understanding of the relevant field and application, their experience and skills, and their ability to provide constructive feedback on applications.

ARPA-E requires all reviewers to complete a Conflict-of-Interest Certification and Nondisclosure Agreement through which they disclose their knowledge of any actual or apparent conflicts and agree to safeguard confidential information contained in Concept Papers, Full Applications, and Replies to Reviewer Comments. In addition, ARPA-E trains its reviewers in proper evaluation techniques and procedures.

Applicants are not permitted to nominate reviewers for their applications. Applicants may contact the Grants Officer by email (<u>ARPA-E-CO@hq.doe.gov</u>) if they have knowledge of a potential conflict of interest or a reasonable belief that a potential conflict exists.

## F. ARPA-E SUPPORT CONTRACTORS

ARPA-E utilizes contractors to assist with the evaluation of applications and project management. To avoid actual and apparent conflicts of interest, ARPA-E prohibits its support contractors from submitting or participating in the preparation of applications to ARPA-E.

By submitting an application to ARPA-E, Applicants represent that they are not performing support contractor services for ARPA-E in any capacity and did not obtain the assistance of ARPA-E's support contractor to prepare the application. ARPA-E will not consider any applications that are submitted by or prepared with the assistance of its support contractors.

## G. RISK REVIEW

If selected for award negotiations, ARPA-E may evaluate the risks posed by the Applicant using the criteria set forth at 2 CFR §200.206(b)(2). ARPA-E may require special award terms and conditions depending upon results of the risk analysis.

Further, as DOE invests in critical infrastructure and funds critical and emerging technology areas, DOE also considers possible vectors of undue foreign influence in evaluating risk. If high risks are identified and cannot be sufficiently mitigated, DOE may elect to not fund the applicant. As part of the research, technology, and economic security risk review, DOE may contact the applicant and/or proposed project team members for additional information to inform the review.

#### ARPA-E will not make an award if ARPA-E has determined that:

- The entity submitting the proposal or application:
  - has an owner or Covered Individual that is party to a malign foreign talent recruitment program of the People's Republic of China or another foreign country of concern;<sup>27</sup>
  - has a business entity, parent company, or subsidiary located in the People's Republic of China or another foreign country of concern; or
  - has an owner or Covered Individual that has a foreign affiliation with a research institution located in the People's Republic of China or another foreign country of concern; and
- The relationships and commitments described above:
  - interfere with the capacity for activities supported by the Federal agency to be carried out:
  - o create duplication with activities supported by the Federal agency;
  - present concerns about conflicts of interest;
  - were not appropriately disclosed to the Federal agency;
  - o violate Federal law or terms and conditions of the Federal agency; or
  - o pose a risk to national security.

If high risks are identified and cannot be sufficiently mitigated, ARPA-E may elect to not fund the applicant.

## VI. AWARD NOTICES AND AWARD TYPES

## A. AWARD NOTICES

Recipients should register with FedConnect in order to receive notification that their funding agreement has been executed by the Grants Officer and to obtain a copy of the executed funding agreement. Please refer to <a href="https://www.fedconnect.net/FedConnect/">https://www.fedconnect.net/FedConnect/</a> for registration instructions.

#### 1. REJECTED SUBMISSIONS

Noncompliant and nonresponsive Concept Papers and Full Applications are rejected by the Grants Officer and are not merit reviewed or considered for award. The Grants Officer sends a notification email to the technical and administrative points of contact designated by the Applicant in ARPA-E eXCHANGE. The notification states the basis upon which the Concept Paper or Full Application was rejected.

#### 2. CONCEPT PAPER NOTIFICATIONS

ARPA-E promptly notifies Applicants of its determination to encourage or discourage the submission of a Full Application. ARPA-E sends a notification letter by email to the technical and administrative points of contact designated by the Applicant in ARPA-E eXCHANGE. ARPA-E provides feedback in the notification letter in order to guide further development of the proposed technology.

Applicants may submit a Full Application even if they receive a notification discouraging them from doing so. By discouraging the submission of a Full Application, ARPA-E intends to convey its lack of programmatic interest in the proposed project. Such assessments do not necessarily reflect judgments on the merits of the proposed project. The purpose of the Concept Paper phase is to save Applicants the considerable time and expense of preparing a Full Application that is unlikely to be selected for award negotiations.

A notification letter encouraging the submission of a Full Application does <u>not</u> authorize the Applicant to commence performance of the project.

#### 3. Full Application Notifications

ARPA-E promptly notifies Applicants of its determination to select, postpone a final decision until a later date, or not select a Full Application for award negotiation. ARPA-E sends a notification letter by email to the technical and administrative points of contact designated by the Applicant in ARPA-E eXCHANGE.

Written feedback on Full Applications is only made available to Applicants in the Replies to Reviewer Comments process. ARPA-E does not offer or provide debriefings.

ARPA-E may stagger its selection determinations. As a result, some Applicants may receive their notification letter in advance of other Applicants.

#### a. SUCCESSFUL APPLICANTS

ARPA-E has discretion to select all or part of a proposed project for negotiation of an award. A notification letter selecting a Full Application for award negotiations does <u>not</u> authorize the Applicant to commence performance of the project. **ARPA-E selects Full Applications for award negotiations, not for award.** Applicants do not receive an award until award negotiations are complete and the Grants Officer executes the funding agreement. The notice of Federal award signed by the Grants Officer is the official document that obligates funds. ARPA-E may terminate award negotiations at any time for any reason.

The Grants Officer is the only individual who can make awards on behalf of ARPA-E or obligate ARPA-E to the expenditure of public funds. A commitment or obligation by any individual other than the Grants Officer, either explicit or implied, is invalid.

ARPA-E awards may not be transferred, assigned, or assumed without the prior written consent of a Grants Officer.

#### **b.** Postponed Selection Determinations

A notification letter postponing a final selection determination until a later date does <u>not</u> authorize the Applicant to commence performance of the project. ARPA-E may ultimately determine to select or not select the Full Application for award negotiations.

#### c. Unsuccessful Applicants

By not selecting a Full Application, ARPA-E intends to convey its lack of programmatic interest in the proposed project. Such assessments do not necessarily reflect judgments on the merits of the proposed project. ARPA-E hopes that unsuccessful Applicants will submit innovative ideas and concepts for future NOFOs.

#### B. Pre-Award Costs

ARPA-E will not reimburse any pre-award costs incurred by Applicants before they are selected for award negotiations. Please refer to Section VI.A of the NOFO for guidance on award notices.

Upon selection for award negotiations, Applicants may incur pre-award costs at their own risk, consistent with the requirements in 2 C.F.R. Part 200, as modified by 2 C.F.R. Part 910, and other Federal laws and regulations. All submitted budgets are subject to change and are

typically reworked during award negotiations. ARPA-E is under no obligation to reimburse preaward costs if, for any reason, the Applicant does not receive an award or the award is made for a lesser amount than the Applicant expected, or if the costs incurred are not allowable, allocable, or reasonable.

## C. RENEWAL AWARDS

At ARPA-E's sole discretion, awards resulting from this NOFO may be renewed by adding one or more budget periods, extending the period of performance of the initial award, or issuing a new award. Renewal funding is contingent on: (1) availability of funds appropriated by Congress for the purpose of this program; (2) substantial progress towards meeting the objectives of the approved application; (3) submittal of required reports; (4) compliance with the terms and conditions of the award; (5) ARPA-E approval of a renewal application; and (6) other factors identified by the Agency at the time it solicits a renewal application.

## D. FUNDING AGREEMENT TYPES

Through cooperative agreements, other transactions, and similar agreements, ARPA-E provides financial and other support to projects that have the potential to realize ARPA-E's statutory mission. ARPA-E does not use such agreements to acquire property or services for the direct benefit or use of the U.S. Government.

#### 1. COOPERATIVE AGREEMENTS

ARPA-E generally uses Cooperative Agreements to provide financial and other support to Recipients.

Cooperative Agreements involve the provision of financial or other support to accomplish a public purpose of support or stimulation authorized by Federal statute. Under Cooperative Agreements, the Government and Recipients share responsibility for the direction of projects.

ARPA-E encourages Recipients to review the Model Cooperative Agreement, which is available at https://arpa-e.energy.gov/technologies/project-guidance.

# 2. FUNDING AGREEMENTS WITH FFRDCs/DOE LABS, GOGOS, AND FEDERAL INSTRUMENTALITIES

Any Federally Funded Research and Development Centers (FFRDC) involved as a member of a Project Team must provide the information requested in the "FFRDC Lab Authorization" and "Field Work Proposal" section of the Business Assurances & Disclosures Form, which is submitted with the Applicant's Full Application.

When a FFRDC/DOE Lab (including the National Energy Technology Laboratory or NETL) is the *lead organization* for a Project Team, ARPA-E executes a funding agreement directly with the FFRDC/DOE Lab and a single, separate Cooperative Agreement with another entity on the Project Team. Notwithstanding the use of multiple agreements, the FFRDC/DOE Lab is the lead organization for the entire project, including all work performed by the FFRDC/DOE Lab and the rest of the Project Team.

When a FFRDC/DOE Lab is a *member* of a Project Team, ARPA-E executes a funding agreement directly with the FFRDC/DOE Lab and a single, separate Cooperative Agreement with the Recipient, as the lead organization for the Project Team. Notwithstanding the use of multiple agreements, the Recipient under the Cooperative Agreement is the lead organization for the entire project, including all work performed by the FFRDC/DOE Lab and the rest of the Project Team.

Funding agreements with DOE/NNSA FFRDCs take the form of Work Authorizations issued to DOE/NNSA FFRDCs through the DOE/NNSA Field Work Proposal system for work performed under Department of Energy Management & Operation Contracts. Funding agreements with non-DOE/NNSA FFRDCs, GOGOs (including NETL), and Federal instrumentalities (e.g., Tennessee Valley Authority) will be consistent with the sponsoring agreement between the U.S. Government and the Laboratory. Any funding agreement with an FFRDC or GOGO will have similar terms and conditions as ARPA-E's Model Cooperative Agreement (<a href="https://arpa-e.energy.gov/technologies/project-guidance/pre-award-guidance/funding-agreements">https://arpa-e.energy.gov/technologies/project-guidance/pre-award-guidance/funding-agreements</a>).

Non-DOE GOGOs and Federal agencies may be proposed to provide support to the Project Team members on an applicant's project, through a Cooperative Research and Development Agreement (CRADA) or similar agreement.

#### 3. OTHER TRANSACTIONS AUTHORITY

ARPA-E may use its "other transactions" authority under the America COMPETES Reauthorization Act of 2010 and DOE's other transactions authority as codified at 42 USC §7256(a) and (g) to enter into an other transaction agreement with Recipients on a case-by-case basis.

ARPA-E may negotiate an other transaction agreement when it determines that the use of a standard cooperative agreement, grant, or contract is not feasible or appropriate for a project.

The federal share of other transactions agreements should meet or exceed \$3,000,000. In general, an other transaction agreement normally requires a minimum cost share of 50%. See Section II.D.2 of the NOFO.

#### VII. POST-AWARD REQUIREMENTS AND ADMINISTRATION

The Recipient is the responsible authority regarding the settlement and satisfaction of all contractual and administrative issues, including but not limited to disputes and claims arising out of any agreement between the Recipient and a FFRDC contractor. Recipients are required to flow down these requirements to their Subrecipients through subawards or related agreements.

## A. NATIONAL POLICY REQUIREMENTS

The following national policy requirements apply to Recipients.

- If an award is made to a DOE/NNSA National Laboratory, all Disputes and Claims will be resolved in accordance with the terms and conditions of the DOE/NNSA National Laboratory's management and operating (M&O) contract, as applicable, in consultation between DOE and the Recipient.
- If an award is made to another Federal agency or its FFRDC contractor, all Disputes and Claims will be resolved in accordance with the terms and conditions of the interagency agreement in consultation between DOE and the Recipient.

#### 1. NATIONAL POLICY ASSURANCES

Project Teams, including Recipients and Subrecipients, are required to comply with the National Policy Assurances in effect on the date of award located at <a href="https://www.nsf.gov/awards/managing/rtc.jsp">https://www.nsf.gov/awards/managing/rtc.jsp</a> in accordance with 2 C.F.R. § 200.300.

## 2. Environmental Impact Questionnaire

By law, ARPA-E is required to evaluate the potential environmental impact of projects that it is considering for funding. In particular, ARPA-E must determine <u>before funding a project</u> whether the project qualifies for a categorical exclusion under 10 C.F.R. § 1021.410 or whether it requires further environmental review (i.e., an environmental assessment or an environmental impact statement).

To facilitate and expedite ARPA-E's environmental review, Recipients are required to complete an Environmental Impact Questionnaire during award negotiations. This form is available at <a href="https://arpa-e.energy.gov/technologies/project-guidance/pre-award-guidance/required-forms-and-templates">https://arpa-e.energy.gov/technologies/project-guidance/pre-award-guidance/required-forms-and-templates</a>. Each Recipient must wait to complete the Environmental Impact Questionnaire (EIQ) until after ARPA-E has notified them that Attachment 3 Statement of Program Objectives is in final form. The completed EIQ is then due back to ARPA-E within 14 calendar days.

#### B. Administrative Requirements

## 1. COST SHARE PAYMENTS. 40

All proposed cost share contributions must be reviewed in advance by the Grants Officer and incorporated into the project budget before the expenditures are incurred.

The Recipient is required to pay the "Cost Share" amount as a percentage of the total project costs in each invoice period for the duration of the period of performance. Small Businesses should refer to Section II.D.3 of the NOFO.

ARPA-E may deny reimbursement requests, in whole or in part, or modify or terminate funding agreements where Recipients (or Project Teams) fail to comply with ARPA-E's cost share payment requirements.

#### 2. Intellectual Property and Data Management Plans

ARPA-E requires every Project Team to negotiate and establish an Intellectual Property Management Plan for the management and disposition of intellectual property arising from the project. The Recipient must submit a completed and signed Intellectual Property Management plan to ARPA-E within six weeks of the effective date of the ARPA-E funding agreement. All Intellectual Property Management Plans are subject to the terms and conditions of the ARPA-E funding agreement and its intellectual property provisions, and applicable Federal laws, regulations, and policies, all of which take precedence over the terms of Intellectual Property Management Plans.

ARPA-E has developed a template for Intellectual Property Management Plans (<a href="https://arpa-e.energy.gov/technologies/project-guidance/post-award-guidance/project-management-reporting-requirements">https://arpa-e.energy.gov/technologies/project-guidance/post-award-guidance/project-management-reporting-requirements</a>) to facilitate and expedite negotiations between Project Team members. ARPA-E does not mandate the use of this template. ARPA-E and DOE do not make any warranty (express or implied) or assume any liability or responsibility for the accuracy, completeness, or usefulness of the template. ARPA-E and DOE strongly encourage Project Teams to consult independent legal counsel before using the template.

Awardees are also required, post-award, to submit a Data Management Plan (DMP) that addresses how data generated in the course of the work performed under an ARPA-E award will be preserved and, as appropriate, shared publicly. The Recipient must submit a completed and signed DMP - as part of the Team's Intellectual Property Management Plan - to ARPA-E within six weeks of the effective date of the ARPA-E funding agreement.

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<sup>&</sup>lt;sup>40</sup> Please refer to Section II.D of the NOFO for guidance on cost share requirements.

#### 3. U.S. COMPETITIVENESS

A primary objective of DOE's multi-billion-dollar research, development and demonstration investments – including ARPA-E awards - is advancement of new energy technologies, manufacturing capabilities, and supply chains for and by U.S. industry and labor. Therefore, in exchange for receiving taxpayer dollars to support an applicant's project, the applicant must agree to the following U.S. Competitiveness Provision as part of an award under this NOFO.

#### U.S. Competitiveness

The Contractor (Recipient in ARPA-E awards) agrees that any products embodying any subject invention or produced through the use of any subject invention will be manufactured substantially in the United States unless the Contractor can show to the satisfaction of DOE that it is not commercially feasible. In the event DOE agrees to foreign manufacture, there will be a requirement that the Government's support of the technology be recognized in some appropriate manner, e.g., alternative binding commitments to provide an overall net benefit to the U.S. economy. The Contractor agrees that it will not license, assign or otherwise transfer any subject invention to any entity, at any tier, unless that entity agrees to these same requirements. Should the Contractor or other such entity receiving rights in the invention(s): (1) undergo a change in ownership amounting to a controlling interest, or (2) sell, assign, or otherwise transfer title or exclusive rights in the invention(s), then the assignment, license, or other transfer of rights in the subject invention(s) is/are suspended until approved in writing by DOE. The Contractor and any successor assignee will convey to DOE, upon written request from DOE, title to any subject invention, upon a breach of this paragraph. The Contractor will include this paragraph in all subawards/contracts, regardless of tier, for experimental, developmental or research work.

A subject invention is any invention of the contractor conceived or first actually reduced to practice in the performance of work under an award. An invention is any invention or discovery which is or may be patentable. The contractor includes any awardee, recipient, sub-awardee, or sub-recipient.

As noted in the U.S. Competitiveness Provision, at any time in which an entity cannot meet the requirements of the U.S. Competitiveness Provision, the entity may request a modification or waiver of the U.S. Competitiveness Provision. For example, the entity may propose modifying the language of the U.S. Competitiveness Provision in order to change the scope of the requirements or to provide more specifics on the application of the requirements for a particular technology. As another example, the entity may request that the U.S. Competitiveness Provision be waived in lieu of a net benefits statement or U.S. manufacturing plan. The statement or plan would contain specific and enforceable commitments that would be beneficial to the U.S. economy and competitiveness. Commitments could include manufacturing specific products in the U.S., making a specific investment in a new or existing U.S. manufacturing facility, keeping certain activities based in the U.S. or supporting a certain number of jobs in the

U.S. related to the technology. If DOE, in its sole discretion, determines that the proposed modification or waiver promotes commercialization and provides substantial U.S. economic benefits, DOE may grant the request and, if granted, modify the award terms and conditions for the requesting entity accordingly.

The U.S. Competitiveness Provision is implemented by DOE pursuant to a Determination of Exceptional Circumstances (DEC) under the Bayh-Dole Act and DOE Patent Waivers. See Section VIII.A, "Title to Subject Inventions", of this NOFO for more information on the DEC and DOE Patent Waiver.

#### 4. Nondisclosure and Confidentiality Agreements Representations

In submitting an application in response to this NOFO the Applicant <u>represents</u> that:

- (1) It does not and will not require its employees or contractors to sign internal nondisclosure or confidentiality agreements or statements prohibiting or otherwise restricting its employees or contractors from lawfully reporting waste, fraud, or abuse to a designated investigative or law enforcement representative of a Federal department or agency authorized to receive such information.
- (2) It does not and will not use any Federal funds to implement or enforce any nondisclosure and/or confidentiality policy, form, or agreement it uses unless it contains the following provisions:
  - a. "These provisions are consistent with and do not supersede, conflict with, or otherwise alter the employee obligations, rights, or liabilities created by existing statute or Executive order relating to (1) classified information, (2) communications to Congress, (3) the reporting to an Inspector General of a violation of any law, rule, or regulation, or mismanagement, a gross waste of funds, an abuse of authority, or a substantial and specific danger to public health or safety, or (4) any other whistleblower protection. The definitions, requirements, obligations, rights, sanctions, and liabilities created by controlling Executive orders and statutory provisions are incorporated into this agreement and are controlling."
  - b. The limitation above shall not contravene requirements applicable to Standard Form 312, Form 4414, or any other form issued by a Federal department or agency governing the nondisclosure of classified information.
  - c. Notwithstanding the provision listed in paragraph (a), a nondisclosure confidentiality policy form or agreement that is to be executed by a person connected with the conduct of an intelligence or intelligence-related activity, other than an employee or officer of the United States Government, may contain provisions appropriate to the particular activity for which such document is to be used. Such form or agreement shall, at a minimum, require that the person will not disclose any classified

information received in the course of such activity unless specifically authorized to do so by the United States Government. Such nondisclosure or confidentiality forms shall also make it clear that they do not bar disclosure to congress, or to an authorized official of an executive agency or the Department of Justice, that are essential to reporting a substantial violation of law.

#### 5. Interim Conflict of Interest Policy for Financial Assistance

The DOE interim Conflict of Interest Policy for Financial Assistance (COI Policy) can be found at https://www.energy.gov/management/financial-assistance-letter-no-fal-2022-02. This policy is applicable to all non-Federal entities applying for, or that receive, DOE funding by means of a financial assistance award (e.g., a grant, cooperative agreement, or technology investment agreement or similar other transaction agreement) and, through the implementation of this policy by the entity, to each Investigator who is planning to participate in, or is participating in, the project funded wholly or in part under the DOE financial assistance award. DOE's interim COI Policy establishes standards that provide a reasonable expectation that the design, conduct, and reporting of projects funded wholly or in part under DOE financial assistance awards will be free from bias resulting from financial conflicts of interest or organizational conflicts of interest. The applicant is subject to the requirements of the interim COI Policy and within each application for financial assistance, the applicant must certify that it is, or will be by the time of receiving any financial assistance award, compliant with all requirements in the interim COI Policy. For applicants to any ARPA-E NOFO, this certification, disclosure of any managed or unmanaged conflicts of interest, and a copy of (or link to) the applicant's own conflict of interest policy must be included with the information provided in the Business Assurances & Disclosures Form. The applicant must also flow down the requirements of the interim COI Policy to any subrecipient non-Federal entities.

## 6. COMPLIANCE AUDIT REQUIREMENT

A recipient organized as a for-profit entity expending \$1,000,000 or more of DOE funds in the entity's fiscal year (including funds expended as a Subrecipient) must have an annual compliance audit performed at the completion of its fiscal year. For additional information, refer to Subpart F of: (i) 2 C.F.R. Part 200, and (ii) 2 C.F.R. Part 910.

If an educational institution, non-profit organization, or state/local government has expended \$1,000,000 or more of Federal funds (including funds expended as a Subrecipient) in the entity's fiscal year, the entity must have an annual compliance audit performed at the completion of its fiscal year. For additional information refer to Subpart F of 2 C.F.R. Part 200.

## 7. RESEARCH SECURITY TRAINING REQUIREMENT

Covered individuals listed on applications under this NOFO are required to certify that they have taken research security training consistent with Section 10634 of the CHIPS and Science

Act of 2022. In addition, applicants who receive an award must maintain sufficient records (records must be retained for the time period noted in 2 CFR 200.334 and made available to DOE upon request) of their compliance with this requirement for covered individuals at the Recipient organization and they must extend this requirement to any and all Subrecipients. To fulfill this requirement, an applicant may utilize the four one-hour training modules developed by the National Science Foundation at <a href="https://new.nsf.gov/research-security/training">https://new.nsf.gov/research-security/training</a> or develop and implement their own research security training program aligned with the requirements in Section 10634(b) of the CHIPS and Science Act of 2022. The submission of an application to this NOFO constitutes the applicant's acceptance of this requirement.

# C. REPORTING

Recipients are required to submit periodic, detailed reports on technical, financial, and other aspects of the project, as described in Attachment 4 to ARPA-E's Model Cooperative Agreement (<a href="https://arpa-e.energy.gov/technologies/project-guidance/pre-award-guidance/funding-agreements">https://arpa-e.energy.gov/technologies/project-guidance/pre-award-guidance/funding-agreements</a>).

## 1. Fraud, Waste, and Abuse

An applicant, recipient, or subrecipient must promptly disclose whenever in connection with the federal award (including any activities or subawards thereunder), it has credible evidence of the commission of a violation of Federal criminal law involving fraud, conflict of interest, bribery, or gratuity violations found in Title 18 of the United States Code or a violation of the civil False Claims Act (31 U.S.C. 3729-3733). The disclosure must be made in writing to the Federal agency, the agency's Office of Inspector General, and pass-through entity (if applicable.) Recipients and subrecipients are also required to report matters related to recipient integrity and performance in accordance with Appendix XII of this part. Failure to make required disclosures can result in any of the remedies described in 2 C.F.R. §200.339. (See also 2 C.F.R. part 180, 31 U.S.C. 3321, and 41 U.S.C. 2313.)

For guidance on reporting such violations and information to the DOE Office of Inspector General (OIG), please visit <a href="https://www.energy.gov/ig/ig-hotline">https://www.energy.gov/ig/ig-hotline</a>.

#### 2. COMMERCIALIZATION PLAN AND SOFTWARE REPORTING

If your project is selected and it targets the development of software, you may be required to prepare a Commercialization Plan for the targeted software and agree to special provisions that require the reporting of the targeted software and its utilization. This special approach to projects that target software mirrors the requirements for reporting that attach to new inventions made in performance of an award.

## VIII. OTHER INFORMATION

## A. TITLE TO SUBJECT INVENTIONS

Ownership of subject inventions is governed pursuant to the authorities listed below:

- Domestic Small Businesses, Educational Institutions, and Nonprofits: Under the Bayh-Dole Act (35 U.S.C. § 200 et seq.), domestic small businesses, educational institutions, and nonprofits may elect to retain title to their subject inventions;
- All other parties: The federal Non-Nuclear Energy Act of 1974, 42. U.S.C. 5908, provides
  that the government obtains title to new subject inventions unless a waiver is granted
  (see below):
  - Class Patent Waiver for Domestic Large Businesses: DOE has issued a class patent
    waiver that applies to this NOFO. Under this class patent waiver, domestic large
    businesses may elect title to their subject inventions similar to the right provided to
    the domestic small businesses, educational institutions, and nonprofits by law. In
    order to avail itself of the class patent waiver, a domestic large business must agree
    to the U.S. Competitiveness Provision in accordance with Section VII.B.3 of this
    NOFO.
  - Advance and Identified Waivers: For applicants that do not fall under the class patent waiver or the Bayh-Dole Act, those applicants may request a patent waiver that will cover subject inventions that may be made under the award, in advance of or within 30 days after the effective date of the award. Even if an advance waiver is not requested or the request is denied, the recipient will have a continuing right under the award to request a waiver for identified inventions, i.e., individual subject inventions that are disclosed to DOE within the time frames set forth in the award's intellectual property terms and conditions. Any patent waiver that may be granted is subject to certain terms and conditions in 10 CFR 784.
- DEC: On June 07, 2021, DOE approved a DETERMINATION OF EXCEPTIONAL CIRCUMSTANCES (DEC) UNDER THE BAYH-DOLE ACT TO FURTHER PROMOTE DOMESTIC MANUFACTURE OF DOE SCIENCE AND ENERGY TECHNOLOGIES. In accordance with this DEC, all awards, including sub-awards, under this NOFO made to a Bayh-Dole entity (domestic small businesses and nonprofit organizations) shall include the U.S. Competitiveness Provision in accordance with Section VII.B.3 of this NOFO. A copy of the DEC may be found on the DoE website. Pursuant to 37 CFR § 401.4, any Bayh-Dole entity affected by this DEC has the right to appeal it by providing written notice to DOE within 30 working days from the time it receives a copy of the determination.

## B. GOVERNMENT RIGHTS IN SUBJECT INVENTIONS

Where Recipients and Subrecipients retain title to subject inventions, the U.S. Government retains certain rights.

#### 1. GOVERNMENT USE LICENSE

The U.S. Government retains a nonexclusive, nontransferable, irrevocable, paid-up license to practice or have practiced for or on behalf of the United States any subject invention throughout the world. This license extends to contractors doing work on behalf of the Government.

#### 2. MARCH-IN RIGHTS

The U.S. Government retains march-in rights with respect to all subject inventions. Through "march-in rights," the Government may require a Recipient or Subrecipient who has elected to retain title to a subject invention (or their assignees or exclusive licensees), to grant a license for use of the invention. In addition, the Government may grant licenses for use of the subject invention when Recipients, Subrecipients, or their assignees and exclusive licensees refuse to do so.

The U.S. Government may exercise its march-in rights if it determines that such action is necessary under any of the four following conditions:

- The owner or licensee has not taken or is not expected to take effective steps to achieve practical application of the invention within a reasonable time;
- The owner or licensee has not taken action to alleviate health or safety needs in a reasonably satisfactory manner;
- The owner has not met public use requirements specified by Federal statutes in a reasonably satisfactory manner; or
- The U.S. Manufacturing requirement has not been met.

## C. RIGHTS IN TECHNICAL DATA

Data rights differ based on whether data is first produced under an award or instead was developed at private expense outside the award.

- Background or "Limited Rights Data": The U.S. Government will not normally require
  delivery of technical data developed solely at private expense prior to issuance of an
  award, except as necessary to monitor technical progress and evaluate the potential
  of proposed technologies to reach specific technical and cost metrics.
- Generated Data: The U.S. Government normally retains very broad rights in technical data produced under Government financial assistance awards, including the right to distribute to the public. However, pursuant to special statutory authority, certain categories of data generated under ARPA-E awards may be protected from public disclosure for up to for up to ten years (or more, if approved by ARPA-E) in accordance with provisions that will be set forth in the award. In addition, invention disclosures may be protected from public disclosure for a reasonable time in order to allow for filing a patent application.

## D. PROTECTED PERSONALLY IDENTIFIABLE INFORMATION

Applicants may not include any Protected Personally Identifiable Information (Protected PII) in their submissions to ARPA-E. Protected PII is defined as data that, if compromised, could cause harm to an individual such as identity theft. Listed below are examples of Protected PII that Applicants must not include in their submissions.

- Social Security Numbers in any form;
- Place of Birth associated with an individual;
- Date of Birth associated with an individual;
- Mother's maiden name associated with an individual;
- Biometric record associated with an individual;
- Fingerprint;
- Iris scan;
- DNA;
- Medical history information associated with an individual;
- Medical conditions, including history of disease;
- Metric information, e.g., weight, height, blood pressure;
- Criminal history associated with an individual;
- Ratings;
- Disciplinary actions;
- Performance elements and standards (or work expectations) are PII when they are so
  intertwined with performance appraisals that their disclosure would reveal an
  individual's performance appraisal;
- Financial information associated with an individual;
- Credit card numbers;
- Bank account numbers; and
- Security clearance history or related information (not including actual clearances held).

#### IX. GLOSSARY

**Applicant:** The entity that submits the application to ARPA-E. In the case of a Project Team, the Applicant is the lead organization listed on the application.

**Application:** The entire submission received by ARPA-E, including the Preliminary Application, Full Application, Reply to Reviewer Comments, and Small Business Grant Application (if applicable).

**ARPA-E:** The Advanced Research Projects Agency – Energy, an agency of the U.S. Department of Energy.

**Covered Individual:** an individual who contributes in a substantive, meaningful way to the scientific development or execution of an R&D project proposed to be carried out with an award from ARPA-E. This includes, but is not limited to, the PI, Co-PI, Key Personnel, and technical staff (e.g., postdoctoral fellows/researchers and graduate students). ARPA-E may further designate covered individuals during award negotiations or the award period of performance.

**Deliverable**: A deliverable is the quantifiable goods or services that will be provided upon the successful completion of a project task or sub-task.

**DOE:** U.S. Department of Energy

**DOE/NNSA:** U.S. Department of Energy/National Nuclear Security Administration.

**FFRDCs:** Federally Funded Research and Development Centers

**Foreign Affiliation:** A funded or unfunded academic, professional, or institutional appointment or position with a foreign government or government-owned entity, whether full-time, part-time, or voluntary (including adjunct, visiting, or honorary).

**For-Profit Organizations (or For-Profit Entities):** Entities organized for-profit that are Large Businesses or Small Businesses as those terms are defined elsewhere in this Glossary.

**GOCOs:** U.S. Government Owned, Contractor Operated laboratories.

**GOGOs:** U.S. Government Owned, Government Operated laboratories.

**Institutions of Higher Education** (or *educational institutions*): Has the meaning set forth at 20 U.S.C. 1001.

**Large Business:** Large businesses are entities organized for-profit other than small businesses as defined elsewhere in this Glossary.

Malign Foreign Talent Recruitment Program: The meaning given such term in section 10638 of the Research and Development, Competition, and Innovation Act (division B of Public Law 117–167) or 42 USC 19237, as of October 20, 2022.

**Milestone:** A milestone is the tangible, observable measurement that will be provided upon the successful completion of a project task or sub-task.

PI: Principal Investigator.

**Small Business:** Small businesses are domestically incorporated entities that meet the criteria established by the U.S. Small Business Administration's (SBA) "Table of Small Business Size Standards Matched to North American Industry Classification System Codes" (NAICS) (<a href="http://www.sba.gov/content/small-business-size-standards">http://www.sba.gov/content/small-business-size-standards</a>).

**Subject Invention:** Any invention conceived or first actually reduced to practice under an ARPA-E funding agreement.

**Task:** A task is an operation or segment of the work plan that requires both effort and resources. Each task (or sub-task) is connected to the overall objective of the project, via the achievement of a milestone or a deliverable.

**Total Project Cost:** The sum of the Recipient share and the Federal Government share of total allowable costs. The Federal Government share generally includes costs incurred by GOGOs, FFRDCs, and GOCOs.

**TT&O:** Technology Transfer and Outreach. (See Section I.H.8 of the NOFO for more information).