FINANCIAL ASSISTANCE
FUNDING OPPORTUNITY ANNOUNCEMENT

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

Design Intelligence Fostering Formidable Energy Reduction and Enabling Novel Totally Impactful Advanced Technology Enhancements (DIFFERENTIATE)

Announcement Type: Initial Announcement
Funding Opportunity No. DE-FOA-0002107
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First Deadline for Questions to ARPA-E-CO@hq.doe.gov:	5 PM ET, Friday, May 10, 2019
Submission Deadline for Concept Papers:	9:30 AM ET, Monday, May 20, 2019
Second Deadline for Questions to ARPA-E-CO@hq.doe.gov:	5 PM ET, TBD
Submission Deadline for Full Applications:	9:30 AM ET, TBD
Submission Deadline for Replies to Reviewer Comments:	5 PM ET, TBD
Expected Date for Selection Notifications:	TBD
Total Amount to Be Awarded	Approximately $15 million, subject to the availability of appropriated funds.
Anticipated Awards	ARPA-E may issue one, multiple, or no awards under this FOA. Awards may vary between $250,000 and $5 million.

- For eligibility criteria, see Section III.A of the FOA.
- For cost share requirements under this FOA, see Section III.B of the FOA.
- To apply to this FOA, Applicants must register with and submit application materials through ARPA-E eXCHANGE (https://arpa-e-foa.energy.gov/Registration.aspx). For detailed guidance on using ARPA-E eXCHANGE, see Section IV.H.1 of the FOA.
- Applicants are responsible for meeting each submission deadline. Applicants are strongly encouraged to submit their applications at least 48 hours in advance of the submission deadline.
- For detailed guidance on compliance and responsiveness criteria, see Sections III.C.1 through III.C.4 of the FOA.

Questions about this FOA? Check the Frequently Asked Questions available at http://arpa-e.energy.gov/faq. For questions that have not already been answered, email ARPA-E-CO@hq.doe.gov (with FOA name and number in subject line); see FOA Sec. VII.A. Problems with ARPA-E eXCHANGE? Email ExchangeHelp@hq.doe.gov (with FOA name and number in subject line).

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REQUIRED DOCUMENTS CHECKLIST

For an overview of the application process, see Section IV.A of the FOA.

For guidance regarding requisite application forms, see Section IV.B of the FOA.

For guidance regarding the content and form of Concept Papers, Full Applications, and Replies to Reviewer Comments, see Sections IV.C, IV.D, and IV.E of the FOA.

SUBMISSION	COMPONENTS	OPTIONAL/ MANDATORY	FOA SECTION	DEADLINE
Concept Paper	• Each Applicant must submit a Concept Paper in Adobe PDF format by the stated deadline. The Concept Paper must not exceed 4 pages in length and must include the following: ○ Concept Summary ○ Innovation and Impact ○ Proposed Work ○ Team Organization and Capabilities	Mandatory	IV.C	9:30 AM ET, Monday May 20, 2019
Full Application	[TO BE INSERTED BY FOA MODIFICATION IN JULY 2019]	Mandatory	IV.D	9:30 AM ET, TBD
Reply to Reviewer Comments	[TO BE INSERTED BY FOA MODIFICATION IN JULY 2019]	Optional	IV.E	5 PM ET, TBD

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) to:

"(A) to enhance the economic and energy security of the United States through the development of energy technologies that result in—
(i) reductions of imports of energy from foreign sources;
(ii) reductions of energy-related emissions, including greenhouse gases; and
(iii) improvement in the energy efficiency of all economic sectors; and
(B) to ensure that the United States maintains a technological lead in developing and deploying advanced energy technologies."

ARPA-E issues this Funding Opportunity Announcement (FOA) under the programmatic authorizing statute codified at 42 U.S.C. § 16538. The FOA and any awards made under this FOA are subject to 2 C.F.R. Part 200 as amended by 2 C.F.R. Part 910.

ARPA-E funds research on and the development of high-potential, high-impact energy technologies that are too early for private-sector investment. 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 to develop drive down 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. By 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 lower than that of the incumbent technology.

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 the clear disruptive potential, e.g., by demonstrating capability for manufacturing at competitive cost and deployment at scale.

ARPA-E funds applied research and development. 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 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 (http://fossil.energy.gov/), the Office of Nuclear Energy (http://www.energy.gov/ne/office-nuclear-energy), and the Office of Electricity Delivery and Energy Reliability (http://energy.gov/oe/office-electricity-delivery-and-energy-reliability).

B. PROGRAM OVERVIEW

1. SUMMARY

In the 250 years since the dawn of the Industrial Revolution, the pace of technology-driven economic growth has dwarfed that achieved in prior centuries.[2] This growth has transformed human life—dramatically enhancing both the quality and duration of it. The emerging artificial intelligence revolution has similar transformational potential, which we seek to leverage to help resolve the energy challenges that are tied to the modern industrial age.

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

[2] Bank of England, A Millennium of Macroeconomic Data

Recent analyses suggest that the energy technologies that currently power our economy are not sustainable economically or environmentally.[3] Fortunately, technological innovation in the energy space has already helped to mitigate these challenges. For instance, while James Watt's transformational steam engine featured a fuel conversion efficiency of ~2% in 1774,[4] today's most modern combined cycle plants have efficiencies approaching 70%. Furthermore, solar, wind, and nuclear plants are capable of providing emission-free electric power (albeit currently with a commensurate loss of flexibility and/or a higher installed cost per unit of output power). However, the most recent climate data and modeling suggests that we must move faster to further reduce the environmental impact associated with the energy sector.[5] In order to achieve the rapid transition to lower-carbon-footprint energy sources and systems, their use must also offer a compelling economic return to their owners and operators.

However, the tremendous technological progress that we have already made can result in diminishing marginal returns on investments in further performance improvements in some areas.[6] Fortunately, rapidly emerging artificial intelligence/machine learning (ML) technologies offer the potential to counteract these otherwise diminishing returns and to enhance the pace of energy innovation by accelerating certain aspects of the energy technology design and development processes.

Specifically, the DIFFERENTIATE program seeks to enhance the pace of energy innovation by incorporating machine learning into energy technology development processes. By doing so, this program aims to enhance the productivity of energy engineers in helping them to develop next-generation energy technologies.

In order to organize the proposed efforts, a simplified engineering design process framework has been adopted and utilized to identify several general mathematical optimization problems that are common to many (perhaps most) engineering design processes and then to conceptualize several machine learning tools that could help engineers to execute and solve these problems in a manner that dramatically accelerates the pace of energy innovation.

The high-level design process framework is illustrated in Figure 1. In this framework:

1. A problem/challenge is posed (e.g. cost-effectively generate electricity from natural gas at an efficiency in excess of 70%),
2. A potential solution is hypothesized and refined with Reduced Order Models (e.g. fuel cell/engine hybrid systems),

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[3] USGCRP, 2018: Impacts, Risks, and Adaptation in the United States: Fourth National Climate Assessment, Volume II [Reidmiller, D.R., C.W. Avery, D.R. Easterling, K.E. Kunkel, K.L.M. Lewis, T.K. Maycock, and B.C. Stewart (eds.)]. U.S. Global Change Research Program, Washington, DC, USA, 1515 pp. doi: 10.7930/NCA4.2018

[4] Lovland, Jorgen, A History of Steam Power, Department of Chemical Engineering, NTNU, Trondheim, Norway, 2007.

[5] USGCRP, 2018.

[6] Bloom, Nicholas et al, Are Good Ideas Getting Harder to Find?, NBER Working Paper No. 23782.

3. The low fidelity concept is further refined and evaluated with high-fidelity partial differential equation-based solvers and/or experiments (e.g. computational fluid dynamics simulations, finite element analyses, full-scale system demonstrations), and
4. The hypothesized solution is updated with knowledge gained during the high-fidelity evaluation process, and iteration continues until either the problem is either solved or deemed insoluble.

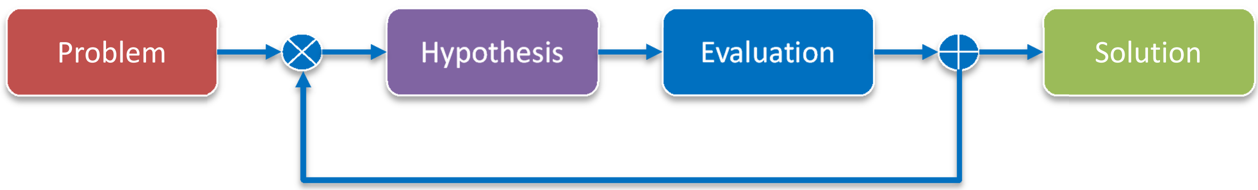

Figure 1: Technology development process framework: pose a problem, hypothesize a solution, evaluate the hypothesis, and iterate as required.

The DIFFERENTIATE program seeks to develop machine learning tools that:

1) Enhance the creativity of the hypothesis generation (i.e. conceptual design) process by helping engineers develop new concepts and by enabling the consideration of a larger and more diverse set of design options during the hypothesis generation phase,
2) Enhance the efficiency of the high-fidelity evaluation (i.e. detailed design) process by accelerating the high-fidelity analysis and optimization of the hypothesized solution, and
3) To ultimately reduce (ideally eliminate) design iteration by developing the capability to execute "inverse design" processes in which the product design is effectively expressed as an explicit function of the problem statement.

In order to facilitate the achievement of the above-mentioned objective, ARPA-E is issuing this FOA to encourage teams consisting of mathematicians, operations research analysts, computer scientists, energy engineers, and others with applicable skills and experience to jointly work on developing the tools required to enhance the creativity and efficiency (i.e. productivity) of the energy technology design process.

Eight example design challenge problem areas that are both of significant importance and for which it is believed that adequate data either are available or can be generated during the program are specified. Briefly, they are the following:

- **Hypothesis Generation (i.e. Conceptual Design)**
    - Thermodynamic Cycles/Chemical Processes (e.g. Gas Separations)
    - Electrical Power Converters
    - Materials/Molecules
- **Hypothesis Evaluation** (i.e. Detailed Design)
    - Heterogeneous Catalysts
    - Turbomachinery
- **Inverse Design**
    - Aerodynamic Devices/Surfaces
    - Photonic Devices

More detailed descriptions of each of the challenge problem areas are provided in the Program Structure Section (Section I.E.) of this FOA.

ARPA-E is soliciting submissions that seek to develop machine learning enhanced tools that facilitate the solution to one of the above challenge problem areas *or a challenge problem developed by the proposing team*. It is expected that each submission will explicitly identify a selected challenge problem, an anticipated solution approach, a data acquisition/creation strategy, the major development risks and associated mitigation plans, and an anticipated path to commercial relevance[7] for the design tool/software to be developed.

ARPA-E is encouraging the formation of well-rounded technical teams where all the requisite technical skills are represented—machine learning, mathematics/optimization, software, and energy (e.g. mechanical, chemical, materials, or electrical) engineering.

C. PROGRAM OBJECTIVES

The objective of the DIFFERENTIATE program is to enhance the pace of energy innovation by accelerating the incorporation of machine learning into the energy technology design process. Specifically, ARPA-E is seeking to develop machine-learning-enhanced—

1. Hypothesis generation (i.e. Conceptual Design) tools,
2. High-fidelity hypothesis evaluation (i.e. Detailed Design) tools, and
3. Inverse design tools.

In the remainder of this section, more detailed descriptions of the abovementioned capabilities are provided after a brief description of the overall design process framework.

[7] Commercial relevance might include—open source software and algorithms; commercial software; proprietary algorithms, software and/or design processes.

Design Process Framework

In the interest of establishing an organizing framework for these efforts, a simplified representation of the engineering design process is utilized that is analogous to the scientific method. A schematic diagram of this process was presented in Figure 1.

In it, a problem is posed and a hypothesized solution is developed and evaluated versus target performance metrics defined in the problem statement. If the targets are not met, repeated adjustments to the hypothesis are made and evaluated until either the targets are achieved or the effort is abandoned.

1. Hypothesis Generation (i.e. Conceptual Design) – Mixed integer optimization

In the Hypothesis Generation phase, engineers:

1. Gather information about prior (now sub-optimal) solutions to the current or previous similar problems,
2. Gather information about relevant emerging technologies,
3. Consolidate this information into a design concept that is "hypothesized" to offer an attractive solution to the target problem, and
4. Iteratively refine the hypothesized concept using low-fidelity but computationally efficient Reduced-Order Models (ROMs).

In Figure 2, a Hypothesis-centric view of the design process framework introduced in Figure 1 is shown. In this view, the hypothesis generation phase is represented as an iterative conceptual design process where computationally efficient Reduced Order Models (ROMs) are used to evaluate low-fidelity candidate concept architectures.

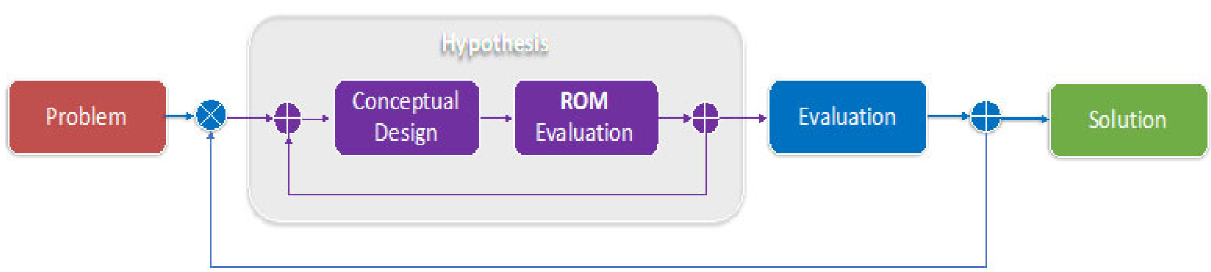

Figure 2: Hypothesis-centric view of the design process framework introduced in Figure 1

In the Hypothesis Generation/Conceptual Design phase, engineers are typically seeking answers to the following questions—

1. Which technologies/components do I need in my system?
2. How are they connected?
3. How do they interact?
4. What are the nominal characteristics of the technologies/components?

As an illustrative example, consider a hypothesized solution to the challenge problem of generating electricity from natural gas at an efficiency of >70% in an economically attractive manner that is presented in Figure 3. This hypothesized system concept includes five components that are connected in the manner illustrated in the figure. Furthermore, several component level design parameters (e.g. compressor pressure ratio, recuperator effectiveness, fuel cell area) must be determined in order to enable useful estimates of the thermo-economic performance of the system subject to known physical conservation laws and/or technology constraints (e.g. conservation of energy, turbine material temperature limits).

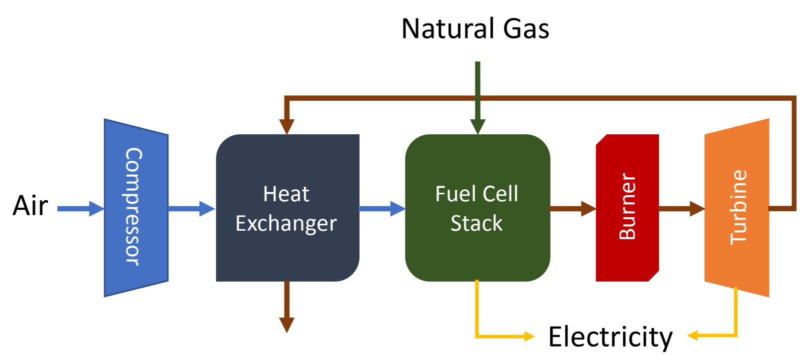

Figure 3: Sample conceptual design of a high efficiency natural gas to electricity conversion system

To clarify, the system concept shown is a potential outcome of the conceptual design process for a challenge problem that calls for an ultra-high efficiency (i.e. >70%) fuel to electricity conversion system. One of the major objectives of the DIFFERENTIATE program is to develop machine-learning-enhanced hypothesis generation/conceptual design tools that automatically determine engineering-optimal[8] solutions for the architectures of systems, such as that shown in Figure 3, subject to problem-specified (e.g. natural gas fuel) and technology-imposed (e.g. material property limits) constraints.

To continue with this example, the desired architectural optimization tool would select system components from an existing database and determine how they can be connected to satisfy the

[8] In the context of this FOA, an 'engineering-optimal' solution is not necessarily the true mathematical global optimum. Rather, it is the most attractive known solution to a problem that is obtained with the resources (e.g. time, money) made available for its solution. It is hoped that the ML-enhanced optimization methodologies developed during the DIFFERENTIATE program will help to either close the "optimality-gap" between the engineering-optimal and globally-optimal solutions or achieve the same gap with the expenditure of fewer development resources.

constraints while improving upon the objective function. For each component, this database would provide interface numbers and types (e.g. flow, mechanical, electrical), technology constraints, and a list of unknown design parameters that must be determined during the optimization.

From a mathematical standpoint, the type of problem that is solved is a Mixed-Integer Problem (MIP) in that the solution vector contains both integer (components and connections) and continuous (design parameters) variables. Depending on the type of component level ROMs employed, the mixed integer problem may be a mixed integer *linear* programming problem or a mixed integer *non-linear* programming problem, which is meant to signify that, when all integer variables are fixed to potential integer solution, the resulting mathematical program is either a linear optimization problem or a nonlinear optimization problem. Furthermore, the resulting nonlinear program may represent a convex optimization problem or a non-convex optimization problem.

The formal mathematical problem may be stated as follows—

$$\min Z = f(x, y)$$

$$g(x, y) = 0$$

$$h(x, y) \leq 0$$

$$x \in \Re^n$$

$$y \in \{0,1\}^m$$

Z is the performance metric to be minimized (e.g. the negative of the efficiency or net present value) by selecting x and y. $g(x, y)$ are the equality constraints. These include technology constraints and the physical conservation laws (e.g. conservation of mass and energy). $h(x, y)$ are the inequality constraints (e.g. maximum temperatures). The x vector represents the continuous design parameters, and the y vector represents the integer/Boolean quantities (e.g. components and connections). n and m represent the number of continuous and integer variables, respectively. Both quantities are also nominally unknown.

While the above example was focused on the optimization of mechanical and electrochemical fuel to electric power conversion systems, similar mixed integer optimizations occur in the conceptual design of many “systems.” Examples include—

1. Thermodynamic cycles/Chemical processes,
2. Electrical power converters, and
3. Materials/molecules.

An example of the desired thermodynamic cycle design capability is provided in Wang *et al*[9], where the ability to develop optimal Combined Heat and Power (CHP) system architectures is demonstrated, albeit for very simple representations of the system components (e.g. microturbine, adsorption chiller). In the context of CHP system architectural design, this FOA would seek to build upon the demonstrated capability by leveraging machine-learning-enhanced approaches to enable an enhancement to the fidelity of the component models that are used in the design of the system at an attractive cost to the design process. These enhancements might include better component representations or perhaps enhanced optimization approaches that are capable of efficiently solving the likely resulting mixed integer nonlinear programming (MINLP) problem.

In sum, the first objective of the DIFFERENTIATE program is the development of machine-learning-enhanced hypothesis generation/conceptual design/mixed integer optimization tools that will help engineers to more rapidly and cost-effectively consider a wider range of more novel concepts before selecting an engineering-optimal architecture for high-fidelity detailed design and evaluation.

2. Hypothesis Evaluation (i.e. Detailed Design) – Nonlinear optimization problems

In the Hypothesis Evaluation (HE) phase, engineers:

1. Add substantial fidelity to their conceptual design to fully define the materials, the sizes and shapes of parts to be fabricated from them, their configurations, and detailed manufacturing approaches,
2. Optimize their higher fidelity concepts with high-fidelity (*e.g.,* Partial Differential Equation based) simulations and targeted risk reduction experiments, and
3. Validate their overall design in full system experimental demonstrations.

In Figure 4, an Evaluation-centric view of the design framework originally presented in Figure 1 is shown. In this view, the evaluation process is nominally modeled as a series of parallel detailed design processes where the individual components that comprise the system conceptual design are fully defined and evaluated with high-fidelity (e.g. partial differential equation based) solvers and experiments. To continue the example used in the "Hypothesis Generation" section, one of these design processes might be focused on defining the physical compressor that would yield the desired pressure ratio at the target efficiency. Another might be focused on defining the physical heat exchanger that would yield the target effectiveness while respecting the pressure drop constraints, and yet another would fully define the fuel cell stack.

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[9] Wang, Yi *et al*, Mixed-integer linear programming-based optimal configuration planning for energy hub: Starting from scratch, Applied Energy 210, 2018, pp. 1141-1150.

In the early stages of the component-level design processes (i.e. component-level conceptual design), component-level ROM-model based (perhaps machine-learning-enhanced) mixed-integer optimization tools are likely to be appropriate, as both integer and continuous variables are required to define the materials and the component-level architectures (e.g. number of cells in the fuel cell stack, number of compressor stages and/or blades). However, as the design matures and the discrete decisions are made, mixed-integer problems frequently give way to optimization problems with only continuous variables (e.g. thicknesses of the various layers in the repeat unit of fuel cell stack, the shapes of compressor blades) that leverage relatively expensive high-fidelity analyses.

From a mathematical standpoint, the type of problem that is commonly solved in the later stages of the hypothesis evaluation/detailed design process is a linear or nonlinear optimization problem. Once again, depending on the high fidelity model employed, the problem may be linear or nonlinear and convex or non-convex.

The formal mathematical problem may be stated as follows—

$$\min Z = f(x)$$

$$g(x) = 0$$

$$h(x) \leq 0$$

$$x \in \Re^n$$

Z is the performance metric to be minimized (e.g. the negative of the efficiency or mass) by selecting x. $g(x)$ are the equality constraints. These include technology constraints and the physical conservation laws (e.g. conservation of mass and energy). $h(x)$ are the inequality constraints (e.g. maximum temperatures). The x vector represents the continuous design variables. n represents the dimensional space of the design variables.

An example of the desired optimization capability can be found in Kaya and Hajimirza,[10] where neural networks were used to develop surrogate-model representations of thin film multi-layered amorphous silicon-based solar cells. These representations were then used to optimize the multi-layer structures of the devices at computational costs that were less than one-fifth of that of the baseline optimizations that were conducted using Finite-Difference-Time-Domain simulations of Maxwell's Equations.

[10] Kaye, Mina and Hajimirza, Shima, Rapid Optimization of External Quantum Efficiency of Thin Film Solar Cells Using Surrogate Modeling of Absorptivity, Nature Scientific Reports, *(2018) 8:8170* DOI: 10.1038/s41598-018-26469-3.

In sum, the second objective of the DIFFERENTIATE program is the development of machine-learning-enhanced hypothesis evaluation/detailed design/real parameter optimization tools that will help engineers to more rapidly and cost-effectively optimize their design concepts.

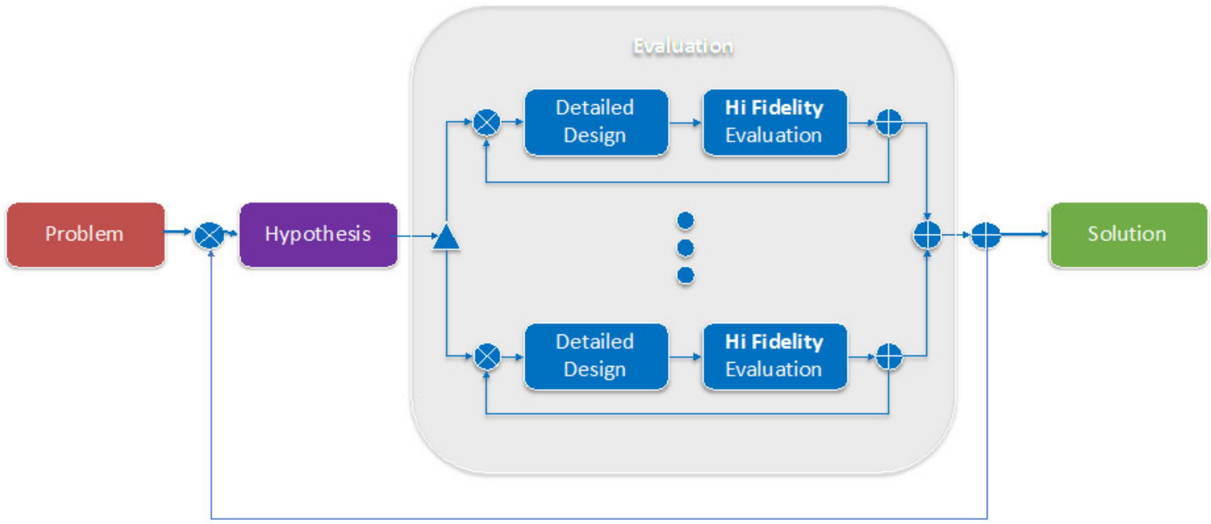

Figure 4: Evaluation-centric view of the design process framework introduced in Figure 1

3. Inverse Design

In an inverse design process, the design is explicitly calculated from the target performance metrics. In the remainder of this sub-section, this process is described and contrasted with traditional forward design processes.

Traditional Forward Design Processes

Traditional forward processes are iterative in that a solution is hypothesized, evaluated against its target performance, and iteratively refined based upon the results of repeated evaluations. To illustrate this process in more mathematical terms, the traditional forward design process originally presented in Figure 1 is shown again in Figure 5 with mathematical annotations. In essence, assuming for sake of simplicity that the design intent is to meet or exceed y_{target}, the hypothesis that is formulated in the hypothesis generation phase may be expressed as follows—

$$H:\ f\left(x_{hypothesis}\right) \geq y_{target}.$$

In the evaluation phase, the actual performance of the hypothesized concept is estimated—

$$y_{actual} = f(x_{hypothesis}).$$

If the actual performance of the concept meets the design intent (i.e. $y_{actual} \geq y_{target}$), the design process has been successfully completed, and the hypothesis becomes the final design (x_{design}). Otherwise, if a performance shortfall exists, the hypothesis is updated—notionally using the difference between the actual and target performance vectors and the gradient of the objective function—

$$\Delta x_{hypothesis} = \frac{y_{target} - y_{actual}}{\nabla f}$$

This iteration process continues until either the target performance is achieved or the effort is deemed infeasible. The cost of traditional design processes is driven by the cost of repeated design evaluation processes.

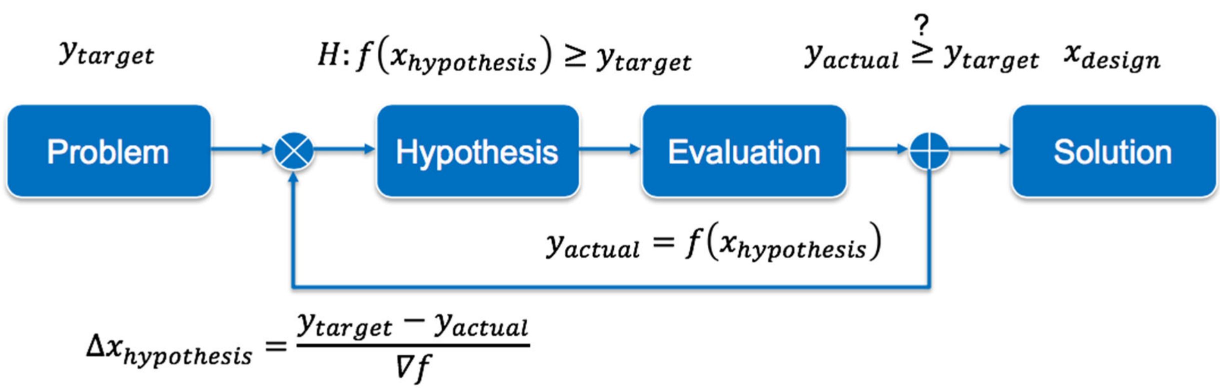

Figure 5: Traditional iterative design process – where it is assumed for simplicity that the design intent is to meet or exceed all the performance metrics identified in the requirements vector y_{target}.

Inverse Design Processes

Alternatively, in an "Inverse Design" process, the design is explicitly calculated from the requirements without iteration. In mathematical terms:

$$x_{design} = f^{-1}(y_{target}).$$

If the inverse function (f^{-1}) is known, inverse design processes have the potential to be appreciably lower cost as the design may be determined from a single explicit function evaluation. A cartoon illustrating the desired capability is presented in Figure 6.

However, the cost of determining the inverse function is potentially significant due to the cost of the required training data and the mathematical risk associated with the potentially ill-posed nature of some inverse problems. Nonetheless, there are examples where non-machine-learning-based inverse design techniques have been successfully applied in optics,[11] aerodynamics,[12] and chemistry.[13]

Consequently, the third and final objective of the DIFFERENTIATE program is the development of useful (i.e. of sufficient accuracy and for acceptable cost) inverse design representations for relatively simple design problems (e.g. compressor blades, nanophotonic devices, simple materials/molecules).

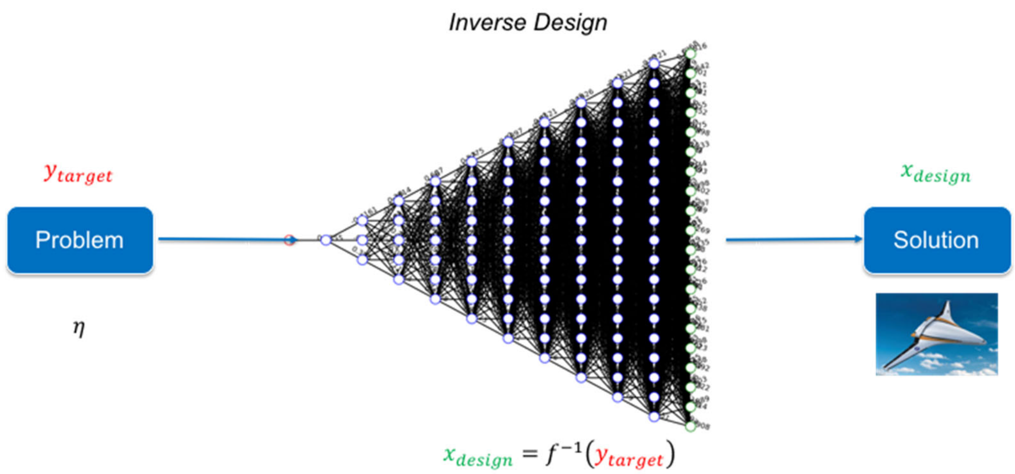

Figure 6: Cartoon illustration desired inverse design capability

D. APPROACH

As discussed in the previous section, the objective of the DIFFERENTIATE program is to accelerate the pace of energy innovation by enhancing our capabilities to formulate novel high-performance system concepts, to efficiently optimize the detailed design of their components, and in some selected instances to solve inverse design problems. The overall approach that the DIFFERENTIATE program seeks to encourage is the leveraging of rapidly advancing machine learning technology in the realization of the three targeted capabilities.

In this section, notional examples of potential solution approaches are presented with the significant caveat that they are provided for illustrative purposes only and have not yet been fully reduced to practice (i.e., They might not work!). This discussion is preceded by a brief

[11] Molesky, Sean *et al*, Inverse Design in Nanophotonics, Nature Photonics, Vol 12, November 2018, pp. 659-670.
[12] Jameson, Antony, Aerodynamic Design Using Control Theory, Journal of Scientific Computing, Vol. 3, No. 3, 1988.
[13] Sanchez-Lengeling, Benjamin and Aspuru-Guzik, Alán, Inverse molecular design using machine learning: Generative models for matter engineering, 27 July 2018, Science 361, pp. 360-365.

review of the three general types of machine learning and a discussion of how each of them might be appropriate (or not) in the context of the DIFFERENTIATE program.

1. Machine Learning

Machine learning algorithms provide computational algorithms the ability to learn and improve from experience without explicit human intervention. Our interest in such algorithms stems from our hypothesis that they may be used to cost-effectively develop models that may be used to help engineers more efficiently develop attractive solutions to challenging problems. As illustrated in Figure 7, there are three general types of machine learning:

1. Unsupervised learning is used to identify "clusters" of data points with common characteristics in unlabeled data. As an example, an unlabeled data set might consist of pictures of elephants and dogs. With luck, when an unsupervised learning algorithm is trained with them, it may (ideally) be able identify that there are at least two overreaching categories. However, as no picture "labels" were provided, the resulting clustering algorithm will not be able to identify the pictures as either elephants or dogs.

2. Supervised learning is used with labeled data to identify data categories (i.e. classification) or to quantitatively predict continuous valued parameters (i.e. regression). For example, if the abovementioned elephant and dog pictures were labeled with the classification "elephant" or "dog", a supervised learning algorithm that is trained using both the pictures and corresponding labels, would (ideally) be capable of identifying whether an individual elephant or dog picture supplied to it is that of an elephant or a dog. Furthermore, in addition to classification, supervised learning is also helpful in the development of regressions that could be used to quantitatively predict parameters of interest (e.g. perhaps the weight of the animals in the pictures if such training data were also provided—to stretch an example perhaps a bit too far).

3. Reinforcement learning is used to develop a reward maximizing strategy/policy for an agent that sequentially interacts with an environment that is influenced by the actions of the agent. In each interaction, the agent assesses the state of the environment and either deterministically or stochastically selects an appropriate action based upon the strategy/policy that it has learned through prior interactions.[14]

[14] Sutton, Richard S. and Barto, Andrew G., Reinforcement Learning: An Introduction, The MIT Press, 2018.

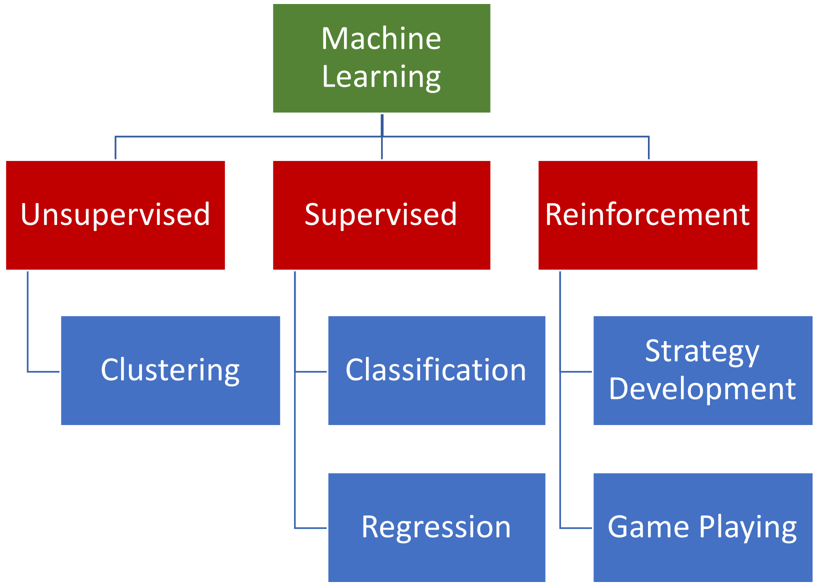

Figure 7: Three types of machine learning and typical uses for each of them

Of the three abovementioned types of machine learning, it is expected that both supervised and reinforcement learning will play the largest roles in the scope of activities envisioned for the DIFFERENTIATE program. In the remainder of this section, these two types of learning will be highlighted in the descriptions of three example approaches to the development of the desired DIFFERENTIATE capabilities—Hypothesis Generation, Hypothesis Evaluation, and Inverse Design. As a reminder, they are described for illustrative purposes only, and it is hoped that Applicants will offer more compelling approaches to the development of the desired capabilities.

2. Hypothesis Generation (i.e. Conceptual Design) – Mixed integer optimization

In the Hypothesis Generation phase (Figure 2), engineers generally use Reduced Order Models to refine a high-level representation of their solution concept (e.g. Figure 3, Table). The DIFFERENTIATE program seeks to enhance the productivity of engineers in the execution of this phase of the technology development process by automating the definition of the system concept and by enhancing the fidelity of or lowering the cost of executing the ROM-based evaluation process. In mathematical terms, as previously suggested, the DIFFERENTIATE program seeks to enhance the capability of engineers to solve the Mixed Integer (frequently) Non-Linear Problems (MINLP) that are characteristic of many conceptual design processes. This overarching MINLP capability may be further sub-divided into two supporting capabilities:

1. Intelligent Automated Conceptual Design/System Configuration, and
2. Enhanced Fidelity and/or Lower Cost Automated Reduced Order Model Construction and Evaluation.

In Table, descriptions of the desired capability, their mathematical roles, and notional ML-enhanced approaches are presented. In the examples provided, it is hypothesized that supervised learning might be used to develop higher fidelity and/or lower cost ROM system models, and that reinforcement learning might be used to enhance the efficiency of the MINLP optimization process by providing "more intelligent" conceptual design updates.

Table 1: Hypothesis Generation sub-capability description, mathematical role, and example ML-enhanced approach

Sub-Capability	Mathematical Role	Example ML Approach
Intelligent Automated System Configuration	Optimizer	Reinforcement Learning
Enhanced Productivity Automated Reduced Order Model Construction and Evaluation	Function Evaluation	Supervised Learning

3. Hypothesis Evaluation (i.e. Detailed Design) – Nonlinear optimization problems

In the Hypothesis Evaluation phase, overall system architectures are generally defined and the task at hand is the development of the detailed (component) designs that enable the realization of the performance and cost targets established during the definition of the system architectures. In the (overly) simplified design process framework utilized in this FOA, the optimization processes in this phase are assumed to be nonlinear optimization problems. A nominal process flow diagram for this phase has been proposed in Figure 4. Each of the parallel iterative hypothesis evaluation/detailed design processes leverage expensive and high-fidelity (relative to ROMs) function evaluations. In practice, evaluation tools frequently include partial differential equation-based solvers or physical experiments.

In order to illustrate potential ML-based productivity enhancement strategies, a notional ML-enhanced optimization process is depicted in Figure 8. In this approach, an initial guess at the solution to the problem posed is encoded (via the Encoder) into a lower dimensional representation that is used in the iterative optimization process to reduce the dimensionality of the design space and thereby reduce the cost of gradient evaluations. In the baseline iteration process, this initial guess and subsequent variations on it are "re-expanded" (via the Decoder) into their full-dimensional representations before their performance is evaluated (via the Evaluator). This evaluation process could be conducted via traditional methods or perhaps via ML-derived "surrogate" models. However, it is also conceivable that a more comprehensive ML-derived surrogate performance model could be developed that is capable of evaluating the design directly from the lower dimensional representation. This more comprehensive (Decoder + Evaluator) is depicted on the bottom of the figure.

Lastly, as was the case with the Hypothesis Generation capability, reinforcement-learning may offer attractive optimizer-level benefits[15].

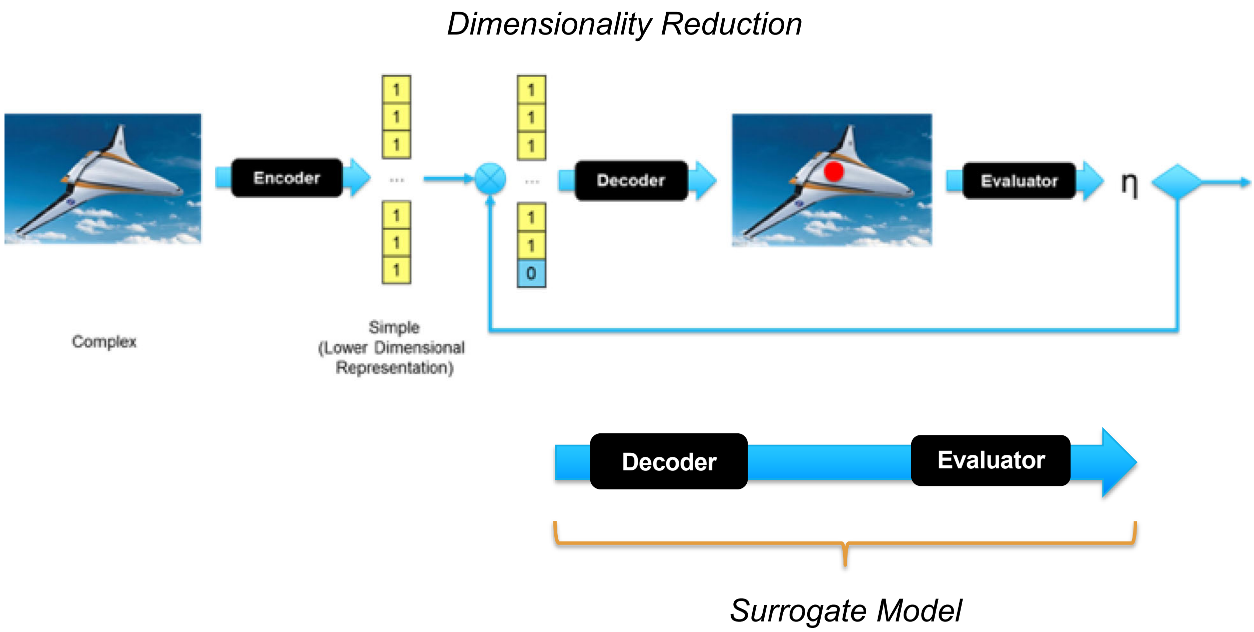

Figure 8: Notional ML-enhanced hypothesis evaluation/detailed design process

4. Inverse Design

As discussed previously, iterative design procedures have the potential to be time-consuming and expensive due to the general requirement for multiple costly objective function evaluations.[16] At the same time, deep neural networks (DNN) offer the potential to be universal function approximators.[17] The DIFFERENTIATE program seeks to reduce design time and iteration by leveraging the universality of DNNs to develop explicit function representations for designs as functions of their performance targets.

As an example of the desired capability, consider the "inverse design" of a simple air-air ejector, where a high-pressure air stream (the primary stream) is used to pump a lower pressure air stream (the secondary stream) through an adverse pressure gradient in a frictionless constant area duct. In this scenario, a fully-mixed ejector model may be used to estimate the ideal

[15] Li, Ke and Malik, Jitendra, Learning to Optimize, https://arxiv.org/abs/1606.01885.
[16] However, it is of course hypothesized that abovementioned ML-enhanced capabilities will reduce both the number and cost of those evaluations.
[17] Cybenko, G., Approximation by Superpositions of Sigmoidal Functions, Mathematics of Control, Signals, and Systems (1989) 2, pp. 303-314.

pumping performance—a convenient approach for this example but likely overly optimistic in practice.

Via this methodology, the fully-mixed ejector exit stream conditions (e.g. density, pressure and velocity) may be readily calculated from the conservations of mass, momentum, and energy given the high and low pressure inflow stream conditions. However, the challenge with this approach in a practical design process is that the exit stream static pressure is generally a known quantity while the primary inflow stream total pressure that is required to pump the desired amount of secondary stream fluid is generally unknown.

However, to expedite the design process via the avoidance of the (apparent) need for design iteration, a DNN-based inverse design approach may be used to develop an explicit functional representation for the unknown primary stream total pressure design parameter given the desired performance (secondary stream mass flow rate) and operating pressure ratio (exit static to secondary stream inflow total pressure ratio).

In this instance, such an approach has been developed and validated by ARPA-E and is pictorially illustrated in Figure 9. In this approach, the pictured network was trained using the fully-mixed analytical forward model to calculate the primary total to exit static pressure ratio (green output node) that is required to pump a desired secondary to primary stream massflow ratio (top red input node) through a specified exit static to secondary stream inflow total pressure ratio (bottom red input node). When trained with >800 data points, the average predicated output error was <2% when evaluated over a random grid of 100x100 input vectors.

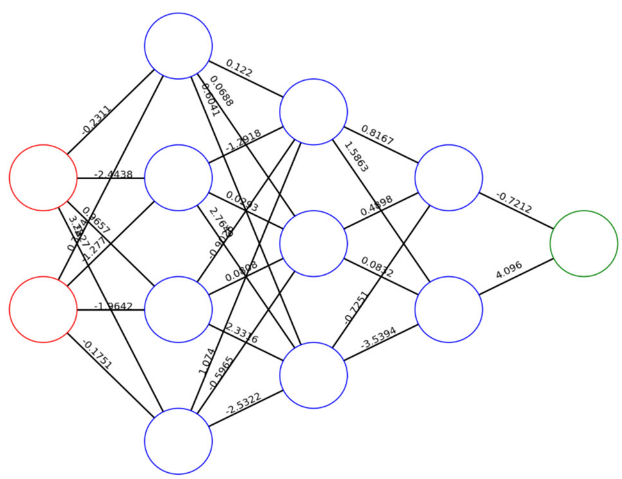

Figure 9: Neural network inverse design representation for the primary total pressure required to pump a desired amount of secondary fluid across a specified outflow static to inflow total pressure ratio

While the above described inverse design methodology was arguably technically successful, in practice, when evaluating whether such an inverse approach is attractive from an economic standpoint, one must weigh the anticipated design cost/time benefits versus the cost of training and testing the neural network. Consequently, inverse methodologies are likely to be most attractive in scenarios where similar design efforts are repeated many times (e.g. custom-designed X).

E. PROGRAM STRUCTURE

The DIFFERENTIATE program is structured to encourage the development of tools that enhance the three aforementioned capabilities. Furthermore, in the interest of focusing limited financial resources on the enhancement of the ability to address important energy-related problems and mitigating the cost of obtaining any required training "data," ARPA-E has selected several challenge problem areas for each of the abovementioned capabilities.

In all submission to this FOA, Applicants are asked to select one capability (i.e. FOA Category[18]) and a challenge problem area for the selected capability. The ARPA-E identified challenge problem areas are as follows—

- **Category #1: Hypothesis Generation (Conceptual Design) – Mixed integer optimization**
    - Thermodynamic Cycles/Chemical Processes (e.g. Gas Separations)
    - Electrical Power Converters
    - Materials/Molecules

- **Category #2: Hypothesis Evaluation (Detailed Design) – Nonlinear optimization problems**
    - Heterogeneous Catalysts
    - Turbomachinery

- **Category #3: Inverse Design**
    - Aerodynamic Devices/Surfaces
    - Photonic Devices

More detailed descriptions of these problem areas are provided in the following three sections. However, if an Applicant feels strongly that it has a qualified (i.e. impactful and tractable) alternative challenge problem for one of the desired capabilities, the Applicant has the option to propose to develop its selected capability on its challenge problem. However, the Applicant must sufficiently justify that the proposed alternative challenge problem is both highly impactful (from a national energy-usage perspective) and especially appropriate for solution-process enhancement via machine learning.

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[18] It is likely (perhaps almost certain) that the lean organizational framework employed in this FOA will be too simple and that some proposed approaches may arguably fit into more than one of the three FOA categories. In this circumstance, Applicants are encouraged to simply pick the category that is most 'correct' for formal submission purposes and discuss the applicability of the proposed approach to one or more additional categories in the technical volume.

1. Category #1: Hypothesis Generation (Conceptual Design) – Mixed integer optimization

In this category, the DIFFERENTIATE program seeks to develop the capability to "automatically" determine an engineering-optimal system configuration for the conversion of available resources to desired outputs—subject to application-driven (e.g. no CO_2 emissions) and/or technology-driven (e.g. Temperature < 1200 °C) constraints. In Figure 10, a notional process flow diagram is presented to illustrate the desired Hypothesis Generation tool inputs, process elements, and outputs. In order to focus tool development efforts on problems of interest to ARPA-E, three broad categories are proposed in the remainder of this section as challenge problem areas for initial tool development. However, it is anticipated that the approaches and algorithms developed will be applicable in areas beyond that of the initial challenge problem.

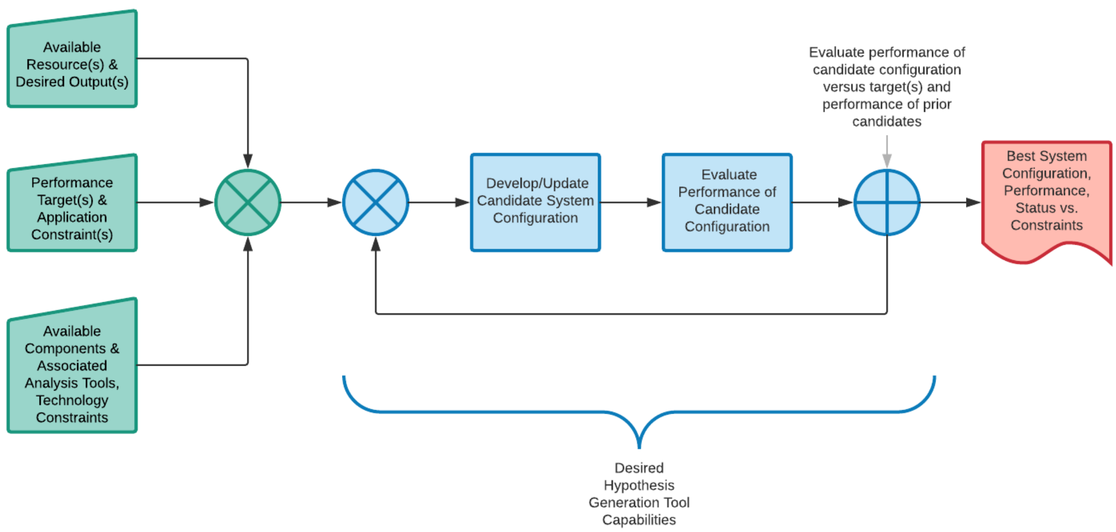

Figure 10: Nominal process flow diagram illustrating the expected Hypothesis Generation Tool inputs (green), process elements (blue) and outputs (red).

Challenge Problem Area 1.1: Thermodynamic Cycle/Chemical Process Optimization

Thermodynamic cycles (work output) and chemical processes (chemical output) are ubiquitous tools in the conversion of natural resources to more economically useful outputs. From a national perspective, they are major economic and energy-usage drivers. For example, in 2018, over 80% of US electricity was generated via thermodynamic cycles,[19] and in 2014, chemical industries accounted for 33% of total US manufacturing energy usage.[20]

In this challenge problem area, the objective of the DIFFERENTIATE program is the development of the ML-enhanced capability to automatically design engineering-optimal thermodynamic cycles and/or chemical processes, given the available resources, desired outputs, available components, and relevant application and technology constraints. In the interest of providing further clarity, four specific example challenge problems are provided in Table 1; two are electrical power generation problems (i.e. thermodynamic cycles), and two are chemical manufacturing process problems.

Table 1: Sample specific thermodynamic cycle/chemical process optimization challenge problems

Description	Available Resources	Desired Outputs	Design Objective	Constraints
Carbon-Neutral Conversion of Natural Gas to Electric Power (e.g. INTEGRATE, IMPACCT)	Air & Natural Gas	Electric Power	Max Fuel to Electricity Conversion Efficiency	CO_2 Emissions ≤ 30 g/kWh_{elec}
Ultra-High Efficiency Conversion of Heat to Electric Power	High (e.g. 1000 °C), Temperature Heat Source & Low (e.g. 25 °C) Temperature Heat Sink	Electric Power	Max Available Heat to Electricity Conversion Efficiency (I.e. Second Law Basis Efficiency)	
Carbon-Neutral Liquid Fuels (e.g. REFUEL)	Heat or Electricity, CO_2, H_2O	Surrogate Jet-A (~$C_{10}H_{23}$)	Max LHV (MJ/kg)	CO_2 Emissions ≤ 30 $g/kWh_{products}$
Methane Pyrolysis (e.g. Half-baked Methane)	Heat, CH_4	H_2, C	Max H_2 + C Yield	CO_2 Emissions ≤ 30 $g/kWh_{products}$

An approach to solution of each of these problems might include the development of an ML-enhanced modeling tool that given the available inputs and desired outputs would be capable of selecting components (e.g. compressor, heat exchanger, distillation column) from a list of

[19] https://www.eia.gov/todayinenergy/detail.php?id=38053 (Natural Gas + Coal + Nuclear)
[20] https://www.eia.gov/consumption/manufacturing/data/2014/pdf/table1_2.pdf

potential options and optimally arranging them while establishing component-level performance targets (e.g. pressure ratio, effectiveness, purity) and rolling these targets into a prediction of the overall system performance. In the performance analysis, reduced order explicit physics-based or ML-derived surrogate (i.e. implicitly physics-based) component models might be employed subject to specified technology and/or application constraints. ML might be used to develop the capability to automatically provide attractive system configurations for performance evaluation subject to overall physical constraints such as the conservations of species, mass, and energy.

Challenge Problem Area 1.2: Electrical Power Converters

Semi-conductor-device-switched electrical power converters[21] are critically important in today's electronic world and are forecast to become even more so in the coming decades. Specifically, a 2005 ORNL study estimated that 30% of all electrical power generated passed through power converters and that this percentage could grow to 80% by 2030.[22]

The value propositions enabled by these devices in stationary applications are driven by their efficiency, reliability, and cost (e.g. $/W). In transportation applications, power-specific device mass (e.g. kg/W) and/or volume (e.g. L/W) are also frequently also critical value drivers.

The converters themselves consist of interconnected individual circuit components (e.g. resistors, capacitors, inductors, diodes, switching devices). As an example, a simple DC to DC buck converter is depicted in Figure 11.

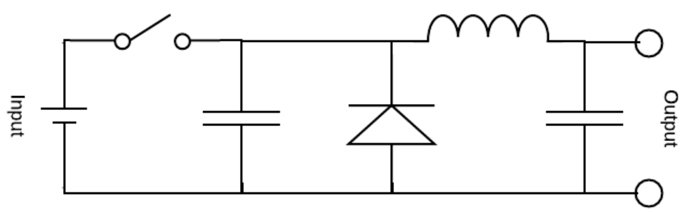

Figure 11: DC to DC Buck (High to Low Voltage DC) Converter[23]

In this challenge problem area, the objective of the DIFFERENTIATE program is to automate the electrical circuit design process by automatically selecting, configuring, and tailoring the individual components that enable available resources (e.g. high voltage DC power) to be converted to the desired output (e.g. lower voltage DC power with a voltage ripple <XX%) subject to the application-specific thermal and packaging considerations.

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[21] These devices are used to convert electric power from one form to another more useful one (e.g. AC to DC, DC to DC, DC to AC).

[22] Tolbert, L.M. et al, Power Electronics for Distributed Energy Systems and Transmission and Distribution Applications, ORNL/TM-2005/230, December 2005.

[23] https://www.mouser.de/pdfdocs/BuckConverterDesignNote.pdf

In the development of the desired ML-enhanced automated design capability, Applicants should leverage existing state-of-the-art (and emerging) circuit design languages (e.g. Verilog, HDL, Modelica, Modia) and analysis software (e.g. SPICE, Cadence) to the maximum extent possible in the interest of focusing the limited available resources on the development of the ML-enhanced automation capability and to facilitate the integration of DIFFERENTIATE-developed tools into existing power converter design work flows.

A potential ML-enhanced approach to the realization of the desired capability in this program area might employ the same strategy utilized in the example provided for Challenge Problem Area 1.1. In this context, given the available resources (e.g. high voltage DC power) and the desired output (e.g. lower voltage DC power), the ML-enhanced optimization tool might select potential components (e.g. resistor, capacitor, inductor, diode) from a list of available options and automatically specify (e.g. resistance, capacitance, inductance, orientation) and configure them into a system that would optimally yield the desired electrical power conversion. In the context of some of the abovementioned available programming tools, the desired ML-design capability might automatically generate Modelica or Modia code for a candidate system architecture so that it can be evaluated with existing physics-based analysis tools.

Challenge Problem Area 1.3: Materials/Molecules

Material properties limit energy system performance in many applications. For instance, the high temperature oxidative and/or strength properties of metals are frequent thermodynamic cycle (e.g. Brayton, Otto) performance limiters. Additionally, the electronic and/or ionic conductivities of materials limit the performance of many electronic and chemical-to-electronic energy-conversion devices.

Given this performance limiting role, the development of new materials with more attractive properties can enable better performing energy systems. This point has, of course, been recognized and acted upon by mankind for at least millennia (e.g. Stone Age, Bronze Age, Iron Age). Investment and development progress continue today; however, the required financial investment is large (e.g. Air Force expenditures of >$100M/year for gas turbine materials alone[24]) and the resulting pace of material property advancement is arguably slower (~20 years/discovery[25]) than would be preferred given our climate and energy challenges.

The search for new materials is frequently an empirical one that is directed by the intuition of skilled engineers and scientists. New compositions are manually and iteratively hypothesized and evaluated with existing databases, experiments and/or high-fidelity (e.g. Density Functional

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[24] National Research Council 2011. Materials Needs and R&D Strategy for Future Military Aerospace Propulsion Systems. Washington, DC: The National Academies Press. https://doi.org/10.17226/13144.

[25] Clean Energy Materials Innovation Challenge Expert Workshop. Materials Acceleration Platform: Accelerating Advanced Energy Materials Discovery by Integrating High-Throughput Methods with Artificial Intelligence. Mission Innovation

Theory) simulations. However, recent work has suggested that machine learning-enhanced material composition design tools can help to accelerate the identification of attractive new material compositions.[26]

In this challenge problem area, the objective of the DIFFERENTIATE program is to accelerate the maturation of emerging ML-enhanced design tools to help identify promising new material compositions for a broad range of potential energy applications. It is hoped that these tools might be used to more efficiently suggest compositions for further evaluation that might yield attractive performance increases (e.g. tensile strength, conductivity) at acceptable costs. In the spirit of the objective of this category (i.e. the acceleration of the solution of MINLP), the specific capability that is sought in this context is the automated selection of the appropriate constituents (e.g. carbon, alkane, asparagine) and/or the automated development of synthesis processes[27] for advanced materials/molecules that have the potential to offer attractive value propositions in one or more energy applications.

2. Category #2: Hypothesis Evaluation (Detailed Design) – Nonlinear optimization problems

In this section, two Hypothesis Evaluation/Detailed Design challenge problems areas are described in more detail in order to illustrate both the energy-related challenge problems and opportunities for ML-enhanced design tools to facilitate their solutions.

The challenge problems areas include:

1. Heterogeneous Catalysts
2. Turbomachinery

These problem areas were selected due to their importance to ARPA-E's mission and the fact that the optimization of designs within each of the two areas nominally requires the repeated solution of a system of partial differential equations (e.g. Schrödinger, Navier-Stokes, Maxwell). Generally speaking, proposed solution approaches might leverage dimensionality reduction and surrogate models and/or new ML-enhanced optimization approaches to reduce the cost and/or number of high-fidelity and cost design performance evaluations.

Challenge Problem Area 2.1: Heterogeneous Catalysts

Heterogeneous catalysts are ubiquitous in many energy applications. They are broadly used to facilitate the synthesis (e.g. NH_3, H_2) and/or the destruction (e.g. CO, NO_x, CH_4, O_2) of many chemical compounds by lowering the activation energies required for reactions to proceed—without being consumed. While they are critical to the economics of many energy-related

[26] Gomez-Bombarelli, R. et al, Automatic Chemical Design Using a Data-Driven Continuous Representation of Molecules, ACS Central Science 2018 4 (2), 268-276.

[27] Kim, E et al, Virtual screening of inorganic materials synthesis parameters with deep learning, npj Computational Materials (2017) 53.

processes (e.g. ammonia synthesis, fuel reformation, oxygen reduction), they are also often major cost drivers in part through the frequent use of platinum group metals. New catalyst design efforts are frequently focused on developing new compositions and/or surface morphologies that offer the potential for lower cost through reduced precious metal usage and/or longer life.

Unfortunately, many of these development processes feature expensive high-fidelity numerical simulations and/or experiments. In posing this challenge problem area, ARPA-E seeks to accelerate the discovery process by reducing the required number of high-fidelity performance evaluations. Potential opportunities in this space include approaches that facilitate the ML-enhanced discovery of low-cost catalyst ‘descriptors’ that are themselves easier to measure/predict than the physical property of interest but still can be used to infer the desired property that is expensive to measure/predict,[28] or approaches that leverage the development and use of, for example, Density Functional Theory and/or Lattice Boltzmann trained neural network surrogate models to predict catalyst performance as a function of its composition, surface morphology, and perhaps its level of contamination.[29]

Challenge Problem Area 2.2: Turbomachinery

Turbomachines (e.g. compressors and turbines) are major performance drivers in many energy systems—including stationary electric power plants (e.g. natural gas combined cycles) and aircraft engines. Their modern multistage industrial design processes nominally include mean-line, streamline, and three-dimensional computational fluid dynamics (CFD) simulations. Each successive design stage employs physics-based models of increasing fidelity and cost. However, at all stages, empirical corrections to the models are typically made for important, but unmodeled, effects. For instance, at the mean-line stage, these empirical corrections include blade incidence angle loss models, and at the 3D CFD stage, the empiricism frequently includes the turbulence models employed in Reynolds-Averaged Navier-Stokes (RANS) models. While the mean-line analyses are efficient at the establishment of target rotor/stator or blade/vane turning angle, and streamline analyses are effective at developing initial stacked two-dimensional blade geometries, relatively expensive RANS simulations are used extensively in the refinement of the full three-dimensional airfoil and end wall (including turbine rim cavity) geometries.

As the cost of executing a design simulation at a given level of fidelity has dropped (some might say plummeted) due to enhancements in both design tool efficiency and computer hardware, turbomachinery component performance (e.g. efficiency) has continued to increase—albeit at the cost of increased design complexity.

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[28] Goldsmith, B. R. et al, Machine Learning for Heterogeneous Catalyst Design and Discovery, AiChE Journal, July 2018, Vol. 64. No. 7.
[29] Ibid.

In parallel, additive manufacturing technologies have been rapidly evolving and are beginning to make inroads into both industrial and aircraft turbine applications.[30] As this manufacturing technology continues to mature, the design flexibility that it offers would potentially make it an attractive manufacturing approach for turbomachinery airfoils—further increasing the number of design options that would be available for designers to leverage in their pursuit of enhanced performance at an attractive cost.

In this challenge problem area, the DIFFERENTIATE program is seeking to develop ML-enhanced design tools to dramatically augment the ability of engineers to optimize the designs of turbomachinery systems with the goal of enabling the attainment of greater thermodynamic performance at lower cost.

Within the context of the current design systems, there are potential opportunities to leverage the flexibility of machine learning to enhance the fidelity of the abovementioned empiricism for the same cost at all stages. It may even be possible to fully replace the mean-line and streamline analyses with a single efficient ML-based design tool. Furthermore, ML-enhanced tools could help engineers to manage the increasing dimensionality of their design spaces by helping to efficiently/automatically develop new parametric representations (e.g. Principal Component Analyses) that would ideally enable them to reap the benefits of their increased flexibility at a reduced design cost. Lastly, ML-based surrogate models of turbomachinery flow fields, structures, or thermal management systems, could be invaluable in the efficient automation of the design of turbomachinery components.

3. Category #3: Inverse Design

In this category, Applicants must develop the capability to express designs as explicit functions of their performance targets, or in other words as inverse problems. This capability would be of tremendous practical interest in situations where similar design efforts are frequently and repeatedly executed (e.g. custom-designed X).

However, generally speaking, the solution of inverse problems is fraught with mathematical peril as they are frequently ill-posed—meaning that a solution may not exist, may not be unique, or may not vary continuously with continuous changes in the initial/boundary conditions. Hence, in this category and in the interest of focusing on the mathematical complexity of this class of problems, Applicants should pursue the development of their inverse capabilities using "simpler" engineering design problems. This approach is encouraged—in the interest of reducing the complexity of the design to be expressed by the inverse capability and in the interest of reducing the cost of individual training data points. For instance, in Challenge Problem Area 3.1, Applicants should pursue the inverse design of aerodynamic devices/surfaces

[30] https://www.ge.com/reports/epiphany-disruption-ge-additive-chief-explains-3d-printing-will-upend-manufacturing/

such as two-dimensional airfoil cross-sections or blades/wings rather than seeking to design an entire multi-stage compressor via inverse methods.

Lastly, while the successful development of an inverse design capability for the selected challenge problem will be a major objective of a project in this category, the development of higher-fidelity understandings of the following are also of significant interest—

1. the types of engineering design problems that are most amenable to inverse approaches and
2. the cost associated with the development of the such capabilities (e.g. training data and network complexity required versus design complexity)

In the following two-subsections, two challenge problems areas are suggested for the development of a machine-learning enhanced inverse design capability.

Challenge Problem Area 3.1: Aerodynamic Devices/Surfaces

In this challenge problem area, the development of commercially-relevant machine-learning-enhanced inverse design methodologies for aerodynamic surfaces are sought. These devices/surfaces might include—for example—aircraft wings, wind turbine blades, radial expander or compressor rotors, mixing devices, or enhanced heat transfer surfaces.

The inverse design capability would be capable of automatically generating engineering-optimal designs of the aerodynamic device/surface that would convert the available inputs (e.g. shaft power and 1 kg/s of air at standard temperature and pressure) to the desired output (e.g. 1 kg/s of air at 10 bar) at minimum cost (e.g. input shaft power).

Notionally speaking, these inverse design representations might consist of adequately trained deep neural networks that would cost-effectively output a commercially-useful design representation given a vector of commercially-relevant inputs. Ideally, these inputs would include the full importance-weighted range of potential operating conditions and associated performance targets, and the (notional) inverse design deep neural network would appropriately weigh these conditions and targets when providing a design.

Challenge Problem Area 3.2: Photonic Devices

In this challenge problem area, the development of commercially relevant machine-learning-enhanced inverse design methodologies for photonic devices are sought. These devices might include, for example, solar/photovoltaic cells, electronic to photonic interconnects, optical demultiplexers, and imaging tools.[31, 32, 33]

The inverse design capability would be capable of automatically generating the design of the photonic device that is capable of converting specified inputs (e.g. sunlight) to the desired outputs (e.g. electric current) at minimum cost (or maximum efficiency).

F. TECHNICAL PERFORMANCE TARGETS

The objective of the DIFFERENTIATE program is to enhance the pace of energy innovation by accelerating the incorporation of machine learning into energy-related engineering design processes. By doing so, it is expected that these processes will be executed at reduced time, cost and risk and/or with increased design performance, robustness and novelty. These benefits would then in turn lead to higher value energy technologies that would help the nation to reduce its energy usage and to enhance the productivity of its economy.

In this section, technical performance targets for each of the desired ML-enhanced capabilities are provided to help focus technical efforts on the program objectives. Generally speaking, as the objective of each of the categories is the development of a capability that is as generally applicable as possible, the choice of problem will not be a selection criterion beyond the Program Policy Factors stated in Section V.B.1. Rather, the performance targets are focused on the potential for the proposed approach to improve status quo design processes through lower cost and/or better performance and for the potential of major elements the proposed approach to be transferable to other system-level architectural optimization problems.

In each of the following three sub-sections, a table of performance targets/development milestones is provided. Given the difficulty of establishing meaningful quantitative performance targets that are universally applicable for both known and unknown (i.e. Applicant defined) challenge problem areas, only the milestones themselves are provided along with an indication of whether they are deemed of 'primary' (need to have) or 'secondary' (nice to have) importance. However, Applicants are encouraged to quantitatively address as many of the criteria as possible in their submissions. (E.g. The baseline design process that we seek to enhance currently takes 2 years and costs $10M, and we expect our ML-enhanced approach to reduce the time and cost of this process by 50% . . .)

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[31] Miller, Owen, Photonic Design: From Fundamental Solar Cell Physics to Computational Inverse Design, UC Berkeley Ph.D. Thesis, Electrical Engineering and Computer Science, 2012.

[32] Piggott et al, Inverse design and demonstration of a compact and broadband on-chip wavelength demultiplexer, Nature Photonics, DOI: 10.1038/NPHOTON.2015.69.

[33] National Research Council 2013. *Optics and Photonics: Essential Technologies for Our Nation*. Washington, DC: The National Academies Press. https://doi.org/10.17226/13491.

1. Category #1: Hypothesis Generation (Conceptual Design) – Mixed integer optimization

The objective of this category is the development of the capability to automatically configure and optimize system architectures. ARPA-E-provided challenge problem areas include the following:

1. Thermodynamic systems/chemical manufacturing processes,
2. Electrical power converters, and
3. Composite materials and/or molecules.

However, Applicants are free to select their own problems with adequate justification. In Table , a list of performance targets /development milestones are provided for the desired hypothesis generation tools.

Table 3: Hypothesis Generation (Conceptual Design) – Mixed integer optimization technical performance targets (notional qualitative program milestones)

#	Milestone	Primary	Secondary
1	Cost & time of baseline (status) design process defined	✓	
2	Machine-learning enhancement strategy with hypothesized design process benefits (e.g. cost, time, risk, performance, robustness, or novelty) established	✓	
3	Initial estimate of training and test data requirements provided (i.e. number of data points and cost per point)	✓	
4	Ability to generate/acquire training and test data with resources expected to be available at the start of the program confirmed	✓	
5	Ability to automatically generate and evaluate (with physics-based ROMs or surrogate models) system architectures for selected challenge problem with speed and accuracy that are consistent with the value proposition defined in Criteria #2 demonstrated	✓	
6	Ability to automatically evolve architecture concepts toward the optimal system configuration demonstrated	✓	
7	Integrated and fully-automated ability to generate, evaluate and optimize architectures with acceptable performance uncertainties given available resources and desired outputs demonstrated	✓	
8	Process to transfer the hypothesis generation capability to another energy-related challenge problem area (with updated physics-based ROMs or surrogate models) at an attractive cost developed		✓

9	Development tools made commercially available (i.e. open source, commercial software, or proprietary toolkits) to energy engineers practicing in the challenge problem areas		✓

2. Category #2: Hypothesis Evaluation (Detailed Design) – Nonlinear constrained optimization

The objective of this category is to dramatically enhance capabilities to optimize the detailed designs of energy technologies that typically require expensive and high-fidelity performance evaluations during state-of-the-art optimization processes. Examples of such evaluations include partial differential equation based numerical simulations and physical experiments. Within this category, ARPA-E seeks approaches to expedite the optimization process via the strategic development and deployment of ML-enhanced tools. It is expected that these tools would reduce the cost of performance evaluations (perhaps through the use of surrogate models) and/or reduce the number of evaluations required by making better iterative choices.

ARPA-E provided challenge problems in this area include the following—

1. Heterogeneous Catalysts and
2. Gas Compressors.

However, Applicants are free to select their own problems with adequate justification. In Table , a list of performance targets/ development milestones are provided for the desired detailed design tools.

Table 4: Hypothesis Evaluation (Detailed Design) – Non-linearly constrained optimization technical performance targets

#	Milestone	Primary	Secondary
1	Cost & time of baseline (status) design process defined	✓	
2	Machine-learning enhancement strategy with hypothesized design process benefits (e.g. cost, time, risk, performance, robustness, or novelty) established	✓	
3	Initial estimate of training and test data requirements provided (i.e. number of data points and cost per point)	✓	
4	Ability to generate/acquire training and test data with resources expected to be available at the start of the program confirmed	✓	
5	Ability to automatically generate, evaluate (with high fidelity partial differential equation-based solvers or surrogate models) and update	✓	

	detailed designs for selected challenge problem with fidelity, speed and accuracy that are consistent with the value proposition defined in Criteria #2 demonstrated (e.g. computational time/cost reduction of >80% demonstrated for the challenge problem)		
7	Process to transfer the optimization capability to another energy-related challenge problem area at an attractive cost developed		✓
8	Development tools made commercially available (i.e. open source, commercial software, or proprietary toolkits) to energy engineers practicing in the challenge problem areas		✓

3. Category #3: Inverse Design

The objective of this category is the development of the ML-enhanced capability to express designs as explicit functions of their performance targets. ARPA-E provided challenge problems include—

1. Aerodynamic Devices/Surfaces and
2. Photonic Devices.

However, Applicants are free to select their own problems with adequate justification.
In Table 5, a list of performance targets/development milestones are provided for the desired inverse design tools.

Table 5: Inverse design capability technical performance targets

#	Milestone	Primary	Secondary
1	Initial estimate of training and test data requirements provided (i.e. number of data points and cost per point)	✓	
2	Ability to generate/acquire training and test data with resources expected to be available at the start of the program confirmed	✓	
3	Ability to execute an inverse design for a “simple” (e.g. two-dimensional wing cross section) design problem in the selected challenge problem area demonstrated	✓	
4	Ability to execute an inverse design for a “moderate” (e.g. full three-dimensional wing) design problem in the selected challenge problem area demonstrated	✓	
5	Design complexity metrics developed with the goal of understanding the relationship between design complexity and the required training data	✓	

	and the complexity of the associated ML-approach (e.g. number of nodes in a deep neural network)		
6	Ability to execute an inverse design for a tractable "complex" (e.g. full aircraft) design problem in the selected challenge problem area demonstrated	✓	
7	Process to transfer the inverse design capability to another energy-related challenge problem area at an attractive cost developed		✓
8	Development tools made commercially available (i.e. open source, commercial software, or proprietary toolkits) to energy engineers practicing in the challenge problem areas		✓

II. AWARD INFORMATION

A. AWARD OVERVIEW

ARPA-E expects to make approximately $15 million available for new awards under this FOA, subject to the availability of appropriated funds. ARPA-E anticipates making approximately 7 awards under this FOA. ARPA-E may, at its discretion, issue one, multiple, or no awards.

Individual awards may vary between $250,000 and $5 million.

The period of performance for funding agreements may not exceed 24 months. ARPA-E expects the start date for funding agreements to be February 2020, or as negotiated.

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 requiring proof-of-concept R&D can propose a project with the goal of delivering on the program metric at the conclusion of the period of performance. These submissions must contain an appropriate cost and project duration plan that is described in sufficient technical detail to allow reviewers to meaningfully evaluate the proposed project. If awarded, such projects should expect a rigorous go/no-go milestone early in the project associated with the proof-of-concept demonstration. Alternatively, submissions requiring proof-of-concept R&D can propose a project with the project end deliverable being an extremely creative, but partial solution. However, the Applicants are required to provide a convincing vision how these partial solutions can enable the realization of the program metrics with further development.

Applicants proposing projects for which some initial proof-of-concept demonstration already exists should submit concrete data that supports the probability of success of the proposed project.

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

ARPA-E plans to fully fund your negotiated budget at the time of award.

B. RENEWAL AWARDS

At ARPA-E's sole discretion, awards resulting from this FOA may be renewed by making a new award, adding one or more budget periods and/or extending the period of performance of the initial 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.

C. ARPA-E 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.

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."[34] Accordingly, ARPA-E has substantial involvement in the direction of every Cooperative Agreement, as described in Section II.D below.

1. COOPERATIVE AGREEMENTS

ARPA-E generally uses Cooperative Agreements to provide financial and other support to Prime Recipients.[35]

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 Prime Recipients share responsibility for the direction of projects.

ARPA-E encourages Prime Recipients to review the Model Cooperative Agreement, which is available at http://arpa-e.energy.gov/arpa-e-site-page/award-guidance.

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

[35] The Prime Recipient is the signatory to the funding agreement with ARPA-E.

2. Funding Agreements with FFRDCs/DOE Labs, GOGOs, and Federal Instrumentalities

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

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

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

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

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

3. Other Transactions Authority

ARPA-E may use its "other transactions" authority under the America COMPETES Reauthorization Act of 2010 to enter into an other transaction agreement with Prime Recipients, on a case-by-case basis.

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

In general, an other transaction agreement would require a cost share of 50%. See Section III.B.2 of the FOA.

D. STATEMENT OF SUBSTANTIAL INVOLVEMENT

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 Prime 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 Prime Recipient fails to achieve any of the "Go/No-Go" milestones or technical milestones and deliverables as determined by the ARPA-E Contracting 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. §§ 200.338 and 200.339.
- ARPA-E may provide guidance and/or assistance to the Prime Recipient to accelerate the commercial deployment of ARPA-E-funded technologies. Guidance and assistance provided by ARPA-E may include coordination with other Government agencies and nonprofits to provide mentoring and networking opportunities for Prime Recipients. ARPA-E may also organize and sponsor events to educate Prime Recipients about key barriers to the deployment 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 deployment of ARPA-E-funded technologies.

III. Eligibility Information

A. Eligible Applicants

This FOA is open to U.S. universities, national laboratories, industry and individuals.

1. Individuals

U.S. citizens or permanent residents may apply for funding in their individual capacity as a Standalone Applicant,[36] as the lead for a Project Team,[37] or as a member of a Project Team. However, ARPA-E will only award funding to an entity formed by the Applicant.

2. Domestic Entities

For-profit entities, educational institutions, and nonprofits[38] that are incorporated in the United States, including U.S. territories, are eligible to apply for funding as a Standalone Applicant, as the lead organization for a Project Team, or as a member of a Project Team.

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

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

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

3. Foreign Entities

U.S. incorporated subsidiaries of foreign entities, whether for-profit or otherwise, are eligible to apply for funding under this FOA as a Standalone Applicant, as the lead organization for a Project Team, or as a member of a Project Team, subject to the requirements in 2 C.F.R. §

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[36] A Standalone Applicant is an Applicant that applies for funding on its own, not as part of a Project Team.

[37] The term "Project Team" is used to mean any entity with multiple players working collaboratively and could encompass anything from an existing organization to an ad hoc teaming arrangement. A Project Team consists of the Prime Recipient, Subrecipients, and others performing or otherwise supporting work under an ARPA-E funding agreement.

[38] 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 Prime Recipient or Subrecipient.

910.124, which includes requirements that the entity's participation in this FOA's Program be in the economic interest of the U.S. The Full Application must state the nature of the corporate relationship between the foreign entity and domestic subsidiary or affiliate.

Entities not incorporated in the U.S., whether for-profit or otherwise, are not eligible to apply for funding, but may be proposed by an Applicant as a member of a Project Team.

All work under an ARPA-E award must be performed in the U.S. The Applicants may request a waiver of this requirement in the Business Assurances & Disclosures Form, which is submitted with the Full Application and can be found at https://arpa-e-foa.energy.gov/. Please refer to the Business Assurances & Disclosures Form for guidance on the content and form of the request.

4. Consortium Entities

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

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

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

B. Cost Sharing[39]

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

[39] Please refer to Section VI.B. of the FOA for guidance on cost share payments and reporting.

1. Base Cost Share Requirement

ARPA-E generally uses Cooperative Agreements to provide financial and other support to Prime Recipients (see Section II.C.1 of the FOA). Under a Cooperative Agreement or Grant, the Prime Recipient must provide at least 20% of the Total Project Cost[40] as cost share, except as provided in Sections III.B.2 or III.B.3 below.[41]

2. Increased Cost Share Requirement

Large businesses are strongly encouraged to provide more than 20% of the Total Project Cost as cost share. ARPA-E may consider the amount of cost share proposed when selecting applications for award negotiations (see Section V.B.1 of the FOA).

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

3. Reduced Cost Share Requirement

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

- A domestic educational institution or domestic nonprofit applying as a Standalone Applicant is not required to provide cost share.
- Project Teams composed exclusively of domestic educational institutions, domestic nonprofits, and/or FFRDCs/DOE Labs/Federal agencies and instrumentalities (other than DOE) are not required to provide cost share.
- Small businesses – or consortia of small businesses – will provide 0% cost share from the outset of the project through the first 12 months of the project (hereinafter the "Cost Share Grace Period").[42] If the project is continued beyond the Cost Share Grace Period, then at least 10% of the Total Project Cost (including the costs incurred during the Cost Share Grace Period) will be required as cost share over the remaining period of performance.

[40] The Total Project Cost is the sum of the Prime Recipient share and the Federal Government share of total allowable costs. The Federal Government share generally includes costs incurred by GOGOs and FFRDCs.
[41] Energy Policy Act of 2005, Pub.L. 109-58, sec. 988.
[42] Small businesses are generally defined as 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). Applicants that are small businesses will be required to certify in the Business Assurances & Disclosures Form that their organization meets the SBA's definition of a small business under at least one NAICS code.

- Project Teams where a small business is the lead organization and small businesses perform greater than or equal to 80%, but less than 100%, of the total work under the funding agreement (as measured by the Total Project Cost) the Project Team are entitled to the same cost share reduction and Cost Share Grace Period as provided above to Standalone small businesses or consortia of small businesses.[43]
- Project Teams where domestic educational institutions, domestic nonprofits, small businesses, and/or FFRDCs perform greater than or equal to 80% of the total work under the funding agreement (as measured by the Total Project Cost) are required to provide at least 10% of the Total Project Cost as cost share. However, any entity (such as a large business) receiving patent rights under a class waiver, or other patent waiver, that is part of a Project Team receiving this reduction must continue to meet the statutory minimum cost share requirement (20%) for its portion of the Total Project Cost.
- Projects that do not meet any of the above criteria are subject to the minimum cost share requirements described in Sections III.B.1 and III.B.2 of the FOA.

4. Legal Responsibility

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

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

5. Cost Share Allocation

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

6. Cost Share Types and Allowability

Every cost share contribution must be allowable under the applicable Federal cost principles, as described in Section IV.G. of the FOA.

[43] See the information provided in previous footnote.

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

The Prime Recipient may not use the following sources to meet its cost share obligations:

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

In addition, Project Teams may not use independent research and development (IR&D) funds[44] to meet their cost share obligations under Cooperative Agreements. However, Project Teams may use IR&D funds to meet their cost share obligations under "other transaction" agreements.

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

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

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

7. COST SHARE CONTRIBUTIONS BY FFRDCS AND GOGOS

Because FFRDCs are funded by the Federal Government, costs incurred by FFRDCs generally may not be used to meet the cost share requirement. FFRDCs may contribute cost share only if

[44] As defined in Federal Acquisition Regulation SubSection 31.205-18.

the contributions are paid directly from the contractor's Management Fee or a non-Federal source.

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

8. Cost Share Verification

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

C. Other

1. Compliant Criteria

Concept Papers are deemed compliant if:

- The Applicant meets the eligibility requirements in Section III.A of the FOA;
- The Concept Paper complies with the content and form requirements in Section IV.C of the FOA; and
- The Applicant entered all required information, successfully uploaded all required documents, and clicked the "Submit" button in ARPA-E eXCHANGE by the deadline stated in the FOA.

Concept Papers found to be noncompliant may not be merit reviewed or considered for award. ARPA-E may not review or consider noncompliant Concept Papers, including Concept Papers submitted through other means, Concept Papers submitted after the applicable deadline, and incomplete Concept Papers. A Concept Paper is incomplete if it does not include required information. ARPA-E will not extend the submission deadline for Applicants that fail to submit required information and documents due to server/connection congestion.

Full Applications are deemed compliant if:

- The Applicant submitted a compliant and responsive Concept Paper;
- The Applicant meets the eligibility requirements in Section III.A of the FOA;
- The Full Application complies with the content and form requirements in Section IV.D of the FOA; and

- The Applicant entered all required information, successfully uploaded all required documents, and clicked the "Submit" button in ARPA-E eXCHANGE by the deadline stated in the FOA.

Full Applications found to be noncompliant may not be merit reviewed or considered for award. ARPA-E may not review or consider noncompliant Full Applications, including Full Applications submitted through other means, Full Applications submitted after the applicable deadline, and incomplete Full Applications. A Full Application is incomplete if it does not include required information and documents, such as Forms SF-424 and SF-424A. ARPA-E will not extend the submission deadline for Applicants that fail to submit required information and documents due to server/connection congestion.

Replies to Reviewer Comments are deemed compliant if:

- The Applicant successfully uploads its response to ARPA-E eXCHANGE by the deadline stated in the FOA; and
- The Replies to Reviewer Comments comply with the content and form requirements of Section IV.E of the FOA.

ARPA-E will not review or consider noncompliant Replies to Reviewer Comments, including Replies submitted through other means and Replies submitted after the applicable deadline. ARPA-E will not extend the submission deadline for Applicants that fail to submit required information due to server/connection congestion. ARPA-E will review and consider each compliant and responsive Full Application, even if no Reply is submitted or if the Reply is found to be noncompliant.

2. RESPONSIVENESS CRITERIA

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 FOA.
- Submissions that have been submitted in response to other currently issued ARPA-E FOAs.
- Submissions that are not scientifically distinct from applications submitted in response to other currently issued ARPA-E FOAs.
- 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 FOA.
- Submissions for proposed technologies that do not have the potential to become disruptive in nature, as described in Section I.A of the FOA. 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.A of the FOA.

3. SUBMISSIONS SPECIFICALLY NOT OF INTEREST

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

- Algorithms and techniques that do not enhance the efficiency of energy technology, product or service design processes.
- Algorithms and techniques that are not enhanced via machine-learning.
- Efforts where the majority (>50%) of the proposed resources would be expended in the acquisition of experimental training data

4. 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 FOA, provided that each application is scientifically distinct.

IV. APPLICATION AND SUBMISSION INFORMATION

A. APPLICATION PROCESS OVERVIEW

1. REGISTRATION IN ARPA-E eXCHANGE

The first step in applying to this FOA is registration in ARPA-E eXCHANGE, ARPA-E's online application portal. For detailed guidance on using ARPA-E eXCHANGE, please refer to Section IV.H.1 of the FOA and the "ARPA-E eXCHANGE User Guide" (https://arpa-e-foa.energy.gov/Manuals.aspx).

2. CONCEPT PAPERS

Applicants must submit a Concept Paper by the deadline stated in the FOA. Section IV.C of the FOA provides instructions on submitting a Concept Paper.

ARPA-E performs a preliminary review of Concept Papers to determine whether they are compliant and responsive, as described in Section III.C of the FOA. Concept Papers 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 Concept Paper based on the criteria and program policy factors in Sections V.A.1 and V.B.1 of the FOA.

ARPA-E will encourage a subset of Applicants to submit Full Applications. Other Applicants will be discouraged from submitting a Full Application in order to save them the time and expense of preparing an application submission that is unlikely to be selected for award negotiations. 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. Unsuccessful Applicants should continue to submit innovative ideas and concepts to future FOAs.

3. FULL APPLICATIONS

Applicants must submit a Full Application by the deadline stated in the FOA. Applicants will have approximately 45 days from receipt of the Encourage/Discourage notification to prepare and submit a Full Application. Section IV.D of the FOA provides instructions on submitting a Full Application.

ARPA-E performs a preliminary review of Full Applications to determine whether they are compliant and responsive, as described in Section III.C of the FOA. 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.A.2 and V.B.1 of the FOA.

4. 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. Applicants may submit an optional Reply to Reviewer Comments, which must be submitted by the deadline stated in the FOA. Section IV.E of the FOA provides instructions on submitting a Reply to Reviewer Comments.

ARPA-E performs a preliminary review of Replies to determine whether they are compliant, as described in Section III.C.1 of the FOA. ARPA-E will review and consider compliant Replies only. ARPA-E will review and consider each compliant and responsive Full Application, even if no Reply is submitted or if the Reply is found to be non-compliant.

5. 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 Contracting 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.

6. 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 and program policy factors in Sections V.A.2 and V.B.1 of the FOA. 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.

Applicants are promptly notified of ARPA-E's selection determination. ARPA-E may stagger its selection determinations. As a result, some Applicants may receive their notification letter in advance of other Applicants. Please refer to Section VI.A of the FOA for guidance on award notifications.

B. APPLICATION FORMS

Required forms for Full Applications are available on ARPA-E eXCHANGE (https://arpa-e-foa.energy.gov), including the SF-424 and Budget Justification Workbook/SF-424A. A sample Summary Slide is available on ARPA-E eXCHANGE. Applicants may use the templates available on ARPA-E eXCHANGE, including the template for the Concept Paper, the template for the Technical Volume of the Full Application, the template for the Summary Slide, the template for the Summary for Public Release, the template for the Reply to Reviewer Comments, and the template for the Business Assurances & Disclosures Form. A sample response to the Business Assurances & Disclosures Form is available on ARPA-E eXCHANGE.

C. CONTENT AND FORM OF CONCEPT PAPERS

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 Funding Requested (Federal and Cost Share), and Project Duration.

Concept Papers found to be noncompliant or nonresponsive may not be merit reviewed or considered for award (see Section III.C of the FOA).

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.

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 below. If Applicants exceed the maximum page length indicated above, ARPA-E will review only the authorized number of pages and disregard any additional pages.

1. Concept Paper

a. Concept Summary

- Describe the proposed concept with minimal jargon, and explain how it addresses the Program Objectives of the FOA.

b. Innovation and Impact

- Clearly identify the problem to be solved with the proposed technology concept.
- Describe how the proposed effort represents an innovative and potentially transformational solution to the technical challenges posed by the FOA.
- Explain the concept's potential to be disruptive compared to existing or emerging technologies.
- To the extent possible, provide quantitative metrics in a table that compares the proposed technology concept to current and emerging technologies and to the Technical Performance Targets in Section I.F of the FOA for the appropriate Technology Category in Section I.D of the FOA.

c. Proposed Work

- Describe the final deliverable(s) for the project and the overall technical approach used to achieve project objectives.
- Discuss alternative approaches considered, if any, and why the proposed approach is most appropriate for the project objectives.
- Describe the background, theory, simulation, modeling, experimental data, or other sound engineering and scientific practices or principles that support the proposed approach. Provide specific examples of supporting data and/or appropriate citations to the scientific and technical literature.
- Describe why the proposed effort is a significant technical challenge and the key technical risks to the project. Does the approach require one or more entirely new technical developments to succeed? How will technical risk be mitigated?
- Identify techno-economic challenges to be overcome for the proposed technology to be commercially relevant.
- Estimated federal funds requested; total project cost including cost sharing.

d. TEAM ORGANIZATION AND CAPABILITIES

- Indicate the roles and responsibilities of the organizations and key personnel that comprise the Project Team.
- Provide the name, position, and institution of each key team member and describe in 1-2 sentences the skills and experience that he/she brings to the team.
- Identify key capabilities provided by the organizations comprising the Project Team and how those key capabilities will be used in the proposed effort.

Identify (if applicable) previous collaborative efforts among team members relevant to the proposed effort.

D. CONTENT AND FORM OF FULL APPLICATIONS

[TO BE INSERTED BY FOA MODIFICATION IN JULY 2019]

E. CONTENT AND FORM OF REPLIES TO REVIEWER COMMENTS

[TO BE INSERTED BY FOA MODIFICATION IN JULY 2019]

F. INTERGOVERNMENTAL REVIEW

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

G. FUNDING RESTRICTIONS

[TO BE INSERTED BY FOA MODIFICATION IN JULY 2019]

H. OTHER SUBMISSION REQUIREMENTS

1. USE OF ARPA-E eXCHANGE

To apply to this FOA, Applicants must register with ARPA-E eXCHANGE (https://arpa-e-foa.energy.gov/Registration.aspx). Concept Papers, Full Applications, and Replies to Reviewer Comments must be submitted through ARPA-E eXCHANGE (https://arpa-e-foa.energy.gov/login.aspx). ARPA-E will not review or consider applications submitted through other means (e.g., fax, hand delivery, email, postal mail). 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 "My Submissions" link 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 FOA, 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.**

ARPA-E may not review or consider incomplete applications and applications received after the deadline stated in the FOA. Such applications may be deemed noncompliant (see Section III.C.1 of the FOA). 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 IV of the FOA;
- 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 FOA;
- 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.

V. APPLICATION REVIEW INFORMATION

A. CRITERIA

ARPA-E performs a preliminary review of Full Applications to determine whether they are compliant and responsive (see Section III.C of the FOA). ARPA-E also performs a preliminary review of Replies to Reviewer Comments to determine whether they are compliant.

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 FOA 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 FOA for the appropriate technology Category in Section I.D of the FOA;
- 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. The above criteria will be weighted as follows:

Impact of the Proposed Technology Relative to FOA Targets	50%
Overall Scientific and Technical Merit	50%

2. Criteria for Full Applications

[TO BE INSERTED BY FOA MODIFICATION IN JULY 2019]

3. Criteria for Replies to Reviewer Comments

[TO BE INSERTED BY FOA MODIFICATION IN JULY 2019]

B. Review and Selection Process

1. 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 US dependence on foreign energy sources;
  b. Stimulation of domestic manufacturing/U.S. Manufacturing Plan;
  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-Leveraging of Federal Funds**. Project leverages Federal funds to optimize advancement of programmatic goals by proposing cost share above the required minimum or otherwise accessing scarce or unique resources.

VI. **High Project Impact Relative to Project Cost.**

2. 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 Contracting 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.

3. ARPA-E SUPPORT CONTRACTOR

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.

C. ANTICIPATED ANNOUNCEMENT AND AWARD DATES

[TO BE INSERTED BY FOA MODIFICATION IN JULY 2019]

VI. Award Administration Information

A. Award Notices

1. Rejected Submissions

Noncompliant and nonresponsive Concept Papers and Full Applications are rejected by the Contracting Officer and are not merit reviewed or considered for award. The Contracting Officer sends a notification letter by email to the technical and administrative points of contact designated by the Applicant in ARPA-E eXCHANGE. The notification letter 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. Please refer to Section IV.G of the FOA for guidance on pre-award costs.

3. Full Application Notifications

[TO BE INSERTED BY FOA MODIFICATION IN JULY 2019]

B. Administrative and National Policy Requirements

[TO BE INSERTED BY FOA MODIFICATION IN JULY 2019]

C. Reporting

[TO BE INSERTED BY FOA MODIFICATION IN JULY 2019]

VII. Agency Contacts

A. Communications with ARPA-E

Upon the issuance of a FOA, only the Contracting Officer may communicate with Applicants. ARPA-E personnel and our support contractors are prohibited from communicating (in writing or otherwise) with Applicants regarding the FOA. This "quiet period" remains in effect until ARPA-E's public announcement of its project selections.

During the "quiet period," Applicants are required to submit all questions regarding this FOA to ARPA-E-CO@hq.doe.gov. Questions and Answers (Q&As) about ARPA-E and the FOA are available at http://arpa-e.energy.gov/faq. For questions that have not already been answered, please send an email with the FOA name and number in the subject line to ARPA-E-CO@hq.doe.gov. Due to the volume of questions received, ARPA-E will only answer pertinent questions that have not yet been answered and posted at the above link.

- ARPA-E will post responses on a weekly basis to any questions that are received that have not already been addressed at the link above. ARPA-E may re-phrase questions or consolidate similar questions for administrative purposes.
- ARPA-E will cease to accept questions approximately 10 business days in advance of each submission deadline. Responses to questions received before the cutoff will be posted approximately one business day in advance of the submission deadline. ARPA-E may re-phrase questions or consolidate similar questions for administrative purposes.
- Responses are published in a document specific to this FOA under "CURRENT FUNDING OPPORTUNITIES – FAQS"" on ARPA-E's website (http://arpa-e.energy.gov/faq).

Applicants may submit questions regarding ARPA-E eXCHANGE, ARPA-E's online application portal, to ExchangeHelp@hq.doe.gov. ARPA-E will promptly respond to emails that raise legitimate, technical issues with ARPA-E eXCHANGE. ARPA-E will refer any questions regarding the FOA to ARPA-E-CO@hq.doe.gov.

ARPA-E will not accept or respond to communications received by other means (e.g., fax, telephone, mail, hand delivery). Emails sent to other email addresses will be disregarded.

During the "quiet period," only the Contracting Officer may authorize communications between ARPA-E personnel and Applicants. The Contracting Officer may communicate with Applicants as necessary and appropriate. As described in Section IV.A of the FOA, the Contracting Officer may arrange pre-selection meetings and/or site visits during the "quiet period."

B. DEBRIEFINGS

ARPA-E does not offer or provide debriefings. ARPA-E provides Applicants with a notification encouraging or discouraging the submission of a Full Application based on ARPA-E's assessment of the Concept Paper. In addition, ARPA-E provides Applicants with reviewer comments on Full Applications before the submission deadline for Replies to Reviewer Comments.

VIII. Other Information

A. Title to Subject Inventions

Ownership of subject inventions is governed pursuant to the authorities listed below. Typically, either by operation of law or under the authority of a patent waiver, Prime Recipients and Subrecipients may elect to retain title to their subject inventions under ARPA-E funding agreements.

- 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. If they elect to retain title, they must file a patent application in a timely fashion.
- All other parties: The Federal Non-Nuclear Energy Research and Development Act of 1974, 42. U.S.C. 5908, provides that the Government obtains title to new inventions unless a waiver is granted (*see below)*.
- Class Waiver: Under 42 U.S.C. § 5908, title to subject inventions vests in the U.S. Government and large businesses and foreign entities do not have the automatic right to elect to retain title to subject inventions. However, ARPA-E typically issues "class patent waivers" under which large businesses and foreign entities that meet certain stated requirements, such as cost sharing of at least 20%, may elect to retain title to their subject inventions. If a large business or foreign entity elects to retain title to its subject invention, it must file a patent application in a timely fashion. If the class waiver does not apply, a party may request a waiver in accordance with 10 C.F.R. §784.
- GOGOs are subject to the requirements of 37 C.F.R. Part 501.
- Determination of Exceptional Circumstances (DEC): DOE has determined that exceptional circumstances exist that warrant the modification of the standard patent rights clause for small businesses and non-profit awardees under Bayh-Dole to maximize the manufacture of technologies supported by ARPA-E awards in the United States. The DEC, including a right of appeal, is dated September 9, 2013 and is available at the following link: http://energy.gov/gc/downloads/determination-exceptional-circumstances-under-bayh-dole-act-energy-efficiency-renewable. Please see Sections IV.D and VI.B for more information on U.S. Manufacturing Requirements.

B. Government Rights in Subject Inventions

Where Prime 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 Prime 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 Prime Recipients, Subrecipients, or their assignees and exclusive licensees refuse to do so.

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

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

C. Rights in Technical Data

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

- Background or "Limited Rights Data": The U.S. Government will not normally require delivery of technical data developed solely at private expense prior to issuance of an award, except as necessary to monitor technical progress and evaluate the potential of proposed technologies to reach specific technical and cost metrics.
- Generated Data: The U.S. Government normally retains very broad rights in technical data produced under Government financial assistance awards, including the right to distribute to the public. However, pursuant to special statutory authority, certain categories of data generated under ARPA-E awards may be protected from public disclosure for up to five years 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.
- ARPA-E is prepared to consider modifications to standard data provisions to facilitate commercialization of software first produced in performance of the award.

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).

E. FOAS AND FOA MODIFICATIONS

FOAs are posted on ARPA-E eXCHANGE (https://arpa-e-foa.energy.gov/), Grants.gov (http://www.grants.gov/), and FedConnect (https://www.fedconnect.net/FedConnect/). Any modifications to the FOA are also posted to these websites. You can receive an e-mail when a modification is posted by registering with FedConnect as an interested party for this FOA. It is recommended that you register as soon as possible after release of the FOA to ensure that you receive timely notice of any modifications or other announcements. More information is available at https://www.fedconnect.net.

F. OBLIGATION OF PUBLIC FUNDS

The Contracting 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 Contracting Officer, either explicit or implied, is invalid.

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

G. REQUIREMENT FOR FULL AND COMPLETE DISCLOSURE

Applicants are required to make a full and complete disclosure of the information requested in the Business Assurances & Disclosures Form. Disclosure of the requested information is mandatory. Any failure to make a full and complete disclosure of the requested information may result in:

- The rejection of a Concept Paper, Full Application, and/or Reply to Reviewer Comments;
- The termination of award negotiations;
- The modification, suspension, and/or termination of a funding agreement;
- The initiation of debarment proceedings, debarment, and/or a declaration of ineligibility for receipt of Federal contracts, subcontracts, and financial assistance and benefits; and
- Civil and/or criminal penalties.

H. RETENTION OF SUBMISSIONS

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.

I. 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 must 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.

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J. Compliance Audit Requirement

A prime recipient organized as a for-profit entity expending $750,000 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 is either a Prime Recipient or a Subrecipient, and has expended $750,000 or more of Federal funds 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.

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 Concept Paper, Full Application, and Reply to Reviewer Comments.

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

Cost Sharing: is the portion of project costs from non-Federal sources that are borne by the Prime Recipient (or non-Federal third parties on behalf of the Prime Recipient), rather than by the Federal Government.

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.

FOA: Funding Opportunity Announcement.

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

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

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

Prime Recipient: The signatory to the funding agreement with ARPA-E.

PI: Principal Investigator.

Project Team: A Project Team consists of the Prime Recipient, Subrecipients, and others performing or otherwise supporting work under an ARPA-E funding agreement.

Standalone Applicant: An Applicant that applies for funding on its own, not as part of a Project Team.

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

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

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

TT&O: Technology Transfer and Outreach. (See Section IV.G. of the FOA for more information).