FINANCIAL ASSISTANCE
NOTICE OF FUNDING OPPORTUNITY

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

CATALYTIC APPLICATION TESTING FOR ACCELERATED LEARNING CHEMISTRIES VIA HIGH-THROUGHPUT EXPERIMENTATION AND MODELING EFFICIENTLY SBIR/STTR (CATALCHEM-E SBIR/STTR)

Announcement Type: Initial Announcement
Notice of Funding Opportunity No. DE-FOA-0003506
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Questions about this NOFO? Check the Frequently Asked Questions available at https://arpa-e.energy.gov/faqs. For questions that have not already been answered, email ARPA-E-CO@hq.doe.gov (with NOFO name and number in subject line). Problems with ARPA-E eXCHANGE? Email ExchangeHelp@hq.doe.gov (with NOFO name and number in subject line).

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BASIC INFORMATION

KEY DATES:	
Notice of Funding Opportunity (NOFO) Issue Date:	November 14, 2024
Deadline for Concept Paper Questions to ARPA-E-CO@hq.doe.gov:	5 PM ET, December 10, 2024
Submission Deadline for Concept Papers:	9:30 AM ET, December 17, 2024
Anticipated Timeframe for Encourage/Discourage Notifications:	March, 2025
Deadline for Full Application Questions to ARPA-E-CO@hq.doe.gov:	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 $35 million, subject to the availability of appropriated funds to be shared between NOFOs DE-FOA-0003505 and DE-FOA-0003506.
Anticipated Number and Value of Awards	ARPA-E anticipates making approximately 10-12 awards between NOFOs DE-FOA-0003505 and DE-FOA-0003506. ARPA-E may issue one, multiple, or no awards. The Federal share of awards may vary between $2.5 million and $3.5 million.
Agency Contact Information	• Questions and answers (Q&As) about ARPA-E and this specific NOFO: http://arpa-e.energy.gov/faq. • Send other questions about the NOFO to: ARPA-E-CO@hq.doe.gov. • Send questions about use of ARPA-E eXCHANGE to: ExchangeHelp@hq.doe.gov. Upon the issuance of a NOFO, only the Grants Officer via ARPA-E-CO@hq.doe.gov 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.

Catalyst discovery, development, and optimization has been critical to the commodity fuels and chemical industry, but it can take years to develop a durable commercial catalyst. Further, the development process often relies on experience, intuition, engineering judgement, and experimental trial and error across multiple length scales. Recent advancements in high-throughput experimentation (HTE) methods using artificial intelligence (AI) and machine learning (ML) present a significant and unique opportunity to accelerate the design and development cycle for catalyst research and development (R&D) workflows.

The CATALCHEM-E program seeks to disrupt and accelerate the traditional heterogeneous catalyst R&D workflows spanning from rational design of research catalyst powders to synthesis, characterization, and reactor-scale testing of technical catalyst composites. These novel workflows will be developed in two phases of 18 months each. In Phase 1, teams will

tightly couple state-of-the-art HTE methods with advanced tools and techniques in AI/ML to achieve more than a ten-time acceleration in the catalyst development cycle. Further impact will be realized in Phase 2 by utilizing the tools developed in Phase 1 to achieve novel catalyst-reaction discovery and co-design. The program encourages the development of closed-loop and other promising, automated workflow topologies that enable inverse design of heterogenous catalysts. Other key program goals include synthesis of new "drop-in" manufacturable technical catalysts in engineered forms at the kilogram scale for thermochemical or electrochemical reactor systems, generation of high-quality databases, and creation of AI/ML models. Various communities, such as subject matter experts in HTE, AI/ML, computational modeling and simulation, traditional experimental catalysis, industrial catalysis, and manufacturing must come together in an unprecedented way to achieve these ambitious, game-changing program goals.

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: http://arpa-e.energy.gov/.

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."[1] 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 early-stage 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 (http://www.eere.energy.gov/), the Office of Fossil Energy and Carbon Management (https://www.energy.gov/fecm/office-fossil-energy-and-carbon-management), the Office of Nuclear Energy (http://www.energy.gov/ne/office-nuclear-energy), and the Office of Electricity (https://www.energy.gov/oe/office-electricity).

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.

[1] OMB Circular A-11 (https://www.whitehouse.gov/wp-content/uploads/2018/06/a11_web_toc.pdf), Section 84, pg. 3.

B. SBIR/STTR PROGRAM OVERVIEW

The Small Business Innovation Research (SBIR) and Small Business Technology Transfer (STTR) programs are Government-wide programs authorized under Section 9 of the Small Business Act (15 U.S.C. § 638). The objectives of the SBIR program are to (1) stimulate technological innovation in the private sector, (2) strengthen the role of Small Business Concerns in meeting Federal R&D needs, (3) increase private sector commercialization of innovations derived from Federal R&D activities, (4) foster and encourage participation by socially and economically disadvantaged and women-owned Small Business Concerns, and (5) improve the return on investment from Federally funded research and economic benefits to the Nation. The objective of the STTR program is to stimulate cooperative partnerships of ideas and technologies between Small Business Concerns and partnering Research Institutions through Federally funded R&D activities.[2]

ARPA-E administers a joint SBIR/STTR program in accordance with the Small Business Act and the SBIR and STTR Policy Directive issued by the U.S. Small Business Administration (SBA).[3] ARPA-E provides SBIR/STTR funding in three phases (Phase I, Phase II, and Phase IIS).

Applicants must apply for a Combined Phase I/II Award or a Combined Phase I/II/IIS Award. Combined Phase I/II and I/II/IIS Awards are intended to develop transformational technologies with disruptive commercial potential. Such commercial potential may be evidenced by (1) the likelihood of follow-on funding by private or non-SBIR/STTR sources if the project is successful, or (2) the Small Business Concern's record of successfully commercializing technologies developed under prior SBIR/STTR awards. Phase IIS awards are a "sequential" (i.e., additional) Phase II award, intended to allow the continued development of promising energy technologies. Combined Phase I/II/IIS awards may be funded up to $4,505,859. Funding amounts will be consistent with the Phase I and Phase II limits posted on SBIR.gov website.[4]

ARPA-E reserves the right to select all or part of a proposed project (i.e., only Phase I, or only Phase I and Phase II). In the event that ARPA-E selects Phase I only or Phase I/II only, then the maximum award amount for a Phase I award is $314,363 and the maximum amount for a Phase I/II award is $2,410,111.

[2] Research Institutions include FFRDCs, nonprofit educational institutions, and other nonprofit research organizations owned and operated exclusively for scientific purposes. Eligible Research Institutions must maintain a place of business in the United States, operate primarily in the United States, or make a significant contribution to the U.S. economy through the payment of taxes or use of American products, materials, or labor.

[3] See 88 Fed. Reg. 19704 (May 3, 2023) or SBIR.gov file at SBIR and STTR Policy Directive - May 2023.

[4] For current SBIR and STTR Phase I and Phase II funding amounts, see https://legacy.www.sbir.gov/about. Phase IIS funding amounts are equal to Phase II funding amounts for both SBIR and STTR awards.

C. PROGRAM OVERVIEW

1. SUMMARY

The Catalytic Application Testing for Accelerated Learning Chemistries via High-throughput Experimentation and Modeling Efficiently (CATALCHEM-E) program aims to disrupt and accelerate the design and development cycle for heterogeneous catalyst R&D workflows. The program will span from rational material discovery to synthesis and final reactor testing. These novel workflows will be developed by coupling the latest advancements in artificial intelligence (AI) and machine learning (ML) with high-throughput experimentation (HTE) to verifiably complete 10–15 years of traditional catalysis R&D work within 12–18 months, thus achieving more than a ten-time acceleration in the catalyst development cycle.[5] The program will then use these new tools to discover and optimize catalytic chemistries relevant to ARPA-E's goals. These new chemistries will ultimately help advance the objective of net-zero carbon emissions by 2050.[6]

Innovations developed under the CATALCHEM-E program will involve:

- Future refinery relevant or other next-generation feedstocks such as hydrogen (H_2), nitrogen (N_2), oxygen (O_2), water (H_2O), carbon dioxide (CO_2), methane (CH_4), ammonia (NH_3), methanol (MeOH), ethanol (EtOH), bio-intermediates ($C_xH_yO_z$), waste plastics, and triglycerides (TAGs); and
- Products like ethylene ($C_2^=$) and propylene ($C_3^=$) as low carbon monomers, and sustainable aviation fuel (SAF), diesel, and syngas as distillate range hydrocarbons.

2. TECHNICAL BACKGROUND

The DOE has set major energy and emissions goals for establishing a net-zero sustainable hydrogen and managed carbon economy within the next few decades.[7,8,9] A feasible transition to this economy by 2050 will require new thermochemical and electrochemical catalytic processes to produce low-emission chemicals, fuels, and materials. Many of the heterogenous catalysts developed to meet 2050 goals have challenges related to throughput, single-pass yield, lifetime, stability, energy requirements (i.e., heat, electricity), manufacturability, supply

[5] Sharon Mitchell, Nina-Luisa Michels, and Javier Pérez-Ramírez, "From Powder to Technical Body: The Undervalued Science of Catalyst Scale Up," *Chemical Society Reviews* 42, no. 14 (June 21, 2013): 6094–6112, https://doi.org/10.1039/C3CS60076A.
[6] U.S. Department of Energy. "How we're moving to net-zero by 2050," (April 2021). https://www.energy.gov/articles/how-were-moving-net-zero-2050.
[7] U.S. Department of Energy. "Hydrogen shot," accessed October 23, 2024. https://www.energy.gov/eere/fuelcells/hydrogen-shot.
[8] U.S. Department of Energy. "Clean Fuels & Products Shot™: Alternative sources for carbon-based products," accessed October 23, 2024. https://www.energy.gov/eere/clean-fuels-products-shottm-alternative-sources-carbon-based-products.
[9] U.S. Department of Energy. "Carbon negative shot," accessed October 23, 2024. https://www.energy.gov/fecm/carbon-negative-shot.

chain security, and cost.[10] To solve these issues in a timely manner, new laboratory-scale powder research catalysts must be quickly discovered, formulated, compounded, and developed into commercial-ready, formed technical catalysts. An overview of the traditional catalysis R&D workflows for research and technical catalyst development is shown in Figure 1.

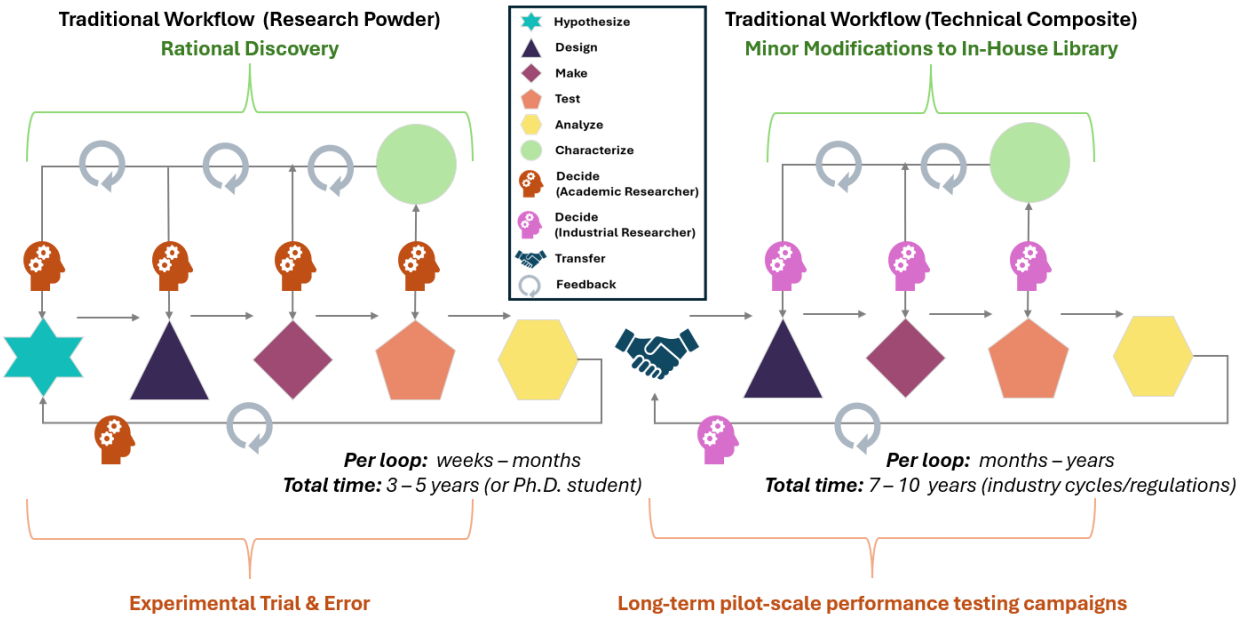

Figure 1. An overview of the traditional catalysis R&D workflows for research and technical catalyst development, which typically takes 10–15 years from conception to pilot-scale testing.

These conventional workflows largely rely on experience, intuition, engineering judgement, and experimental trial and error, followed by long-term pilot-scale performance testing campaigns to derisk the technologies. Additionally, the transfer of research catalyst knowledge and data to the industrial technical catalyst development community must take place for successful commercialization.

Research Catalyst Development (State-of-the-Art): Traditional laboratory-scale research catalyst R&D workflows are based on rational surface science, synthesis, characterization, pre-treatment, and activity testing of new materials. Research catalysts are typically synthesized in powder form at milligram-to-gram quantities and tested over relatively short time periods (hours-to-days) for material compositional screening purposes.[5] Many of these laboratory-scale prepared materials struggle to meet the first-tier performance targets set by catalyst manufacturers (e.g., yield, durability, stability, lifetime) or are too expensive to risk developing into a technical catalyst. Consequently, for some novel materials, the R&D cycle for powder research catalysts focuses on reactive surface fundamentals and the scientific discovery process can take decades to complete.

[10] Yixiao Wang et al., "Catalytic Processes to Accelerate Decarbonization in a Net-Zero Carbon World," *ChemSusChem* 15, no. 24 (December 20, 2022): e202201290, https://doi.org/10.1002/cssc.202201290.

In the past, experimental attempts to accelerate these R&D cycles involved brute force, combinatorial synthesis, and screening of powders to explore compositional space. These techniques were hindered by scale (microgram-to-milligram), reactor geometry, and the rational material design challenge of covering the vast compositional space across the periodic table with just human experience and intuition. Thus, the latter challenge was addressed using in-silico approaches leveraging high-performance computing hardware resources to solve *ab initio* chemistry methods like density functional theory (DFT). Although these approaches have traditionally been limited by computational time, calculation accuracy, and lack of connection to synthesis procedures, commercial technology organizations specializing in software platforms have recently made significant strides in accelerating these techniques.[11,12]

Technical Catalyst Development (State-of-the-Art): On the other hand, commercial-scale industrial catalysis researchers follow materials development workflows, taking months-to-years. Whereas laboratory-scale catalysis often tests research catalysts in powder form, commercial-scale industrial catalysis focuses on the engineered forms known as catalyst composites or technical catalysts. Technical catalysts are compounded with highly active and durable powder research catalysts as key ingredients along with multiple additives enhancing operability, selectivity, manufacturability, lifetime, resilience, and stability.[13] These technical catalysts are typically synthesized in kilogram-to-ton quantities. The materials are then loaded into reactors and devices requiring operational time-on-stream (TOS) periods over several months (more than 2,000 hours) at length-scales (over 1 inch) where both heat and mass transfer effects are more pronounced.[14] Examples of technical catalyst engineered forms include catalytic pellets, extrudates, coatings, washcoated reticulated structures, washcoated foams, washcoated monoliths, porous catalytic membranes, membrane electrode assemblies (MEAs), and gas diffusion electrodes (GDEs). There is no compelling evidence within the body of published literature suggesting the use of computational chemistry or AI/ML methods to design these commercial-ready technical catalysts.

Recent R&D workflow advancements that couple HTE methods with modern AI/ML tools and techniques present a significant and unique opportunity to accelerate the entire development cycle from research to technical catalyst. While a few existing R&D acceleration platforms for materials discovery have begun to utilize some of these developments, the majority of the reported work in catalysis has focused primarily on developing powder research catalysts tested in laboratory settings, as opposed to engineered forms of technical catalysts at

[11] Physics-Based Software Platform for Molecular Discovery & Design, Schrödinger, accessed October 23, 2024, https://www.schrodinger.com/.
[12] Azure Quantum Elements, Azure Quantum, accessed October 23, 2024, https://quantum.microsoft.com/.
[13] Julieth T. García-Sánchez and Víctor G. Baldovino-Medrano, "Elements of the Manufacture and Properties of Technical Catalysts," *Industrial & Engineering Chemistry Research* 62, no. 20 (May 24, 2023): 7769–7838, https://doi.org/10.1021/acs.iecr.3c00369.
[14] Susannah L. Scott, "A Matter of Life(time) and Death," *ACS Catalysis* 8, no. 9 (September 7, 2018): 8597–99, https://doi.org/10.1021/acscatal.8b03199.

industrially relevant testing conditions.[15,16,17,18] Additionally, there are major challenges associated with establishing an accelerated workflow that includes technical catalyst development. The CATALCHEM-E program seeks to address those challenges by creating AI/ML-enabled workflows that integrate technical catalyst performance testing data together with multi-scale theoretical predictions, synthesis protocols, characterization data, and experimental research catalyst optimization cycles. Some of the notable challenges include but are not limited to:

- **Uncertainty in maintaining the integrity of the key intrinsic active site distribution during high-throughput synthesis of technical composite engineered forms from research powders.** In the CATALCHEM-E program, this challenge will be addressed by incorporating advanced characterization data for both virgin and spent materials into a single AI-ready database enabling modeling and cross-performance relationships between research and technical catalysts.
- **Challenges with parallel reactor performance site precision and reproducibility between both research and technical catalyst testing campaigns.** This challenge will be addressed by keeping a commercial control sample during all experimental testing, conducting intra-team validation, and performing appropriate statistical quality control analysis.
- **Insufficient amount of multi-scale, high-quality research and technical catalyst activity data along with the corresponding long-term reactor performance data.** This challenge will be addressed by utilizing HTE, advanced characterization techniques, open-source and proprietary databases, data from reactor-scale simulations, and data augmentation methods to increase the size of the training dataset. "High-quality" is defined as the characteristics of data being highly repeatable and reproducible with high levels of accuracy and precision as defined by industry-accepted standardization bodies such as the American Society for Testing and Materials (ASTM), International Organization for Standardization (ISO), or National Institute for Standards and Technology (NIST).[19,20,21]
- **Difficulty in establishing multi-scale structure-activity relationships between research and technical catalysts.** This challenge will be addressed by developing AI-ready databases combining various forms of data from synthesis, characterization,

[15] Adrian Ramirez et al., "Accelerated Exploration of Heterogeneous CO2 Hydrogenation Catalysts by Bayesian-Optimized High-Throughput and Automated Experimentation," *Chem Catalysis* 4, no. 2 (February 2024): 100888, https://doi.org/10.1016/j.checat.2023.100888.

[16] Nathan J. Szymanski et al., "An Autonomous Laboratory for the Accelerated Synthesis of Novel Materials," *Nature* 624, no. 7990 (November 29, 2023): 86–91, https://doi.org/10.1038/s41586-023-06734-w.

[17] Malcolm Sim et al., "Chemos 2.0: An Orchestration Architecture for Chemical Self-Driving Laboratories," *Matter* 7, no. 9 (September 2024): 2959–77, https://doi.org/10.1016/j.matt.2024.04.022.

[18] Martin Seifrid et al., "Autonomous Chemical Experiments: Challenges and Perspectives on Establishing a Self-Driving Lab," *Accounts of Chemical Research* 55, no. 17 (August 10, 2022): 2454–66, https://doi.org/10.1021/acs.accounts.2c00220.

[19] "American Society for Testing and Materials." ASTM International. Accessed October 23, 2024. https://www.astm.org/

[20] "International Organization for Standardization." ISO, June 12, 2024. https://www.iso.org/.

[21] "National Institute of Standards and Technology." NIST, October 16, 2024. https://www.nist.gov/.

performance testing (including language and annotations), and creating subsequent AI/ML models which effectively stitch together data and information across scales.

Key program elements include, but are not limited to:

- **Novel workflow topologies:** A workflow topology is a diagram designating key task nodes involved in the development of a technical catalyst from conception through reactor-scale testing. An example of a traditional, non-automated closed-loop workflow spanning from hypothesis to technical catalyst performance testing is illustrated in Figure 1. The CATALCHEM-E program envisions creating novel closed-loop workflow topologies that strategically remove bottlenecks and time-consuming tasks ultimately resulting in significant acceleration when compared to the traditional workflow.
- **Enhanced data integrity and benchmarking through reference chemistries:** The program will use reference chemistries for workflow validation. These reference chemistries have been proven at the commercial scale and are relevant to both ARPA-E's goals and the U.S. goal of net-zero carbon emissions by 2050. Specifically, the reference chemistries recommended in this program have been selected to provide applicants with feedstock phase flexibility across thermochemical and electrochemical reaction classes. Here, commercially available catalysts operating in real-world industrial-scale reactor units will serve as controls to ensure data integrity within each task node in the workflow, and as benchmarks when assessing the performance of AI/ML models.
- **High-quality data generation via HTE:** Autonomous or automated HTE methods are necessary to generate high-quality experimental data in large quantities to train and validate AI/ML models. HTE techniques operating over complex, wide parameter spaces can increase the efficiency of experimentation across all stages of the catalyst development cycle, from research catalyst (synthesis, characterization, and validation) to technical catalyst (formulation, characterization, and validation). In addition, the quality of data and ability to identify the most optimal experimental conditions is expected to be enhanced dramatically with these approaches.
- **AI/ML-ready catalysis databases and informatics:** As a result of creating effective CATALCHEM-E workflows, projects must create a set of robust databases in tandem populated with high-quality, multi-scale, multi-modal data as generated and gathered from synthesis, characterization, and performance testing tasks at the *ab initio* and research and technical catalyst levels. Further, these novel workflows will take advantage of the tools for automation and database management to streamline the storage, access, and processing of collected data that is findable, accessible, interoperable, and reusable (FAIR) to accomplish AI/ML tasks.[22]
- **Transformational multi-scale, multi-modal modeling using AI/ML:** As shown in Figure 2 in Section I.D, there are several ways to leverage the AI/ML tools and techniques to understand heterogenous catalyst surfaces starting from known theoretical predictions

[22] Mark D. Wilkinson et al., "The FAIR Guiding Principles for scientific data management and stewardship", *Sci Data* 3, 160018 (2016), https://doi.org/10.1038/sdata.2016.18.

or prior knowledge in literature coupled with CATALCHEM-E workflow data (including language) from synthesis, advanced characterization, and reactor-scale testing activities.

- **Surrogate AI/ML assisted computational modeling and simulations:** ML-based surrogate models can be used in two ways in the program. First, these models can accelerate the parametric testing space for the reactor-scale performance. Projects may accelerate the simulation of technical catalyst performance at engineering-scale by training surrogate models on data generated using various computational fluid dynamics and multi-physics approaches (e.g., COMSOL, Ansys, and OpenFOAM).[23,24,25] These simulations can be used to expand the training set of the CATALCHEM-E learning model. Second, these models can accelerate the elucidation of fundamental reaction mechanisms and networks by including atomic scale, *ab initio* approximations along with microkinetic modeling for more rigorous calculations involving surface transition states and adsorption energetics**.**

D. PROGRAM OBJECTIVES

The CATALCHEM-E program is seeking to support the development of fundamentally disruptive technologies that can achieve R&D acceleration from research to technical catalyst levels by tightly coupling state-of-the-art high-throughput catalyst design experimental methods and advancements in AI/ML with industrially relevant catalyst forms and conditions. If successful, these technologies will address the ARPA-E goals by improving energy efficiency, reducing energy-related emissions, and reducing imports, while contributing to the U.S. goal of achieving net-zero carbon emissions by 2050.[6]

The novel accelerated workflows created under CATALCHEM-E (see Figure 2) will address the major bottlenecks (described in Section I.C.2) impacting catalyst development at the reactor unit-scale by adopting the latest methods and tools in HTE and AI/ML. Starting from research catalyst rational design (i.e., composition and structure) and continuing through reactor-scale testing of technical catalysts, CATALCHEM-E aims to drastically reduce the development time for heterogeneous catalysts. The program will first deliver accelerated workflow tools validated on reference chemistries (Phase 1) and then use these same high-quality, developed workflow tools to co-optimize new reactions and technical catalysts that are relevant to ARPA-E's goals and the net-zero carbon emissions 2050 goals (Phase 2). For more details on program phases, see Section I.F.

[23] "Multiphysics Software for Optimizing Designs." COMSOL. Accessed October 23, 2024. https://www.comsol.com/.
[24] Ansys Engineering Simulation Software. Accessed October 23, 2024. https://www.ansys.com.
[25] OpenFOAM. Accessed October 23, 2024. https://www.openfoam.com/.

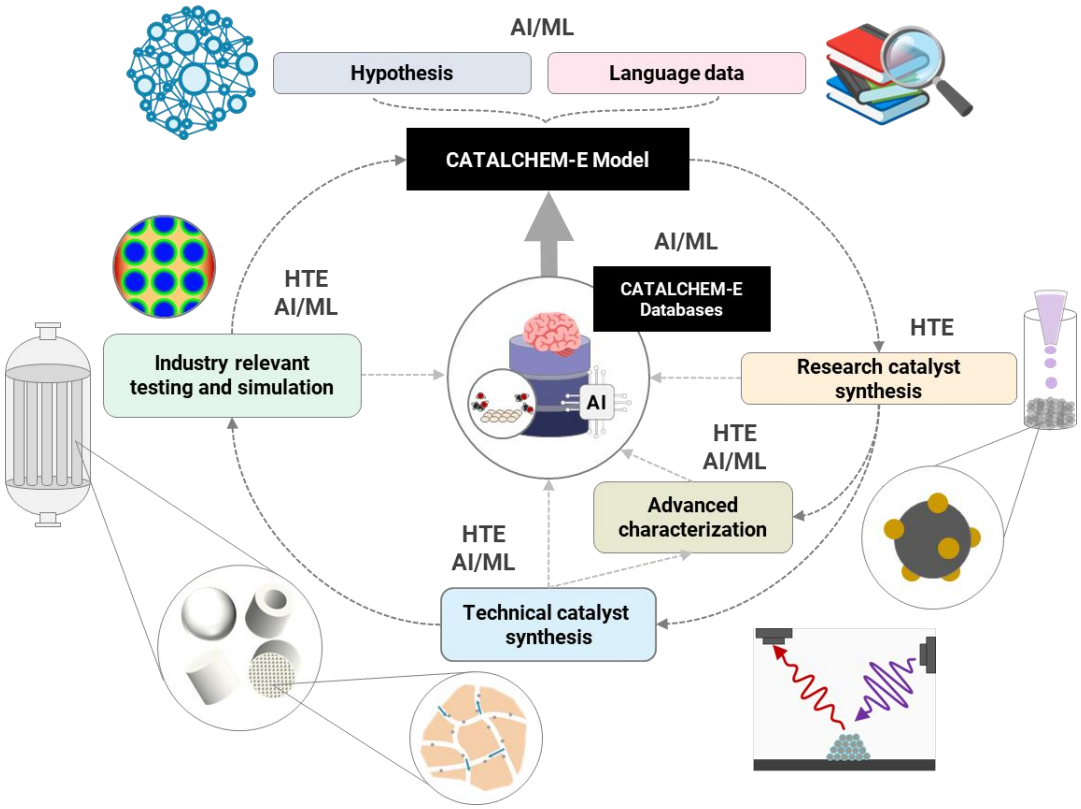

Figure 2. An overview of the CATALCHEM-E program illustrating an integrated AI-enabled workflow.

Through the development of novel heterogenous catalysts and/or catalytic reactions, this program aims to support the following objectives:

- **Synthesis of new drop-in manufacturable technical catalysts** in engineered forms at kilogram scale for thermochemical or electrochemical reactor systems, as well as evaluation of these technical catalysts for performance under realistic, industrial conditions for reactions that generate key commodity fuels and chemical intermediates projected by the net-zero carbon emissions by 2050 scenarios.[26] The identified chemical reactions have significant potential to further ARPA-E's statutory goals by cumulatively impacting quad-scale levels of energy or gigaton-scale reductions in CO_2-equivalent greenhouse gas (GHG) emissions.
- **Develop AI-enabled closed-loop or other potentially disruptive acceleration workflow topologies** for specific reference chemistries. The methodology should be applicable to relevant chemistries that can help achieve ARPA-E's goals and advance the goal of net-zero carbon emissions by 2050 and should meet the required performance targets outlined in Table 2 in Section I.F.1 and Table 3 in Section I.F.2. These workflows will lead to an equivalent of 10–15 years of traditional catalysis R&D work verifiably completed through rediscovery within 12–18 months, and then to novel catalyst-reaction discovery

[26] Eelco T.C. Vogt and Bert M. Weckhuysen, "The refinery of the future", *Nature* 629, 295–306 (2024), https://doi.org/10.1038/s41586-024-07322-2.

and co-design.[27] Further impact will be realized in Phase 2 where novel catalyst-reaction discovery and co-design will be achieved by utilizing the acceleration methods advanced in Phase 1 of the program.

- **Generate AI-Ready searchable databases** by combining and pre-processing high-quality, multi-scale, multi-modal data as generated and gathered from synthesis, characterization, and performance testing tasks at the atomistic, research, and technical catalyst scales. The impact will be unprecedented research-to-technical catalyst datasets elucidating structure-activity relationships and synthesis insights. The program sets the stage for a long-term future trajectory towards generative AI for catalysis.

E. REQUIRED TECHNICAL APPROACHES

The following technical approaches are necessary to achieve more than a ten-time relative acceleration compared to traditional catalyst R&D workflow. Submissions must address all four of the technical approaches. Submissions which attempt to address only a subset of the "Required Technical Approaches" stated below instead of the complete set may be deemed nonresponsive (see Section V.A.1). At a minimum, each team must include partners from the HTE, catalyst manufacturing, technical catalyst performance testing, and AI/ML communities by the submission of the Full Application. All applicant teams must have access to HTE hardware and data infrastructure and not have to undertake initiatory system design, procurement, construction, and development tasks.

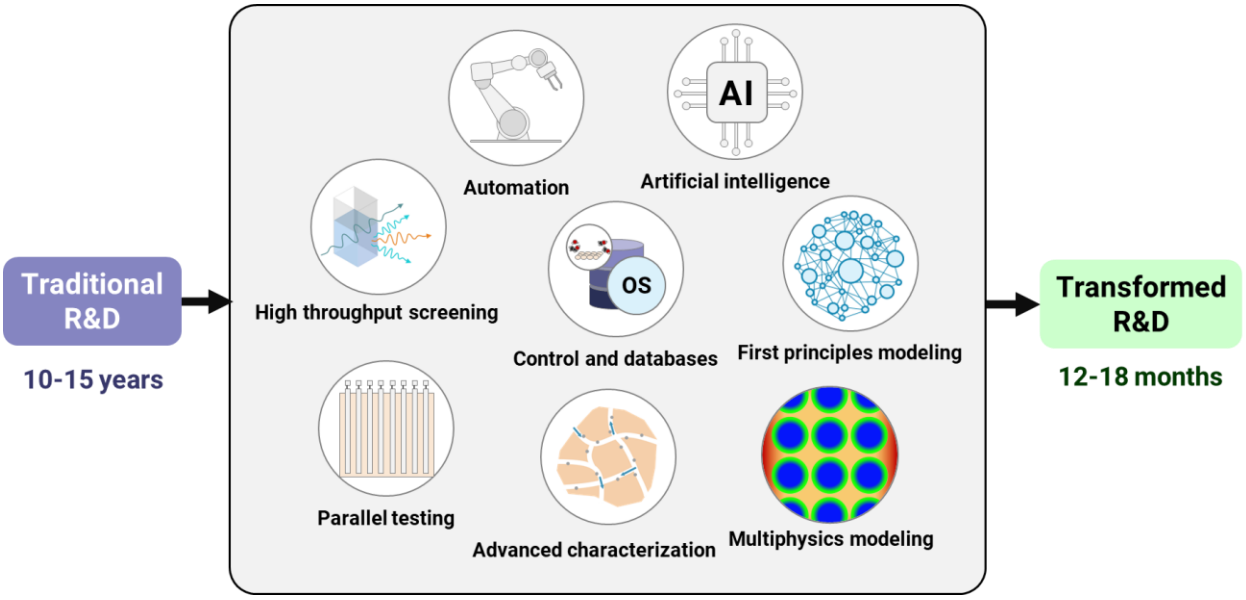

Figure 3. Types of hardware and software tools which can be leveraged to understand chemically active surfaces, synthesize materials, and accelerate the overall heterogeneous catalysis R&D workflow.

[27] Rediscovery is the R&D process of reaching the same scientific conclusions or outcomes as those reported in previous published studies. In this case, rediscovery involves showing that an accelerated workflow has reached the same composition and structure as those known for a reference catalyst and reference chemistry combination.

Technical Approach 1 (TA1): Integrated AI-enabled workflow topology. An overview of the CATALCHEM-E program is shown in Figure 2. Additionally, the types of hardware and software tools that can be leveraged for workflow acceleration are illustrated in Figure 3. This program requires project teams to develop a closed-loop, automated workflow topology, starting from hypothesis to reactor-scale testing of technical catalysts, that ultimately enables inverse design of heterogenous catalysts. However, ARPA-E will also consider alternative promising topologies where the loop is "closed" by a human expert but holds the clear promise of a more than a ten-time relative acceleration compared to traditional workflows (see Figure 1, and validation explanation in Table 2 in Section I.F.1). While a combination of different AI/ML and multi-scale computational modeling and simulation tools could be used for specific R&D tasks, it is expected that the data generated through the workflow will help each project team create AI-ready databases ("CATALCHEM-E databases") and an overarching AI model ("CATALCHEM-E model") to close the loop by providing feedback to improve hypothesis on material composition and structure. This would thereby enhance exploration of non-intuitive chemical spaces. The program also has a strong interest in inverse design approaches that can take pilot-scale testing data as inputs (e.g., yield profile, catalyst specific features, multi-physics adjusted parameters from simulation) to provide insights into the synthesis, formulation, and testing conditions for potential technical catalyst candidates. The CATALCHEM-E model must be validated using reference and other related commercially available catalysts with known compositions (see validation explanation in Table 2).

TA1 has the following elements:

- Accelerated catalysis R&D workflow: The accelerated workflow must integrate theoretical predictions with technical catalyst performance testing by addressing challenges under the four technical approaches discussed in this section and achieve more than a ten-time acceleration compared to a baseline traditional R&D workflow. Projects must use reference chemistries from Table 1 for workflow validation. Commercially available catalysts operating in real-world industrial-scale reactor units must serve as controls to ensure data integrity and as benchmarks when ranking the multi-scale performance between newly synthesized catalysts suggested by the CATALCHEM-E learning model.
- CATALCHEM-E databases and informatics: Each project must create high-quality databases with theoretical data, synthesis, and characterization data for research and technical catalysts, reactor-scale performance data for technical catalysts, as well as any additional data generated via simulations or experiments within a project. It is appropriate for the project teams to draw upon theoretical knowledge, publicly available and/or in-house proprietary data, and data augmentation techniques to address data limitations, especially in the beginning of a proposed workflow. Applicant teams must clearly describe how to stitch together multiple databases in the workflow, for example:
    - Open-source databases with atomistic scale simulation data to train ML-based surrogate models for efficient computational modeling and predicting research catalyst structure and performance leveraging raw characterization data;

  - The research catalyst database for predicting technical catalyst synthesis protocol, structure, and performance; and
  - The technical catalyst database created using engineered catalysts forms and macroscale (e.g., greater than 1 inch O.D. packed-bed reactor or greater than 144 cm^2 solid oxide electrochemical cell) reactor testing coupled with data from multi-physics simulations that ultimately feeds back into the CATALCHEM-E model, enabling inverse design.

- Closed-loop CATALCHEM-E model: AI/ML model(s) must be trained with data in the CATALCHEM-E databases. Projects can make use of supplemental theoretical knowledge, proprietary databases, journal articles, and open-source databases (e.g., Materials Genome Initiative, Open Catalyst Project, CatTestHub) as additional sources of data to enable discovery and optimization of heterogenous catalysts.[28,29,30] Ultimately, each team must train a model for the prediction of technical catalyst performance starting from an input vector that is driven by research catalyst structure, composition, and can include technical catalyst characteristics (forward); and conversely, the prediction of research catalyst compositions and structures starting from technical catalyst performance (inverse). Projects will use advanced AI/ML tools and techniques applicable to small (sample size more than 100) or large (sample size more than 1,000) quantities of data, including but not limited to artificial neural networks, Gaussian processes, random forests, variational autoencoders, generative adversarial networks, recurrent neural networks, graph neural networks, convolutional neural networks, deep reinforcement learning, Bayesian optimization, active learning, natural language processing, and transfer learning. Applicants must propose innovative AI-enabled pathways that have the potential to drastically reduce the time it takes to develop technical catalysts starting from a hypothesis. For instance, it is quite possible to use a combination of learning (AI/ML) and optimization approaches in the same workflow for both research and technical catalyst development, including establishing cross-performance relationships between research and technical catalysts. It is anticipated that the project teams will need multiple iterations of the workflow loop to generate the experimental data required to train the closed-loop model. Incorporation of different types of fundamental atomic-scale catalyst surface, spatial, and electronic descriptors for the active site and the neighboring environment may be helpful in this effort.
- Theoretical support and rational inverse design: Theory-driven prediction and elucidation of catalytic material compositional and structural space using various features (e.g., quantum-level 3D descriptors, structural characterization information) are important in this effort. This work can benefit from advancements in utilizing reactor-scale technical catalyst performance data as input to improve theoretical rational design predictions for research catalysts. Project teams must make use of

[28] Materials Genome Initiative. Accessed October 23, 2024. http://www.mgi.gov/.
[29] "Open Catalyst Project." Open Catalyst Project. Accessed October 23, 2024. https://opencatalystproject.org/.
[30] "CatTestHub: Center for Programmable Energy Catalysis." CatTestHub: Center for Programmable Energy Catalysis. Accessed October 23, 2024. https://cpec.umn.edu/cattesthub.

existing models and/or publicly available open-source datasets to accomplish tasks.

Technical Approach 2 (TA2): High-throughput research catalyst synthesis and characterization. Traditional research catalyst synthesis, multi-modal characterization, and validation are crucial in this effort, especially advanced *in operando* and/or dynamic working surface sensitive techniques where applicable. This technical approach can benefit from autonomous or automated parallel experimentation and closed-loop optimization, similar to those used in self-driving laboratories. Additionally, applicants must utilize AI/ML and data science approaches with research catalyst data to accelerate the workflow and support discovery and optimization tasks.

Technical Approach 3 (TA3): Technical catalyst synthesis and characterization. Technical catalyst formulation, compounding, characterization, and scale up represents the core of this technical approach. The synthesis of technical catalyst mitigates the manufacturability risk often associated with novel research catalyst synthesis methods. Such manufacturing techniques include but are not limited to granulation, extrusion, pelletization, spray drying, hot-pressing, material layer deposition, and ink jetting. This technical approach can benefit from the same innovations as those indicated under TA2, but the formulation and optimizations required are not well-documented in the literature. Structural, physical, and chemical properties such as particle size distribution, surface area, pore structure, pore volume, pore size distribution, texture, morphology, crush strength, average bulk density, shape factor (e.g., characteristic length, diameter), attrition resistance, ionomer binding, hydrophobicity/hydrophilicity balance, chemical stability, corrosion resistance, conductivity, and homogeneity should be considered and reported when relevant. Additionally, applicants must utilize AI/ML and data science approaches with technical catalyst data to accelerate the workflow and support discovery and optimization tasks. Applicants should consider innovative ways to establish cross-performance relationships between research and technical catalysts with data generated using TA2 and TA3.

Technical Approach 4 (TA4): Industry-relevant reactor testing and simulation. Technical catalyst performance testing under realistic, industry-relevant feed and operating conditions along with corresponding reactor modeling/simulation is important in this approach. This performance is observed and measured as yield structure, lifetime, stability, durability, and resiliency. An empirical rate expression form can be used to assist with the simulation effort if needed. Other operational effects must be monitored, such as temperature and pressure profiles. Additionally, applicants may utilize surrogate AI/ML models for computationally intensive simulations of reactor-scale performance data.

F. TECHNICAL PERFORMANCE TARGETS

The CATALCHEM-E program consists of a single category. The program is composed of two phases, each lasting 18 months. Phase 1 (Development) includes the development of an accelerated workflow around one of the specifically defined reference chemistries, and Phase 2 (Discovery) will utilize the accelerated workflows from Phase 1 efforts to optimize new relevant reactions. These phases enable the program to discover and optimize catalytic chemistries that

are relevant to ARPA-E's goals while achieving more than a ten-time acceleration in the catalyst development cycle over traditional R&D workflows. Submissions must propose project plans and budgets for both Phase 1 and Phase 2. Funding for both phases will be obligated at the start of the Period of Performance, but advancement from Phase 1 to Phase 2 at the end of 18 months is at ARPA-E's sole discretion based on the degree to which the project teams exceed the targets mentioned in Tables 2 and 3, the quality of deliverables (e.g., technical catalyst synthesized, ease and efficiency of developed accelerated workflow, and the degree of data quality in the database), and the availability of appropriated funds. The transition from Phase 1 to Phase 2 represents a portfolio-wide down-select, so advancement is not guaranteed even if all milestones from Phase 1 are met.

Table 1: List of reference chemistries recommended for this program.

Feed phase	Class	Reaction	Reactor type	Technical catalyst form
Gas	Thermo	$CO_2 + 3H_2 \rightarrow CH_3OH + H_2O$	Multi-Tube Packed Bed	Pellet/Extrudates
Gas	Electro	$H_2O \rightarrow H_2 + ½\ O_2$	SOEC[31] cathode	Ceramic Support
Liquid	Thermo	$C_6H_{14}O_6 \rightarrow 6\ CO + 7\ H_2$	Fixed Bed	Ceramic Support
Liquid	Electro	$H_2O \rightarrow H_2 + ½\ O_2$	PEM[32] anode	MEA or GDE
Mixed	Thermo	$C_{60}H_{104}O_6$ (TAGs) + $3\ H_2 \rightarrow 3\ C_{16}H_{32} + C_3H_8 + 3\ CO + 3\ H_2O$	Trickle-Bed	Various Supports
Mixed	Electro	$CO_2 \rightarrow CO + ½\ O_2$	PEM or AEM[33] cathode	MEA or GDE

1. PHASE 1: WORKFLOW DEVELOPMENT USING REFERENCE CHEMISTRY

Phase 1 (Development) aims to develop accelerated closed-loop workflows validated on reference chemistries. More detail is provided below.

- ARPA-E has identified reactions of interest, which cover thermochemistry and electrochemistry across different streams of feedstock phase and are listed in Table 1. Applicant teams should select a reaction from Table 1 to develop the workflow in Phase 1 required in the submission.
- Applicants selecting other reference chemistries outside of Table 1 should provide a strong justification for their choice in terms of: 1) quad-level energy impact, 2) availability of data from a commercial reactor and data across multiple scales (laboratory, pilot, commercial), 3) existing need for catalyst discovery with reasonable opportunities for optimization, 4) catalyst composition known for re-discovery, 5)

[31] SOEC: Solid oxide electrolysis cell
[32] PEM: Proton exchange membrane
[33] AEM: Anion exchange membrane

availability of kinetics/rate laws, and 6) importance of reference chemistry, feedstocks and products for ARPA-E goals and the net-zero carbon emissions 2050 goals.

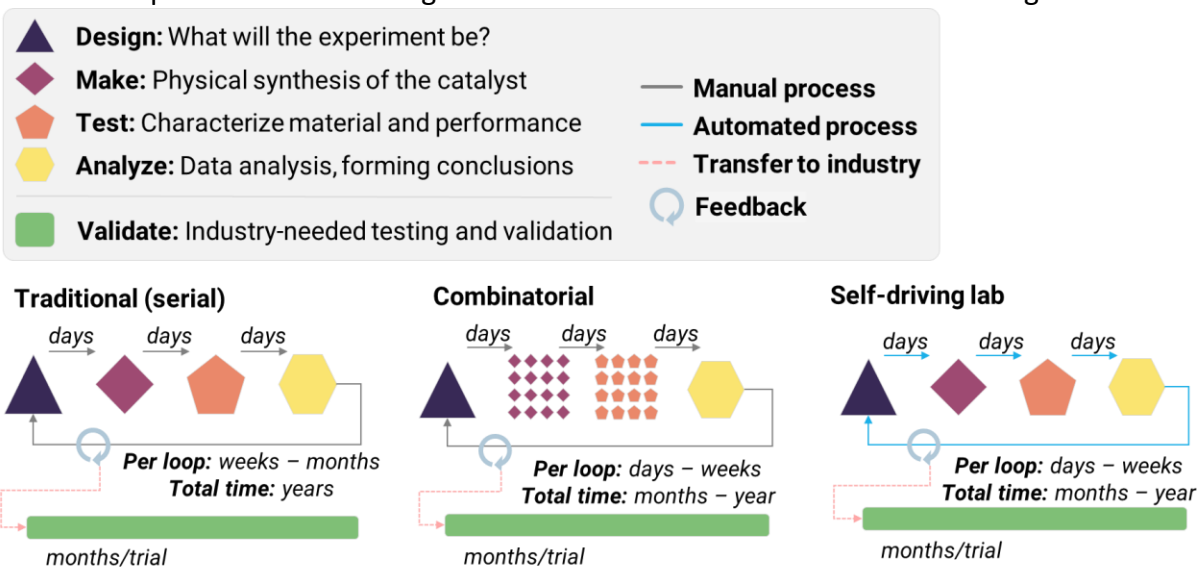

Figure 4. Examples of workflow topologies for the development of research catalysts. Applicant teams are required to submit their proposed workflow topology at both the research and technical catalyst scales.

- Applicant teams must propose a workflow topology in their application that follows a more detailed and granular approach than the example given in Figure 4. Teams can achieve this by using the design template provided or a representative schematic. Workflows must show how the steps lead to technical catalyst performance testing and how the feedback loop is closed, as well as denote which steps occur due to parallelization or automation. The figure should be provided with the application (see Sections III.B and III.C for detail on submitting the proposed workflow topology with both the Concept Paper and Full Application).
- Applicants should provide the information requested in Table 4 in Section I.F.3 based on their specific reference chemistry and workflow in Phase 1.

Table 2. Phase 1 summary of the workflow and reference reaction targets.

Workflow Metrics	Target	Rationale
Overall acceleration	≥ 10x	This is the overall workflow acceleration goal. The target for this metric is based on the proposed workflow topology relative to the more granular baseline methods shown in Figure 4. Applicants should clearly show timescales for task nodes and how removing bottlenecks will accelerate the proposed workflow. More importantly, re-discovery of the commercial reference research powder and corresponding technical catalyst composition and structure as guided by the CATALCHEM-E model will validate this metric. *(TA1)*
Level of workflow automation	> 90%	Task nodes in the overall proposed workflows must be greater than 90% automated. *(TA1)*

Number of research catalysts synthesized in gram (g) quantities and screened after *N* workflow iterations	> 1000	*N* = number of workflow iterations required to reach Phase 1 objectives. Screening must be experimental work and can be supported by *in silico* efforts. This work includes characterization on greater than 50 down-selected research catalysts. *(TA2)*
Number of technical catalysts synthesized in kilogram (kg) quantities after *N* workflow iterations	> 50	*N* = number of workflow iterations required to reach Phase 1 objectives. This work includes characterization on greater than 50 technical catalyst formulations. *(TA3)*
CATALCHEM-E model fidelity (forward)	Within 10% deviation from the known performance	The forward model predicts pilot-scale technical catalyst performance from an input vector that is driven by research catalyst structure and composition and can also include technical catalyst characteristics (e.g., formulation, microstructure). The target is to show model predicted performance within 10% deviation from the known performance (see example of metric types below under "catalyst performance" row). Here, a separate technical "validation catalyst" (other than the reference catalyst) and the corresponding research catalyst component of known pilot-scale performance, composition, and structure is used to make this prediction. *(TA1)*
CATALCHEM-E model fidelity (inverse)	Within 20% deviation from the compositional and structural characteristics	The inverse model predicts research catalyst composition and structure from pilot-scale technical catalyst performance. The target is to show inverse model predicted compositions and structures within 20% deviation from the known physical properties as determined by well-accepted material characterization measurements (e.g., elemental analysis, x-ray analysis and microscopy) of research powders for validation catalyst. Here, a separate technical "validation catalyst" and the corresponding research catalyst of known pilot-scale performance, composition, and structure is used to make this prediction. *(TA1)*
Reference Reaction Metrics	**Target**	**Rationale**
Research and technical catalytic performance	$\frac{\varphi_{\text{CATALCHEM-E}}}{\varphi_{\text{benchmark}}} \geq 0.9$ (across all relevant metrics)	φ_j denotes a specific type of catalytic performance metric. The benchmark catalyst for a specific reference chemistry is measured here. These types of metrics can include, but are not limited to: • Carbon efficiency • Single-pass selectivity of species *i* (S_i) • Single-pass conversion (X) • Single-pass yield of species *i* (Y_i) • Space-time-yield of species *i* (STY_i) • Current density (J)

		• Overpotential (η_{over}) • System efficiency (η_{sys}) • Degradation rate (r_{deg}) Example metrics are cited from published government reports or other applicant proposed sources, such as industry reports or literature.[34,35,36] Applicants are expected to report on all relevant metrics. *(TA2, TA3)*
Technical catalyst batch synthesis size	> 1 kg	Minimum synthesis gravimetric size targets for technical catalysts for application in various engineered forms (e.g., coatings, MEAs, PBRs). *(TA3)*
Technical catalyst continuous TOS	> 2000 hours	Kg scale performance testing of technical catalysts as engineered forms (e.g., coatings, MEAs, PBRs) with < 3% loss of activity. *(TA4)*
Carbon balance closure	95% < x <105%	Gravimetric, volumetric, and various analytical methods used to validate mass balances, as well as carbon present in all feed and product streams. *(TA4)*
Technoeconomic performance	$\frac{\beta_{\mathrm{CATALCHEM-E}}}{\beta_{\mathrm{benchmark}}} \leq 1$ See rationale	β denotes a specific technoeconomic metric targets for reference chemistries based on known commercial processes. Metrics can include, but are not limited to: • Catalyst cost reductions; • Capital expenditure (CAPEX) reductions for major equipment; • Operating expenditure (OPEX) reductions; and • Margins. Applicants to provide basic technoeconomic targets that meet or exceed commercial targets based on a "drop in" catalyst replacement scenario in Phase 1 or preliminary rough estimate for Phase 2.

ARPA-E recognizes that each unique workflow may have distinct challenges. The overall acceleration metric should establish how the baseline value is calculated and how the more than ten-time acceleration will be achieved. In addition, the reaction metrics will significantly vary between project teams based on reference chemistries. Justification for the choice of metrics is required in Table 4 (see Section I.F.3).

[34] U.S. Department of Energy. "Technical Targets for Proton Exchange Membrane Electrolysis," Hydrogen and Fuel Cell Technologies Office, accessed October 8, 2024. https://www.energy.gov/eere/fuelcells/technical-targets-proton-exchange-membrane-electrolysis.

[35] U.S. Department of Energy. "Technical Targets for High Temperature Electrolysis Hydrogen and Fuel Cell Technologies Office, accessed October 8, 2024. https://www.energy.gov/eere/fuelcells/technical-targets-high-temperature-electrolysis.

[36] National Renewable Energy Laboratory. "Economic Feasibility for CO_2 Utilization," accessed October 8, 2024. https://www.nrel.gov/bioenergy/co2-utilization-economics/index.html.

2. PHASE 2: NEW CATALYST AND CHEMISTRY DISCOVERY

Phase 2 aims to utilize the workflow tools developed in Phase 1 to discover new catalysts for reactions of interest. Applicants must include the plans for Phase 2 in their submission. The Phase 2 reaction of interest should be related to the reference chemistry chosen in Phase 1. The type of reaction must be consistent between the two phases, i.e., a Phase 1 reference chemistry using electrochemical membrane electrode assemblies (MEAs) must also utilize an electrochemical MEA (or analogous) in Phase 2.

Potential (but not exclusive) Phase 2 reactions of interest are shown in blue ("Research") and purple ("Unknown") cells in the matrix in Figure 5. For any selected Phase 2 reaction (metrics provided in Table 3), applicants are required to address the questions in Table 4 (see Section I.F.3). Modifications to the Phase 1 workflow are expected in Phase 2.

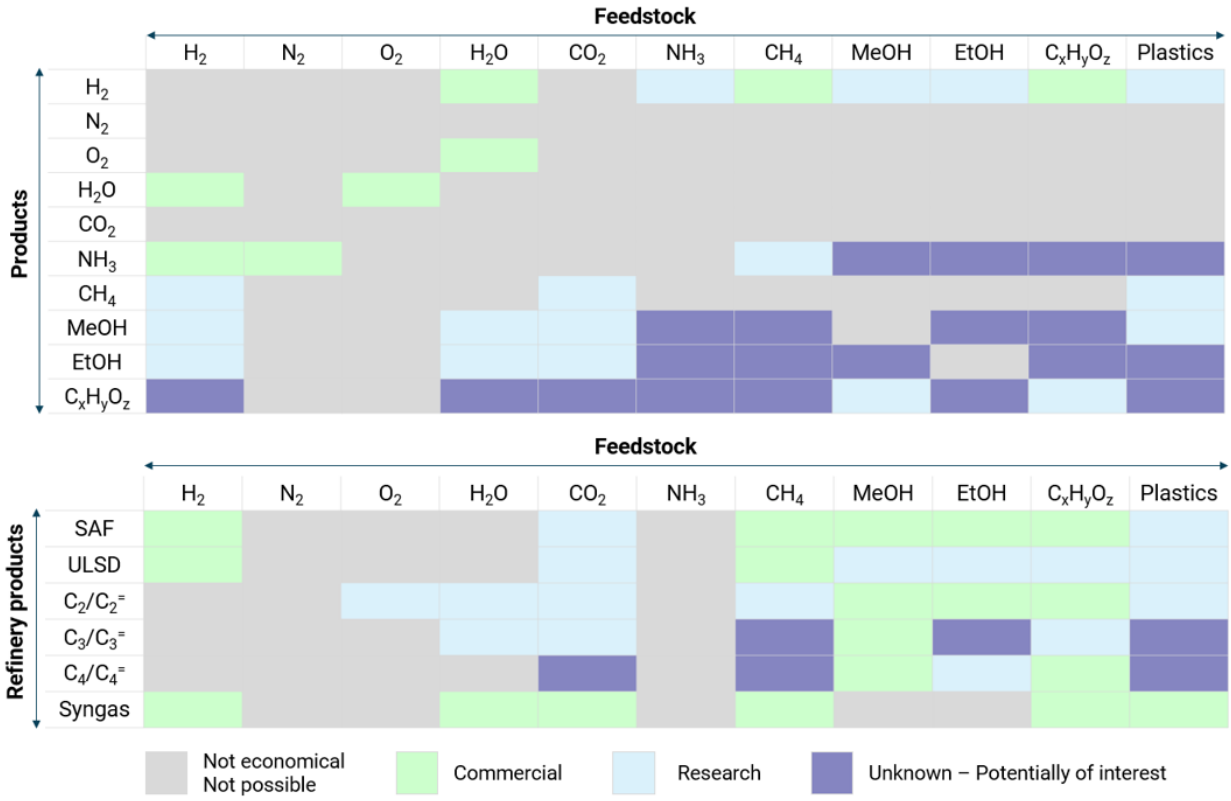

Figure 5. Matrix of potentially relevant net-zero 2050 reaction permutations given select future refinery feedstocks and key chemical intermediates, including SAF, ultra-low sulfur diesel (ULSD), $C_2/C_2^=$, $C_3/C_3^=$, $C_4/C_4^=$, and syngas.

Table 3. Phase 2 reaction metrics and targets.

Reaction Metrics	Target	Rationale
GHG emissions reduction	> 75% over baseline	Feedstocks selected should have a carbon intensity that enables a reduction in GHG by greater than 75% over the widely accepted fossil fuel conventional baseline.
Research and technical catalytic performance	$\frac{\beta_{\text{CATALCHEM-E}}}{\beta_{\text{reported}}} > 1$ (across all relevant metrics)	β_j denotes a specific catalytic performance metric target. No reference catalyst is measured here. Only reported performance in literature (e.g., patents, journals) of nascent proof (X > 5%) is benchmarked. These types of metrics can include, but are not limited to: • Carbon efficiency • Single-pass selectivity of species *i* (S_i) • Single-pass conversion (X) • Single-pass yield of species *i* (Y_i) • Space-time-yield of species *i* (STY_i) • Current density (J) • Overpotential (η_{over}) • System efficiency (η_{sys}) • Degradation rate (r_{deg}) Example metrics are cited from published government reports or other applicant proposed sources, such as industry reports or literature.[34,35,36] Applicants are expected to report on all relevant metrics. *(TA2, TA3)*
Number of technical catalysts synthesized after *N* workflow iterations	> 5	*N* = number of workflow iterations required to reach Phase 2 objectives. This work includes characterization on greater than five technical catalyst formulations. Discovery approach can include: • Phase 1 catalyst library + Net-Zero 2050 Chemistry (Figure 5) • Phase 2 catalyst candidate + Net-Zero 2050 Chemistry (Figure 5) *(TA3)*
Margin	> $100 per tonne product	Economics based on the projected feedstock and product pricing. Provide justification for the reaction of choice as requested in Table 4.

3. JUSTIFICATION TABLE

Applicants are required to address the questions in Table 4 as a component of their Full Application (see Section III.C).

Table 4. Questions for justifying selection of metrics in Tables 2–3.

Workflow Questions
W A. What is the proposed workflow topology? (Submit a more detailed and granular product than the example given in Figure 4 using the design template provided or a representative schematic. Supply this as a separate document per instructions in Section III.C.)
W B. What is the justification for measuring workflow acceleration using metrics in Table 2? Explain why the compositional space used to initiate the workflow is broad enough to justify time for rediscovery.
W C. What are the proposed multi-modal data sources to intake from and what are their forms (e.g., image, text, spectra)? What does a catalyst sample row with a unique identifier look like in the database(s)?
W D. What is the general plan for ensuring data quality and data management? (See also Section I.G.)
W E. Identify and justify which performance metrics will be selected in the validation of forward and inverse models.
Phase 1 Questions
P1 A. What is the selected reference reaction?
P1 B. What is the selected benchmark catalyst for the chosen reaction? Will it be available in both research and technical catalyst forms?
P1 C. What are the proposed performance testing metrics for both the research and technical catalyst? What is the justification for the metrics and targets chosen?
P1 D. What are the minimum required and relevant methods that should be employed for characterizing the chemical, physical, and structural properties of research and technical catalysts (including standard methods) based on the proposed workflow?
Phase 2 Questions
P2 A. What is the selected Phase 2 reaction(s) of interest and why?
P2 B. What is the most recent information available about newly discovered catalysts capable of carrying out these reactions of interest? Provide corresponding references (i.e., articles, reports, patents).
P2 C. What is the scientific justification and merit for Phase 2 chemistry being achievable? Please provide references (i.e., articles, reports, patents).
P2 D. How is the Phase 2 reaction(s) of interest related to the Phase 1 reference chemistry (i.e., feed state of matter, related chemical mechanism, reaction type/class)?

4. SUMMARY OF PROJECT REQUIREMENTS

This section outlines the tasks that CATALCHEM-E project teams must complete, at a minimum, during the course of their award.

Using the technical approaches discussed in Section I.E, each project team must complete the following critical Phase 1 task:

- ***Develop*** an optimized heterogeneous technical catalyst within the first 18 months of the project using one of the reference chemistries from Table 1 while meeting the performance targets in Table 2.

Project teams selected for Phase 2 must complete the following critical task:

- ***Discover*** and optimize catalytic chemistries that are potentially relevant to ARPA-E goals and the U.S. goal of net-zero carbon emissions by 2050 within the next 18 months by meeting the performance targets in Table 3 and addressing the questions in Table 4.

The following requirements apply to both phases. Each project team must complete the following critical tasks for each phase they are active in:

- ***Perform*** reactor-scale testing and simulation of the engineered catalyst forms (technical catalysts) at industrially relevant time and length scales using realistic feeds (see Table 1 for Phase 1 and Figure 5 for Phase 2), pre-treatment and operating conditions. In this case "realistic" means feeds as acquired from commercial partners or relevant industrial sources that includes impurities and not surrogate prepared research feeds;
- ***Develop*** a CATALCHEM-E workflow by integrating HTE and AI/ML throughout the closed-loop topology;
- ***Generate*** CATALCHEM-E databases of all experimental and simulated data generated through the workflow across multiple scales (e.g., atomic to macro), including synthesis, characterization, and reactor performance at engineering scale; and
- ***Develop*** an AI/ML CATALCHEM-E model at the workflow level using CATALCHEM-E databases to enable inverse design within an automated, closed-loop or another promising scheme.

G. ADDITIONAL PROJECT REQUIREMENTS

Database Management: Each team must create a single database repository combining various forms of data (including language and annotations) from computational results, synthesis information, characterization tools, multi-scale reactor performance testing, and from other disparate sources (e.g., instruments, spreadsheets, open-source databases, published literature). The use of professional analytical data management systems, such as Lab Information Management Systems (LIMS), is highly recommended for this purpose.

Databases should be internally consistent within a team with respect to the schema representation. All generated datasets are required to be FAIR. Applicants are required to discuss a plan in the full application which explains the storage, processing, and analysis of multi-scale, multi-modal catalysis data to ensure data quality and support AI/ML tasks, as well as cybersecurity and information handling protocols.

Industry Relevant Support. For the Full Application only, project teams must submit:

- A letter-of-intent from a catalyst manufacturer or a third party toller that can synthesize the catalyst to appropriate mass scale (kg scale);
- A letter of intent from a testing service provider capable of evaluating technical catalyst performance at reactor-scale (e.g., lab prototype or pilot scale) at appropriate time scales (typically, thousands of hours);
- A letter of intent from an HTE hardware resource provider enabling autonomous or automated parallel testing capabilities; and
- A letter of intent from a data infrastructure resource provider enabling database management as discussed above.
  The entities mentioned above could be a participant on the submission or a third-party vendor. See Section III.C for additional information.

H. 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."[37] 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, 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

[37] U.S. Congress, Conference Report to accompany the 21st Century Competitiveness Act of 2007, H. Rpt. 110-289 at 171-172 (Aug. 1, 2007).

ARPA-E may include coordination with other Government agencies and nonprofits[38] 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.

I. 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 pre-award 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).

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.I.8 of the NOFO below) and should be requested as such.

[38] "Nonprofits" or "nonprofit organizations" has the meaning set forth at 2 C.F.R. § 200.70.

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 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" (https://www.gsa.gov/forms-library/disclosure-lobbying-activities) 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 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 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[39] who are proposed to work on the project, both at the Recipient and subrecipient level, and a list of all participating[40] 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.D.

15. PAYMENT OF FEE OR PROFIT

ARPA-E will pay a fee or profit to Recipients in an amount not to exceed 7% of total project cost under any agreement resulting from this NOFO, subject to negotiations. Any fee or profit paid by Recipients to their subrecipients (but not commercial suppliers, vendors, or contractors) must be paid from fee or profit paid to Recipients by ARPA-E. Any fee or profit must be included in the budget submitted with Recipients' Full Applications and will be payable to Recipients upon: (i) completion of all work required by the agreement, (ii) submission and acceptance of all for-profit audit reports and resolution of all findings (if any) identified in the reports, (iii) submission and acceptance by the Government of all closeout documentation required by

[39] See Section IX, Glossary, for the definition of Covered Individual.
[40] For a definition of "participation" please see footnote 51.

Attachment 4 to the agreement (refer to ARPA-E's Model Cooperative Agreement found at https://arpa-e.energy.gov/technologies/project-guidance/pre-award-guidance/funding-agreements), and (iv) submission of an acceptable invoice.

II. ELIGIBILITY INFORMATION

A. ELIGIBLE APPLICANTS

1. SBIR ELIGIBILITY

SBA rules and guidelines govern eligibility to apply to this NOFO. For information on program eligibility, please refer to the SBIR/STTR website, available at https://www.sbir.gov, and to the "Eligibility" section for SBIR/STTR programs at https://www.sbir.gov/apply.

A Small Business Concern[41] may apply as a Standalone Applicant[42] or as the lead organization for a Project Team.[43] If applying as the lead organization, the Small Business Concern must perform at least 66.7% of the work in Phase I and at least 50% of the work in Phase II and Phase IIS, as measured by the Total Project Cost.[44]

2. STTR ELIGIBILITY

SBA rules and guidelines govern eligibility to apply to this NOFO. For information on STTR program eligibility, please refer to the websites in section II.A.1.

Only a Small Business Concern may apply as the lead organization for a Project Team under STTR. The Small Business Concern must perform at least 40% of the work in Phase I, Phase II, and/or Phase IIS, as measured by the Total Project Cost. A single Research Institution must perform at least 30% of the work in Phase I, Phase II, and/or Phase IIS, as measured by the Total Project Cost. Please refer to Section II.B.1 of the NOFO for guidance on Research Institutions' participation in STTR projects.

3. JOINT SBIR AND STTR ELIGIBILITY

An Applicant that meets both the SBIR and STTR eligibility criteria above may request both SBIR and STTR funding if:

- The Small Business Concern is partnered with a Research Institution;
- The Small Business Concern performs at least 66.7% of the work in Phase I and at least 50% of the work in Phase II and/or Phase IIS (as applicable), as measured by the Total Project Cost;

[41] A Small Business Concern is defined by the SBA. Please see SBA.gov for guidelines, including Does Your Small Business Qualify? | U.S. Small Business Administration (sba.gov).
[42] A "Standalone Applicant" is an Applicant that applies for funding on its own, not as part of a Project Team.
[43] A Project Team consists of the Recipient, Subrecipients, and others performing or otherwise supporting work under an ARPA-E funding agreement.
[44] The Total Project Cost is the Federal Government share of total allowable costs. The Federal Government share generally includes costs incurred by GOGOs and FFRDCs.

- The partnering Research Institution performs 30-33.3% of the work in Phase I and 30-50% of the work in Phase II and/or Phase IIS (as applicable), as measured by the Total Project Cost; and
- The Principal Investigator (PI) is employed by the Small Business Concern. If the PI is employed by the Research Institution, submissions will be considered only under the STTR program.

B. ELIGIBLE SUBRECIPIENTS

1. RESEARCH INSTITUTIONS

A Research Institution[45] may apply only as a member of a Project Team (i.e., as a Subrecipient to a Small Business Concern). In STTR projects, a single Research Institution must perform at least 30%, but no more than 60%, of the work under the award in Phase I, Phase II, and/or Phase IIS (as applicable), as measured by the Total Project Cost.

2. OTHER PROJECT TEAM MEMBERS

The following entities are eligible to apply for SBIR/STTR funding as a member of a Project Team (i.e., as a Subrecipient to a Small Business Concern):

- For-profit entities (which includes large businesses and small businesses)
- Nonprofits other than Research Institutions[46]
- Government-Owned, Government Operated laboratories (GOGOs)
- State, local, and tribal government entities
- Foreign entities[47]

In SBIR projects, Project Team members other than the lead organization, including but not limited to Research Institutions, may collectively perform no more than 33.3% of the work under the award in Phase I and no more than 50% of the work under the award in Phase II and/or Phase IIS. This includes efforts performed by Research Institutions.

[45] Research Institutions include FFRDCs, nonprofit educational institutions, and other nonprofit research organizations owned and operated exclusively for scientific purposes. Eligible Research Institutions must maintain a place of business in the United States, operate primarily in the United States, or make a significant contribution to the U.S. economy through the payment of taxes or use of American products, materials, or labor.

[46] 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 Subrecipient.

[47] All work by foreign entities must be performed by subsidiaries or affiliates incorporated in the United States (see Section II.B.3 of the NOFO). However, the Applicant may request a waiver of this requirement in the Business Assurances & Disclosures Form submitted with the Full Application.

In STTR projects, Project Team members (other than the lead organization and the partnering Research Institution) may collectively perform no more than 30% of work under the award in Phase I, Phase II, and/or Phase IIS.

3. FOREIGN ENTITIES

If a Foreign Country of Concern[48] 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.[49]

C. ELIGIBLE PRINCIPAL INVESTIGATORS

1. SBIR

For the duration of the award, the PI for the proposed project (or, if multiple PIs, at least one PI) must be employed by, and perform more than 50% of his or her work for, the Prime Recipient. The Grants Officer may waive this requirement or approve the substitution of the PI after consultation with the ARPA-E SBIR/STTR Program Director.

For projects with multiple PIs, at least one PI must meet the primary employment requirement. That PI will serve as the contact PI for the Project Team.

2. STTR

For the duration of the award, the PI for the proposed project (or, if multiple PIs, at least one PI) must be employed by, and perform more than 50% his or her work for, the Prime Recipient or the partnering Research Institution. The Grants Officer may waive this requirement or approve the substitution of the PI after consultation with the ARPA-E SBIR/STTR Program Director.

For projects with multiple PIs, at least one PI must meet the primary employment requirement. That PI will serve as the contact PI for the Project Team.

[48] "Foreign Countries of Concern", as defined by the State Department, 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.

[49] The contents of a Foreign Entity Waiver request can be found in the Business Assurances & Disclosures Form.

D. FOREIGN PARTICIPATION

1. 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 Countries of Concern[50] 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.

2. FOREIGN PARTICIPATION CONSIDERATIONS

Foreign participation[51] 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.I.6 and the Business Assurances & Disclosures Form).

E. ELIGIBILITY OF PRIOR SBIR AND STTR AWARDEES: SBA BENCHMARKS ON PROGRESS TOWARDS COMMERCIALIZATION

Applicants awarded multiple prior SBIR or STTR awards must meet DOE's benchmark requirements for progress towards commercialization before ARPA-E may issue a new Phase I award. For purposes of this requirement, Applicants are assessed using their prior Phase I and Phase II SBIR and STTR awards across all SBIR agencies. If an awardee fails to meet either of the benchmarks, that awardee is not eligible for an SBIR or STTR Phase I award and any Phase II award for a period of one year from the time of the determination.

ARPA-E applies two benchmark rates addressing an Applicant's progress towards commercialization: (1) the DOE Phase II Transition Rate Benchmark and (2) the SBA Commercialization Rate Benchmark:

[50] Please see footnote 48 for list of Foreign Countries of Concern.

[51] "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.

- The DOE Phase II Transition Rate Benchmark sets the minimum required number of Phase II awards the Applicant must have received for a given number of Phase I awards received during the specified period. **This Transition Rate Benchmark applies only to Phase I Applicants that have received more than 20 Phase I awards during the last five (5) year period, excluding the most recently completed fiscal year**. DOE's Phase II Transition Rate Benchmark requires that 25% of all Phase I awards received over the past five years transition to Phase II awards.

  The SBIR/STTR Phase II transition rates and commercialization rates are calculated using the data in the SBA's TechNet database. For the purpose of these benchmark requirements, awardee firms are assessed once a year, on June 1st, using their prior SBIR and STTR awards across all agencies. SBA makes this tabulation of awardee transition rates and commercialization rates available to all federal agencies. ARPA-E uses this tabulation to determine which companies do not meet the DOE benchmark rates and are, therefore, ineligible to receive new Phase I awards.

- The Commercialization Rate Benchmark sets the minimum Phase III[52] commercialization results that an Applicant must have achieved from work it performed under prior Phase II awards (i.e., this measures an Applicant's progress from Phase II or Phase IIS to Phase III awards). **This benchmark requirement applies only to Applicants that have received more than 15 Phase II awards during the last 10 fiscal years, excluding the two most recently completed fiscal years.**

  The current Commercialization Benchmark requirement, agreed upon and established by all 11 SBIR agencies, is that the Applicants must have received, to date, an average of at least $100,000 of sales and/or investments per Phase II award received, or have received a number of patents resulting from the relevant SBIR/STTR work equal to or greater than 15% of the number of Phase II awards received during the period.

- On June 1 of each year, SBIR/STTR awardees registered on SBIR.gov are assessed to determine if they meet the Phase II Transition Rate Benchmark requirement. (At this time, SBA is not identifying companies that fail to meet the Commercialization Rate Benchmark requirement). Companies that fail to meet the Phase II Transition Rate Benchmark as of June 1 of a given year will not be eligible to apply to an SBIR/STTR NOFO for the following year.

[52] Phase III refers to work that derives from, extends or completes an effort made under prior SBIR/STTR funding agreements, but is funded by sources other than the SBIR/STTR Program. Phase III work is typically oriented towards commercialization of SBIR/STTR research or technology. For more information please refer to the Small Business Administration's "Small Business Innovation Research (SBIR) and Small Business Technology Transfer (STTR) Program Policy Directive" at https://www.sbir.gov/sites/default/files/2024-07/SBA SBIR_STTR_POLICY_DIRECTIVE_May2023.pdf.

F. COMPLIANCE AND RESPONSIVENESS

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

G. 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" may apply to only one of the two ARPA-E CATALCHEM-E NOFOs: DE-FOA-000 3506 (CATALCHEM-E SBIR/STTR), or DE-FOA-000 3505 (CATALCHEM-E). Small businesses that qualify as "Small Business Concerns" are strongly encouraged to apply under the former (SBIR/STTR NOFO). To determine eligibility as a "Small Business Concern" under DE-FOA-0003506 (SBIR/STTR), please review the eligibility requirements in Sections II.A – II.C above.

H. COST SHARING

Cost sharing is not required for this FOA.

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

The Concept Paper is mandatory (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 Federal Funding Requested, and Project Duration.

A fillable Concept Paper template is available on ARPA-E eXCHANGE at https://arpa-e-foa.energy.gov. 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.F of the NOFO).

2. SECOND COMPONENT: SUMMARY SLIDE AND WORKFLOW TOPOLOGY

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.

In this same PowerPoint file, applicants are required to provide a Proposed Accelerated Heterogenous Catalysis R&D Workflow Topology. An example and a template are provided in the summary slide template file on slides 2 and 3.

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 https://arpa-e-foa.energy.gov.
- 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 https://arpa-e-foa.energy.gov.

Full Applications found in any component to be noncompliant or nonresponsive may not be merit reviewed or considered for award (see Section II.F 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. However, all relevant technical information should be included in the body of the Technical Volume.

2. SECOND COMPONENT: JUSTIFICATION TABLE

Applicants must submit responses to the questions posted in the Justification Table (Table 4) in Section I.E.3 of this NOFO. Applicants must denote each response with the respective question label (e.g., W2, W3). This Justification Table component must not exceed three pages to answer all questions (excluding W1, which will be a part of the Seventh Component, Summary Slide) and must be in Adobe PDF format.

3. THIRD COMPONENT: LETTERS OF INTENT

Project teams must submit four letters of intent as described in Section I.F. Letters must be signed and on the appropriate entity's letterhead. The letters of intent from the following four entities: 1) Technical catalyst manufacturer; 2) Reactor-scale testing service provider; 3) HTE hardware resource provider; and 4) Data infrastructure resource provider must be submitted in Adobe PDF format and combined into one file. Letters should clearly state which of the above responsibilities they intend to fulfill.

4. FOURTH 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: https://www.cdfifund.gov/opportunity-zones.

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 https://www.energy.gov/management/articles/certifications-and-assurances-use-sf-424.
- The dates and dollar amounts on the SF-424 are for the entire period of performance, 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.

5. FIFTH 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.

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 the Recipient's Budget Justification.
- Subrecipients incurring less than 10% of the Total Project Cost are not 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.

6. SIXTH 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.

7. SEVENTH COMPONENT: SUMMARY SLIDE AND WORKFLOW TOPOLOGY

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.

In this same PowerPoint file, applicants are required to provide the proposed Workflow Topology as described in W A in the Justification Table (Table 4 in Section I.E.3). An example and a template are provided in the summary slide template file on slides 2 and 3.

8. EIGHTH 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.

6. NINTH COMPONENT: SBIR.GOV COMPANY REGISTRATION

Applicants are required to provide a copy of the SBIR.gov Company Registration confirmation document generated from SBIR.gov (see Section IV.A of the NOFO) in Adobe PDF form. Applicants that have previously completed SBIR.gov Company Registration need not register again and may submit a copy their existing Registration.

7. TENTH COMPONENT: ADDITIONAL OWNERSHIP CERTIFICATIONS

Only those Applicants that are (a) majority-owned by multiple venture capital operating companies, hedge funds, or private equity firms and/or (b) joint ventures minority-owned by a foreign entity are required to complete the Certification for Applicants Majority-Owned by Multiple Venture Capital Operating Companies, Hedge Funds, and Private Equity Funds and Joint Venture Applicants Minority-Owned by Foreign Business Entities (VCOC/FJV Certification). The certification must be submitted in Adobe PDF format.

In the VCOC/FJV Certification, the Applicant is required to self-identify as an entity that falls into one of those categories, provide certain information, verify its ownership status, and verify that it has completed SBIR.gov Company Registration (see Section IV.A) as such an entity.

Applicants that are neither (a) majority-owned by multiple venture capital operating companies, hedge funds, or private equity firms nor (b) joint ventures minority-owned by a foreign entity are not required to complete the VCOC/FJV Certification.

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 https://arpa-e-foa.energy.gov.

Concept Papers, Full Applications, and Replies to Reviewer Comments must be submitted through ARPA-E eXCHANGE. ARPA-E will not review or consider applications submitted through other means (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. COMPLETION OF SBIR.GOV COMPANY REGISTRATION

The first step in applying to this NOFO is completing the SBIR.gov Company Registration (https://app.www.sbir.gov/company-registration/overview). Upon completing registration, Applicants will receive a unique Small Business Concern (SBC) Control ID and SBC Registration confirmation document in Adobe PDF format. Applicants that have previously completed SBIR.gov Company Registration need not register again.

Applicants must submit their Registration confirmation document with SBC Control ID as part of their Full Application (see Section III.C.6 of the NOFO).

B. UNIQUE ENTITY IDENTIFIER AND SAM REGISTRATION

Applicants must register with the System for Award Management (SAM) at www.sam.gov/SAM 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 highest-level 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.

C. USE OF ARPA-E EXCHANGE

To apply to this NOFO, Applicants must register with ARPA-E eXCHANGE (https://arpa-e-foa.energy.gov/Registration.aspx). For detailed guidance on using ARPA-E eXCHANGE, please refer to the "ARPA-E eXCHANGE Applicant Guide" (https://arpa-e-foa.energy.gov/Manuals.aspx).

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 (https://arpa-e-foa.energy.gov/login.aspx), 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.**

D. 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	• Concept Paper (Adobe PDF format)
	  ○ Sections 1-4 (4 pages max.)
	  ○ Bibliographic References (no page limit)
	• Summary Slide and Proposed Workflow Topology (2 page limit, Microsoft PowerPoint format)
		Mandatory	III.B	December 17, 2025

Full Application	• Technical Volume (Adobe PDF format):
	  ○ Cover Page (1 page max.)
	  ○ Executive Summary (1 page max.)
	  ○ Sections 1-5 (20 pages max.)
	  ○ Bibliographic References (no page limit)
	  ○ Personal Qualification Summaries (each summary limited to 5 pages in length, no cumulative page limit)
	• Justification Table (3 pages max., Adobe PDF format)
	• Letters of Intent (no page limit, 4 letters required, Adobe PDF format)
	• Signed SF-424 (Adobe PDF format);
	• Budget Justification Workbook/SF-424A (Microsoft Excel format);
	• Summary for Public Release (250 words max., Adobe PDF format);
	• Summary Slide and Proposed Workflow Topology (1 slide limit, Microsoft PowerPoint format); and
	• Signed Business Assurances & Disclosures Form(s) (no page limit, Adobe PDF format);
	• SBA Company Registration Certificate generated in the SBA Company Registry; (http://sbir.gov/registration) (Adobe PDF format); and
	• If applicable, Certification for Applicants that are (a) Majority-Owned by Multiple Venture Capital Operating Companies, Hedge Funds, or Private Equity Firms; and/or (b) joint ventures minority-owned by a foreign entity (Adobe PDF format).
		Mandatory	III.C	TBD

Reply to Reviewer Comments	• Reply to Reviewer Comments (3 page max., Adobe PDF format)	Optional	III.D	TBD

E. 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.F 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.

F. 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:

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

- Reactions and submissions which do not use heterogeneous electrochemical or thermochemical catalysis, including:
  - Homogeneous catalysis
  - Plasma catalysis
  - Photocatalysis
  - Biocatalysis
  - Gas adsorption-only approaches
  - Battery chemistry
- Purely synthetic data approaches without experimental validation;
- Generation of new atomistic scale simulation data using high-performance computing platforms;
- Work focused on basic research aimed purely at fundamental knowledge generation; and
- Submissions addressing only a subset of the "Required Technical Approaches" discussed in Section I.E instead of the complete set.

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.F of the NOFO for the appropriate technology Category 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;
b. 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: https://www.cdfifund.gov/opportunity-zones.

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 (ARPA-E-CO@hq.doe.gov) 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;[27]
    - 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;
    - create duplication with activities supported by the Federal agency;
    - present concerns about conflicts of interest;
    - were not appropriately disclosed to the Federal agency;
    - violate Federal law or terms and conditions of the Federal agency; or
    - 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 https://www.fedconnect.net/FedConnect/ 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 not 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 not 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 not 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 pre-award 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 AGREEMENTS

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.

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 Recipient share responsibility for the direction of projects.

Phase I will be made as a fixed-amount award. Phase II and Phase IIS of Combined Phase I/II/IIS awards will be made on a cost-reimbursement basis.

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

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 https://www.nsf.gov/awards/managing/rtc.jsp 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 before funding a project 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 https://arpa-e.energy.gov/technologies/project-guidance/pre-award-guidance/required-forms-and-templates. 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. 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 (https://arpa-e.energy.gov/technologies/project-guidance/post-award-guidance/project-management-reporting-requirements) 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.

2. 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.

3. NONDISCLOSURE AND CONFIDENTIALITY AGREEMENTS REPRESENTATIONS

In submitting an application in response to this NOFO the Applicant represents 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.

4. 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.

5. 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.

6. 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 https://new.nsf.gov/research-security/training 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 (https://arpa-e.energy.gov/technologies/project-guidance/pre-award-guidance/funding-agreements).

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 https://www.energy.gov/ig/ig-hotline.

You may report fraud, waste, mismanagement, or misconduct involving SBA programs or employees either online (https://www.sbir.gov/fraud-waste-abuse) or by calling the OIG Hotline toll-free at (800) 767-0385.

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.2 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.2 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: Pursuant to special statutory authority for SBIR/STTR awards, data generated under ARPA-E SBIR/STTR awards may be protected from public disclosure for twenty years from the date of award 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.

SBA: U.S. Small Business Administration.

SBIR: Small Business Innovation Research Program.

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) (http://www.sba.gov/content/small-business-size-standards).

STTR: Small Business Technology Transfer Program.

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.

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