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

Announcement of Teaming Partner List for Upcoming Funding Opportunity Announcement: Quantum Computing for Computational Chemistry and Materials Science

The Advanced Research Projects Agency – Energy (ARPA-E) is considering issuing a Funding Opportunity Announcement (FOA) to support the development of quantum computing technologies aimed at accelerating energy innovation. This potential FOA would focus on quantum computing for advances in chemistry and materials that significantly address ARPA-E mission areas, such as improving energy efficiency and reducing energy-related emissions, including greenhouse gas emissions. The purpose of this announcement is to facilitate the formation of new project teams to respond to a potential future FOA. Any FOA issued in the future would provide specific program goals, technical metrics, and selection criteria. FOA terms would be controlling.

The anticipated goals of the program include developing scalable quantum algorithms for chemistry and materials simulations. The program is expected to culminate in a three-year performance period, resulting in transformative quantum applications with disruptive performance increases compared to classical calculations in metrics such as speed or accuracy. The FOA is expected to require that performance be validated on quantum hardware, either outperforming the classical state-of-the-art or showing a clear path to do so in a scalable manner.

Expertise in the following areas may be useful in responding to the potential FOA:

- Chemistry and Materials Applications: Teams must plan to solve an impactful chemistry or materials problem in the energy space and quantify the relevance to ARPA-E's mission. Therefore, expertise in the specific application in materials science or chemistry may be useful to ensure that the problem is indeed of interest to that field, that solving it would represent a major—not incremental—advance in the field, and that the problem is unlikely to be solved by another approach.
- Classical High-Performance Computing: Experts in classical computational methods used to study chemistry and materials may be useful to ensure that quantum results are compared to and validated against the best available classical methods.
- Quantum Algorithms and Software Engineering: Experts in the design of quantum algorithms, specifically those relevant to chemistry and materials science, may be useful to address the core goals of the potential FOA.
- Quantum Compilation, Embedding, and Error-Correction: Specialists in optimizing circuits and error-correction protocols may be useful to optimize higher-level algorithms for maximum performance on the specific quantum hardware.
- Quantum Hardware: It may be useful to include experts in the specific qubits and architecture that will be used to solve the problem and the likely state of hardware by the end of the period of performance.

Successful teams are likely to include experts from all identified areas of expertise in order to be able to design an approach that leverages quantum computing hardware to solve a practical problem related to ARPA-E's mission in energy. Although a single person may be able to fill more than one of these expert roles, a complete set of experts is unlikely to exist within any single organization. We anticipate effective teaming will be **critical** for project success.

As a general matter, 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 August 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 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 a response to this Notice, 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 teaming list and participation in the list has no bearing whatsoever on the evaluation of applications submitted to the potential FOA.

This Notice does not constitute a FOA. No FOA exists at this time. Applicants must refer to the FOA, expected to be issued by October 2024, for instructions on submitting an application and for the terms and conditions of funding.