U.S. Department of Energy
Advanced Research Projects Agency-Energy

Announcement of Teaming Partner List for Upcoming Notice of Funding Opportunity: Accelerating the Heterogeneous Catalyst Development Cycle for the Net-Zero Emissions via Coupled High Throughput Experimentation and Artificial Intelligence

The Advanced Research Projects Agency – Energy (ARPA-E) is considering issuing a Notice of Funding Opportunity (NOFO) to support the development of artificial intelligence (AI)-enabled, accelerated research and development (R&D) workflows for energy-relevant, heterogeneous, thermochemical, and electrochemical catalysts. The purpose of this announcement is to facilitate the formation of new, multi-disciplinary project teams to respond to a potential future NOFO. Any NOFO issued in the future would provide specific program goals, technical metrics, and selection criteria. If there are any inconsistencies between this announcement and the potential NOFO, the NOFO language would be controlling.

This potential NOFO would focus on:

- Innovations in high-throughput catalyst design experimental methods and state-of-the-art AI and machine learning (ML) algorithms and models; and
- Integration of these innovations into catalysis R&D workflows to automate and accelerate the development of heterogeneous catalysts.

These technology developments would significantly contribute toward ARPA-E's statutory goals by improving energy efficiency, reducing energy-related emissions through new feedstocks, and reducing imports associated with critical materials.

The anticipated goals of the potential program include the following:

- Development of AI-enabled "closed-loop" or other potentially disruptive workflows to accelerate the design and development cycle for chemistries relevant to ARPA-E's mission, which will ultimately help advance the goal of net-zero carbon emissions by 2050 (e.g., "future refinery relevant" or other next generation feedstocks and products);
- Synthesis of new "drop-in" manufacturable technical catalysts in engineered forms at kilogram scale for thermochemical or electrochemical reactor systems, as well as evaluation of these technical catalysts for performance under realistic, industrial conditions; and
- Generation of AI-ready databases by combining and pre-processing high-quality, multi-scale, multi-modal data as generated and gathered from synthesis, characterization, and performance testing tasks at the ab initio, as well as at the research and technical catalyst levels.

The potential program is expected to consist of a three-year performance period. It is anticipated that the program will transform and disrupt traditional catalysis R&D workflows by tightly coupling state-of-

the-art advances in hardware for high-throughput catalyst design experimental methods with modern software tools and techniques in AI/ML, data science, and data engineering such that an equivalent 10 – 15 years of traditional catalysis R&D work can be verifiably completed (through rediscovery) within 12 – 18 months, effectively demonstrating a more than 10x acceleration in the catalyst development cycle. Further impact will be realized by utilizing these acceleration methods for novel catalyst-reaction discovery and co-design. The potential NOFO encourages the development of closed-loop and other promising, automated workflow topologies that enable inverse design of heterogenous catalysts.

Teams composed of experts in the following areas may be useful in responding to the potential NOFO:

- **Materials acceleration and high-throughput experimentation (HTE)**: Teams would be expected to accelerate conventional workflows using a combination of hardware and software tools that can impact both theoretical and experimental aspects of the catalysis R&D.
  From a **hardware** perspective this includes, but is not limited to, expertise with:
  - HTE, including synthesis and parallel testing; and
  - Laboratory automation and robotics, including self-driving laboratories.

  From a **software** perspective this includes, but is not limited to, expertise with:
  - Organization and management of large, HTE-generated datasets (e.g., lab information management systems);
  - Data engineering and data science to connect, structure, and transform diverse datasets to an applicable form while ensuring data quality; and
  - ML and AI that support acceleration and automation of the closed-loop workflow.

- **AI/ML:** This includes, but is not limited to, expertise with:
  - Creation and management of AI-ready databases with data generated across the workflow, as well as supplemental theoretical knowledge and relevant open-source or proprietary databases;
  - Data engineering and data science to connect, structure, and transform diverse datasets for AI/ML tasks while ensuring data quality;
  - Advanced ML and AI tools and techniques that support acceleration and automation of the closed-loop workflow; work with limited and large quantities of data (including language); and enable inverse design of heterogeneous catalysts; and
  - Multi-physics and ML-based surrogate models to simulate technical catalyst performance and accelerate the elucidation of fundamental reaction mechanisms and networks.

- **Catalysis:** Theoretical and experimental catalysis experts whose understanding ranges from first principles to industry-scale validation would be needed to ensure commercial success. This includes, but is not limited to, expertise with:
  - Catalysis theory, modeling, and rational design fundamentals;
  - Catalyst formulation and synthesis. Specifically, expertise in high-throughput synthesis of heterogeneous catalytic materials;
  - Multi-modal catalyst characterization, including traditional X-ray techniques, microscopy techniques, spectroscopy techniques, sorption-based techniques, other material science-based methods along with advanced dynamic, as well as in-situ and operando

characterization methods of heterogeneous catalytic materials for both research and technical catalytic materials; and
    - Chemical reaction engineering, including modeling, operability, and understanding of multi-scale heat, mass and momentum transfer effects as related to reactor configuration, catalyst properties, reaction kinetics.

- **Industrial catalysis and manufacturing:** Teams would require the capability to generate and test technical catalyst composites (e.g., pellets, membrane electrode assemblies) at industrially relevant processes and time and length scales. This industry-relevant testing would be expected to require thousands of hours of time on stream with kilogram-scales of catalysts. While this metric may vary depending on the reaction, a trial at a pilot facility would be essential to project success.

Successful teams are likely to include subject matter experts from all of the identified areas above. Although a single person may be able to fill more than one of these roles, a complete set of experts is unlikely to exist within any single organization. Furthermore, due to timing and resource constraints typical of ARPA-E programs, it is generally recommended that any applicant project team would need to secure access to existing HTE hardware.

ARPA-E strongly encourages outstanding scientists and engineers from different organizations, scientific disciplines, and technology sectors to form new project teams. Interdisciplinary and cross-sector collaboration spanning organizational boundaries enables and accelerates scientific and technological outcomes that were previously viewed as extremely difficult, if not impossible, to achieve.

The Teaming Partner List is being compiled to facilitate the formation of new project teams. The Teaming Partner List will be available on ARPA-E eXCHANGE (http://arpa-e-foa.energy.gov), ARPA-E's online application portal, starting in October 2024. The Teaming Partner List will be updated periodically until the close of the Full Application period to reflect new Teaming Partners who have provided their information.

Any organization that would like to be included on this list should complete all required fields in the form found at the following link: https://arpa-e-foa.energy.gov/Applicantprofile.aspx . Required information includes the following: Organization Name, Contact Name, Contact Address, Contact Email, Contact Phone, Organization Type, Area of Technical Expertise, and Brief Description of Capabilities.

By submitting your information to this Teaming Partner List, you consent to the publication of the above-referenced information. **By facilitating this Teaming Partner List, ARPA-E does not endorse or otherwise evaluate the qualifications of the entities that self-identify for placement on the Teaming Partner List.** ARPA-E will not pay for the provision of any information, nor will it compensate any respondents for the development of such information. Responses submitted to other email addresses or by other means will not be considered. **Participation in and utilization of this list is completely voluntary.** ARPA-E will not identify or facilitate connections through the list and participation in the list has no bearing whatsoever on the evaluation of applications submitted to the potential funding opportunity.

<u>This list does not constitute a Notice of Funding Opportunity (NOFO). A NOFO does not exist at this time.</u> Applicants must refer to the funding opportunity, expected to be issued by November 2024, for instructions on applying and for details on how projects will be funded.