HPC4EnergyInnovation Program:
Collaborations for U.S. Manufacturers

The High-Performance Computing for Energy Innovation (HPC4EI) Program seeks qualified industry partners to participate in short-term, collaborative projects with the Department of Energy's (DOE) National Laboratories. HPC4EI is the umbrella initiative for the HPC4Manufacturing (HPC4Mfg) and HPC4Materials (HPC4Mtls) Programs which are sponsors of this solicitation. Through support from DOE's Office of Energy Efficiency and Renewable Energy (EERE) Advanced Materials and Manufacturing Technologies Office (AMMTO) and Office of Fossil Energy and Carbon Management (FECM), the selected industry partners will be granted access to high performance computing (HPC) facilities and world-class scientists at DOE's National Laboratories.

DOE's HPC4Mfg Program is interested in establishing collaborations that address key energy and decarbonization related challenges for domestic manufacturers. The HPC4Mfg Program is designed to improve manufacturing processes, address products' lifecycle energy consumption, and increase the efficiency of energy conversion and storage technologies. The HPC4Mtls Program is interested in collaborations that address key challenges in developing, modifying, and/or qualifying new or modified materials that perform well in severe or complex environments through the application of HPC, modeling, simulation, and data analysis. These objectives are met by providing access to national laboratory supercomputing resources and expertise for high performance computing projects. This program harnesses the raw processing power of national laboratory supercomputers to decarbonize U.S. industries and move us closer to an equitable, clean energy future that benefits all Americans.

Eligibility for the HPC4EI Program is limited to entities that manufacture in the United States for commercial applications and the organizations that support these entities.

The solicitation will encourage applicants to partner with a diverse range of universities, community colleges, and non-profit organizations, especially those located in disadvantaged communities, to ensure the equitable use and benefits of HPC National Laboratory resources and technologies.

Selected projects will be awarded up to $300,000 to support compute cycles and work performed by the National Laboratory. The industry partner must provide a participant contribution of at least 20% of the total project funding. The industry contribution must come from non-federal funding sources.

In addition, follow-on projects to previously awarded, successful projects in these areas will be considered. Follow-on projects should focus on the further implementation of the demonstrated HPC application in the industrial setting, taking it closer to operational use and broad national impact. Selected follow-on projects will be awarded up to $300,000 to support computing cycles and work performed by the National Laboratory, university, and non-profit partners. The industry partner must provide a participant contribution of at least 33.3% of the total project funding; of this, at least half must be in cash to support the National Laboratory work.

Background

DOE maintains world-class HPC expertise and facilities, currently hosting several of the top 20 most powerful computers in the world as ranked by TOP500 in June 2022. From detailed subatomic-level simulations to massive cosmological studies, researchers use HPC to probe science and technology questions inaccessible by experimental methods. Scientific insights gained from these computational studies have drastically impacted research and technology across industrial sectors and scientific fields. Examples include additive manufacturing, aerospace, oil recovery, drug development, climate science, genomics, and exploration of fundamental particles that make up our universe. From industry to academia, the scientific need for advanced computing continues to drive innovation and development for future high-performance computers and their capabilities.

There is high potential for U.S. industry to utilize the power of HPC. The HPC4EI Program is intended to provide HPC expertise and resources to industry to lower the risk of HPC adoption and broaden its use to support transformational and early-stage technology development. The HPC4EI Program hopes to provide this HPC expertise by supporting targeted collaborations between industry and DOE's National Laboratories.

Successful applicants will work collaboratively with staff from one or more of the DOE National Laboratories to conduct project activities across the various HPC areas of expertise, including development and optimization of modeling and simulation codes, porting and scaling of applications, application of data analytics, as well as applied research and development of tools or methods.

To make the broadest impact across the industry, the project teams are expected to present their results at workshops associated with the program and at regional and national conferences. Publications are also encouraged.

Area 1: HPC4Mfg

DOE's Advanced Materials and Manufacturing Technologies Office (AMMTO) within the Office of Energy Efficiency and Renewable Energy (EERE) is the primary sponsor of the HPC4Mfg Program. Other Technology Offices within EERE and DOE's Office of Fossil Energy and Carbon Management may also sponsor select projects in this portfolio. AMMTO partners with private and public stakeholders to decarbonize industry, lower energy demand, and increase the competitiveness of the U.S. manufacturing and clean energy sectors through process innovations, research and development, and technical assistance and workforce training. AMMTO supports cost-shared research, development, and activities in support of crosscutting next-generation technologies and processes that hold high potential to significantly improve energy efficiency and reduce emissions, industrial waste, and the life- cycle energy consumption of manufactured products.

The primary goal of the HPC4Mfg Program is to reduce carbon emissions across the industrial sector and improve the efficiency and productivity of U.S. manufacturing. The program solicits proposals that require HPC modeling and simulation to overcome impactful manufacturing

process challenges resulting in reduced energy consumption, greenhouse gas emissions, and/or increased productivity. Proposals should provide a realistic assessment of the carbon emissions reduction, energy impact, emission reduction, the improvement in U.S. manufacturing competitiveness, and the increase in U.S. manufacturing jobs that a successful outcome of the project could have across the industrial sector.

Of particular interest to AMMTO are:

- Improvements in manufacturing processes which result in significant national carbon emissions reduction and energy savings. Examples include:
    a. Process improvements in industries with high decarbonization potential such as chemicals, primary metal manufacturing, cement, food processing industries, paper and pulp, and glass;
    b. Improvements in material performance in harsh service environments such as very high temperature or highly corrosive processes (e.g. high-temperature thermal energy storage and conversion);
    c. Improvements in modeling prediction and closed-loop control for smart manufacturing systems (e.g., advanced sensors and process controls);
    d. Improvements in recyclability or material recovery from systems or components at their end of life, or from waste products generated along the supply chain;
    e. Improvements of material quality or purity from materials recovery that facilitate requalification or remanufacturing processes that have lower energy or carbon footprints than mining and refinement of equivalent materials;
    f. Improvements in separation and processing for critical materials (e.g., rare earth elements); and
    g. Electrification of industrial processes.
- Improvements in semiconductor technologies that will result in operational energy efficiency improvements. Examples include:
    a. Improvements in modeling of advanced materials crucial to more energy efficient semiconductor devices and systems.
    b. Process improvements in semiconductor manufacturing that lower the embodied energy of or otherwise result in more energy efficient semiconductor systems.
- Carbon emissions reduction and efficiency improvements in energy conversion and storage technologies. Examples include:
    a. Improvements in waste heat recovery for thermal energy storage systems.
    b. Improvements in design and process optimization for battery component manufacturing and system assembly that improve capacity, operational lifetime, or reduce embodied energy/carbon.

c. Conversion of combined heat and power units to low carbon fuels.

- Reductions in CO2 or CO2-equivalent emissions. Examples include improvement in the performance of carbon-capturing processes; modification of fossil-fueled systems to accept low-to-zero carbon fuels; and electrification of processes to replace combustion-driven processes.

Area 2: HPC4Mtls

The Advanced Energy Materials program, funded by DOE's Office of Fossil Energy and CarbonManagement (FECM) and managed by DOE's National Energy Technology Laboratory, is the primary sponsor of the High Performance Computing for Materials program. FECM funds research, development, demonstration, and deployment projects to decarbonize power generation and industrial production, remove carbon dioxide from the atmosphere, and mitigate the environmental impacts of fossil fuel production and use.

The Advanced Energy Materials program works to characterize, produce, and certify advanced alloys and high-performance materials that are key to realizing dispatchable, reliable, high-efficiency, decarbonized power generation from gas, biomass, or hydrogen. In addition, the program aims to encourage change and stimulate innovation in the high-performance materials value chain to spur U.S. competitiveness.

FECM partners with industry, academia, national labs, and research facilities on research, development, demonstration, and deployment of carbon management technologies that are essential for decarbonizing key sectors, including power and industrial sectors, some of the largestsources of carbon emissions today. Clean hydrogen is expected to play a considerable role in decarbonizing these sectors. Today, roughly 95% of the hydrogen in the United States is producedfrom natural gas without carbon capture, which is not clean. However, there is significant potential in applying carbon capture technologies to help advance a cost-effective and low-carbon hydrogen economy.

Proposals for the HPC4Materials Program should provide a realistic assessment of the proposed project's benefits to the domestic materials supply chain and/or fossil energy application (e.g. reduced energy consumption and/or greenhouse gas emissions for power plants or clean hydrogenproducers/users).

Of particular interest to FECM in this solicitation are:

Advanced Materials for Carbon Conversion Applications

- Improving the understanding of the materials in catalytic conversion reactors to reduce carbon oxides, principally carbon dioxide, into valuables products. Of particular interest is electron-mediated conversion such as electrolyzers, low-temperatures plasma systems, microwave systems and hybrid bio-electrochemical systems.
- Use of computational databases and machine learning for development of

catalyst and catalyst support structures.

Advanced Structural Materials for Hydrogen Applications

- Improving the understanding of the materials impacts including corrosion and erosion effects of gasification of feedstock blends of waste coal, sustainably sourced biomass, and waste plastics on materials in high temperature regions of a gasifier, including sensitivity analysis of blend percentages and types of feedstocks.
- Improving the understanding of the material impacts including hydrogen embrittlement effects of blends of natural gas and hydrogen on materials in pipelines, welded joints, or compressors, including sensitivity analysis of blend percentages.
- Use of computational databases and machine learning for thermal barrier coating(TBC) development for hot gas path components of combustion turbines firing natural gas-hydrogen blends or 100% hydrogen.
- Use of computational databases and machine learning for development of ceramicmetal composites for use in components of combustion turbines firing natural gas-hydrogen blends or 100% hydrogen.

Advanced Functional Materials for Hydrogen Applications

- Use of computational databases and machine learning for catalyst development to synthesize, test, characterize, and scale materials which convert carbon oxides into value-added products with increased energy efficiency, higher selectivity, and lower environmental impacts based on a lifecycle analysis relative to conventional products.
- Use of computational databases and machine learning for catalyst development to synthesize, test, characterize, and scale materials for reforming of natural gas/methane to produce syngas or hydrogen.
- Developing machine learning capabilities to predict composition, thermal performance, and mechanical properties of new materials for thermal energy storage.
- Developing machine learning capabilities to identify promising new materials for non-battery energy storage technologies that can integrate with fossil energy power generating units.
- Improving performance and performance stability of fuel and oxygen electrocatalysts in reversible solid oxide fuel cells (R-SOFCs).
- Understanding and mitigation of microstructural changes due to uneven heat transfer into the reversible solid oxide fuel cells (R-SOFCs) for the oxygen-ion conducting R-SOFCs.

Eligibility

Eligibility is limited to U.S. manufacturers, defined as entities that are incorporated (or otherwise formed) under the laws of a particular state or territory of the United States, and that manufacture products in the United States or that manufacture, distribute, or otherwise deploy software and/or hardware systems as described above or that develop and/or manufacture new or modified materials in the United States. Project work must be executed in the United States.

U.S. universities, institutes, and other non-profit organizations are also eligible to participate as collaborators. The solicitation will encourage applicants to partner with a diverse range of universities, community colleges, and non-profit organizations, especially those located in disadvantaged communities, to ensure the equitable use and benefits of HPC National Laboratory resources and technologies. Funding for university and/or non-profit participants may be provided by the National Laboratory or the industrial partner. If the funding for a university or non-profit participant is to be provided by DOE through the DOE laboratory partner, funding requests must be less than half of the total DOE funds. Funding provided to a university and/or non-profit by the industrial partner can be considered a component of the industrial partner's in-kind funding contribution.

An entity may only submit one Full Application per area (Area 1 HPC4Mfg; Area 2 HPC4Mtls). If an entity submits more than one Concept Paper in an area, the review committee will select no more than one proposal from this entity to advance to the Full Proposal (Full Application) stage. This limitation does not prohibit an applicant from collaborating on other applications (e.g., as a potential subrecipient or partner) so long as the entity is only listed as the applicant on one Full Application per area for this solicitation. In organizations with more than 5,000 employees, an "entity" can be considered to be a major business unit within the company, for example, an Aerospace Division as distinct from a Central Research Division.

Funding Requirements

The DOE monetary contribution for each project will not exceed $300,000. For new initial (not follow-on) projects, an industry partner must provide a participant contribution of at least 20% of the total project funding to support industry expertise to the project. Total project funding is defined as the DOE contribution plus the contributions (in-kind and cash) from the industry partner. Cash contributions are funds supplied by the industry partner to collaborators external to the company. The participant contribution can take the form of monetary funds in or "in-kind" contributions and must come from non-federal sources unless otherwise allowed by law. For follow-on projects, defined as a project that is using the results of a previously funded project within the HPC4EI portfolio, the industry contribution is 33.3% of the total project funding of which at least half of this amount is a cash contribution. Sample budgets are shown below. Total project size cannot exceed $500,000. DOE funding will be provided to the National Laboratory (or laboratories) in support of their work under the HPC4EI Program.

Sample Budget

Project (New project; total project funding of $375K)

TASK	DOE Funds	Industry Partner Cash Contribution	Industry Partner In-kind
Total Project Funding = $375K	**$300K**		**$75K**

Follow-on Project (Uses results from a previously funded project; total project funding of $450K)

TASK	DOE Funds	Industry Partner Cash Contribution	Industry Partner In-kind
Total Project Funding = $450K	**$300K**	**$75K**	**$75K**

Note: THIS IS NOT A PROCUREMENT REQUEST.

Solicitation Process and Timeline

This solicitation comprises a two-stage process consisting of the submission and evaluation of a two-page concept paper and six-page full proposal submitted by the industrial principal investigator (PI). These will be evaluated by a technical review committee on the technical challenge to overcome; how this advances the state of the art for the industrial sector; how HPC can uniquely contribute to the solution of the technical challenge; and the company specific and broad national impact that a successful project can have. A notional project plan should be included.

Successful concept papers will be paired with a National Laboratory partner for the development of the full proposal. Full proposals will be reviewed by a technical committee against the criteria given below. The portfolio of proposals recommended by the committee will be submitted to DOE senior managers for final selection, subject to the availability of funding. All DOE funding decisions shall be final.

Upon approval of funding selections by DOE, the HPC4EI Program will issue a written response to each applicant in the form of an email. Applicants selected for funding will subsequently engage in a formal agreement with the partnered laboratory before work may begin.

Private sector applicants will engage in a DOE Short Form Cooperative Research and Development Agreement (CRADA) for the successful proposal. Once both parties approve the Short Form CRADA, project execution may begin. Failure to engage promptly in CRADA negotiations can result in rejection of the project.

The portfolio of projects will be posted on the HPC4EI website. The HPC4EI Program reserves the right to select all, a portion, or none of the submissions.

If a concept paper or full proposal is technically strong, but is not selected for funding, the program management team may share them with other DOE program offices for consideration for possible funding through those offices.

Timeline

Current solicitation schedule dates will be posted on the HPC4EI website www.hpc4energyinnovation.org. Event dates are subject to change.

Event	**Dates (2022-2023)**
Call for Proposal	November 4, 2022
Concept Paper Due	December 6, 2022
Request for Full Proposal	January 2023
Full Proposal Due	March 2023
Finalists Notified	May 2023

Concept Paper Guidelines

Interested parties will submit a concept paper describing the project objectives by the due date provided above. The concept paper will be evaluated against the documented criteria. Successful concept papers will be invited to submit a full proposal.

The concept paper template can be downloaded from the HPC4EI website (www.hpc4energyinnovation.org) and the electronic proposal system (https://proposalshpc4.inl.gov). The template should be used to prepare your submission. The concept paper should not exceed two (2) single-spaced pages using 12-point Times New Roman font, 1" margins, and formatted in a PDF file. The concept paper **must include** the following components under the corresponding headings below. A concept paper that does not meet the guidelines may be rejected for review. A concept paper template is provided.

- **Title Page: (not included in page limit)** *Include proposal tracking number, the project title,and company name.*

- **Abstract: (150 words or less):** *Provide a* ***non-proprietary, publishable*** *summary of the problem being addressed, why the problem is important to the energy future of the United States, a plan to address the problem, and the impact the solution will have.*

- **Background:** *Explain the technical challenge to be addressed; the state of the art in this area and how this work advances the state of the art; how solving this problem will meet the goals of the HPC4EI Program as defined by the list of topics of interest; the relevant expertise of the industry partners; what National Laboratory expertise is*

needed; and why National Laboratory HPC resources are required and how they will be used.

- **Project Plan and Objectives:** *Describe the technical scope of work to be performed and how this project fits into an overall solution strategy for the challenges being addressed. Describe how the results of the project will be validated, including availability of data. If possible, identify specific simulation codes to be used in this effort. Summarize how your project plan will address the key proposal review criteria: advances the current state of the art in the industrial sector; technical feasibility, relevance to high performance computing.*

- **Impact:** *Estimate how this specific HPC effort will result in national-scale, long-term energy savings and emissions reductions across the industry; the performance improvements that are expected over existing technologies; and the ability of industry to accelerate the adoption of energy-efficient technologies. Describe how this specific HPC work contributes to a transformational change in the energy sector and enduring economic impact. Describe how this effort will result in changes in the way your company operates. Describe the alternative actions if this effort is not funded including reliance on experimental technologies or other courses of action. Include metrics for energy improvements, carbon reductions, performance increases, cost savings, and/or time reductions.*

Changes from Previous Submissions (Reapplications): *For proposals that have been re-submitted from a previous solicitation, briefly describe how you have incorporated changes based on reviewer comments from the previous submission.*

For follow-on projects, the concept paper should not exceed three (3) single-spaced pages using 12-point Times New Roman font, 1" margins, PDF file format, and should include all the components described above. In addition, the following component is required:

- **Results from the prior funded project (one page maximum with figures):** *Review the results and knowledge gained from the prior funded project. Explain how these results will be used to address the objectives of this proposal. If you believe that the current proposal is distinctly different from the previous project and should not be considered as a follow-on project, please articulate the differences.*

- Appendix A: References (not included in page count) *References are considered to be citations of publications or conference proceedings. Additional information such as company descriptions, graphics or other descriptions are not considered appropriate for this section and will not be reviewed by the reviewers.*

Completed concept papers, derived from the provided template, must be submitted to the electronic proposal system at https://proposalshpc4.inl.gov by 5:00 p.m. PT on the deadline indicated on the submission website. Submission includes completion of electronic applicant form and upload of concept paper in PDF file format. Concept papers will be evaluated against the criteria listed in the Evaluation Criteria Section.

Full Proposal Guidelines

Successful concept paper submissions will be notified and paired with a PI from one or a combination of the following laboratories:

- Ames Laboratory
- Argonne National Laboratory
- Idaho National Laboratory
- Los Alamos National Laboratory
- Lawrence Berkeley National Laboratory
- Lawrence Livermore National Laboratory
- National Energy Technology Laboratory
- National Renewable Energy Laboratory
- Oak Ridge National Laboratory
- Pacific Northwest National Laboratory
- Sandia National Laboratories
- Other participating laboratories

Partners will then collaborate on the development of a full proposal. Full proposals will be evaluated against the criteria described in the Evaluation Criteria Section.

The full proposal template can be downloaded from the HPC4EI website and the electronic application system. Template should be used to prepare your submission. Proposals should not exceed six (6) single-spaced pages using 12-point Times New Roman font, 1" margins, and formatted in a PDF file. Follow-on project proposals should not exceed eight (8) single-spaced pages using 12-point font Times New Roman font, 1" margins, in PDF file format, and should include all the components with additional Results from Prior Funded Project section. The full proposal **must include** the following components under the corresponding headings below. Proposals that do not meet the guidelines may be rejected for review.

- **Title Page: (not included in page limit)** *Include the proposal tracking number, the project title, and company name.*

- **Abstract: (150 words or less):** *Provide a* ***non-proprietary, publishable*** *summary of the problem being addressed, why the problem is important to the energy future of the United States, a plan to address the problem, and the impact of the solution. If selected for the HPC4EI Program, this abstract will appear on award announcements sent to the press and posted on the program website.*

- **Background:** *Describe the technical challenge to be addressed; the state of the art in this area and how this work advances the state of the art; how solving this problem will meet the goals of the HPC4EI Program as defined by the list of topics of interest; the relevant expertise of the industry partners; what National Laboratory expertise is needed; and why National Laboratory HPC resources are required and how they will be used. Indicate if the proposed project will accelerate transformational technological*

advances in areas that industry by itself is not likely to undertake because of technical and financial uncertainty.

- **Follow-on Projects Only - Results from the Prior Funded Project (two pages maximum with figures):** *Review the results and knowledge gained from the prior funded project. Explain how these results will be used to address the objectives of this proposal. If you believe that the current proposal is distinctly different from the previous project and should not be considered as a follow-on project, please articulate the differences.*

- **Project Plan and Objectives:** *Describe the technical scope of work to be performed and how this scope will fit into the broader solution for the challenges being addressed, including, for example, relevant experimental work. Outline a set of tasks to be performed and state what work industry partners will perform and what work laboratory partners will perform. Describe how the results of the project will be validated, including availability of data. If possible, identify simulation codes to be used in this effort and any modifications to the software that are needed to solve the proposed problem.*

- **Tasks, Milestones, Deliverables, and Schedules:** *Include goals, timelines, and due dates throughout the life of the project. Not every milestone needs to have a deliverable. Include deliverables from all partners, not just the National Laboratory partner(s). Indicate responsible party(ies) for each deliverable. Include deliverables from one partner to another,as well as those to the DOE program sponsors.*

- **Validation and Verification Plan:** *Summarize how the model will be validated and the simulations verified. Include information about the experimental data that will be used for verification, its nature and source.*

- **Impact:** *Estimate how this specific HPC effort will result in national-scale, long-term energy savings and emissions reductions across the industry; the performance improvements that are expected over existing technologies; and the ability of industry to accelerate the adoption of energy-efficient technologies. Explain how this specific HPC work contributes to a transformational change in the energy sector and enduring economic impact. Describe the alternative actions if this effort is not funded including reliance on experimental technologies or other courses of action. Describe how this effort will specifically impact your company/entity. Include metrics for energy improvements, carbon reduction, performance increases, cost savings, and/or time reductions.*

- **Energy Savings Estimates:** *HPC4Mfg proposals must include numerical estimates for annual energy savings, carbon savings, and justifications for these estimates. Energy and carbon savings should be on an annual basis, assuming successful implementation of the technology being enabled by the HPC effort. Estimates for market penetration used for the savings should be realistic and conservative.*

- **Implementation and Adoption:** *Describe how this work will be incorporated into companyand industry-wide operations. Describe the follow-on activities to extend this effort to solve the broader problem being addressed.*

Appendixes

Appendix A: **References (not included in page count)**

Appendix B: **Project Summary of Tasks and Schedule** (not included in page count): *Provide a summary of the tasks and subtasks in a table format that includes the milestones,deliverables, and schedule. Include a schedule summary in Gantt chart format.*

Appendix C: Project Budget (not included in page count) *Summarize project costs including amount and source of participant contribution in the table provided. Indicate in- kind and/or cash contribution for industry funding. Include a description of how this fundingwill make a large difference relative to existing funding from other sources, including the private sector and why the government should fund this work. Funding for university and/or non-profit participants may be provided by the National Laboratory or the industrial partner. If the funding for a university or non-profit participant is to be provided by DOE through the DOE laboratory partner, funding requests must be less than half of the total DOE funds. Funding provided to a university and/or non-profit by the industrial partner can be considered a component of the industrial partner's in-kind funding contribution.*

Appendix D: Computational Resources (not included in page count) *Describe the computational approach, the performance of the codes, and the resources requested (platform and number of core hours). Provide information about whether the code can run efficiently on a GPU platform or requires a CPU platform. If the estimated computational resource requirement is over 10 million CPU core-hours or 1 million node hours on a GPU platform, describe how these resources will be obtained.*

Appendix E: Pictures for Publication (not included in page count) *Include one or two* ***non-proprietary*** *pictures/images with a short caption and photo credit that can be used in a press release and posted on the website should this project be funded. If project is selected, high resolution image (s) will be requested by HPC4EI administrator.*

Appendix F: Discussion of How This Work Benefits the Laboratory (not included in page count) *Briefly discuss new or enhanced capabilities that will be gained by the partnering laboratory. Or, explain how this will help to maintain existing laboratory capabilities.*

Appendix G: Biographies (not included in page limit) *Include one paragraph* ***non-proprietary*** *biography for the industrial PI(s) and partnering laboratory PI(s). These may be posted on the HPC4EI website should this project be funded.*

Appendix H: Resumes (not included in page limit) *Include resumes of participants.*

Completed proposals, derived from the provided template, must be submitted to the electronic proposal system at https://proposalshpc4.inl.gov by 5:00 p.m. PT on the deadline

indicated on the submission website. Submission includes completion of electronic applicant form and upload of full proposal in PDF file format. This date will be approximately five weeks after concept paper notifications have been issued.

Evaluation Process and Criteria

Both concept papers and full proposals will be evaluated by a Technical Merit Review Committee consisting of experts in the application of HPC modeling, simulation, and data analysis from each of the principal DOE National Laboratories, and members of the DOE program offices with knowledge of the U.S. industry. Subject Matter Experts will be consulted to verify claims, including the description of current state of the art and estimate of project impact (e.g., cost and energy savings).

Concept papers will be evaluated primarily on the technical challenge and potential impact of using HPC to solve the industrial challenge. Concept papers should articulate, to the extent possible, the technical plan for performing the work. The committee recognizes that those industrial PIs who have not yet identified a National Laboratory partner to work with may not have a complete picture of the technical solution techniques that are possible.

Full proposals will be evaluated against all the criteria listed below. Because the industrial partner will have an assigned laboratory partner to work with to develop the full proposal, the technical plan and feasibility will be expected to be well articulated. In addition, strong evidence of communication and planned collaborations between the National Laboratory and industrial participants is expected in the full proposals.

Final funding decisions will be made by the sponsoring DOE office. DOE reserves the right to fund none, one, several or all the submitted proposals. All DOE funding decisions will be final.

Evaluation Criteria

- **Advances the State of the Art in the Industrial Sector: (Weight 20%)**
    - Does the proposed work take the industrial sector to a new level; provide a wholly new capability; or make an existing, energy-intensive technology obsolete in the manufacturing sector?
    - Does the proposed work take materials performance and behavior to a new level in a specific energy application environment; scale up the production of a new or modified material; provide a wholly new capability; or dramatically decrease the time required to certify or qualify a new or modified material?
    - Is the technical readiness level appropriate for a one-year project to produce meaningful results for the industrial sector?

- **Technical Feasibility: (Weight 20%)**

  - Does the proposal have a clearly stated technical approach including a description of the software to be used and any needed modifications?
  - Does the proposal match team expertise to the problem to be solved; have modeling expertise on both the National Laboratory and industry sides; and process experts for the model validation if necessary?
  - Does the proposal clearly state roles and responsibilities for the participants and provide evidence of a strong collaboration between the industrial and national partners through joint milestones and deliverables?
  - Is the project plan clearly constructed with realistic time frames for each technical step?
  - Is there a solid verification and validation plan with validation data available?

- **Relevance to HPC: (Weight 20%)**

  - Does the proposed work fully utilize the unique expertise and capabilities at the DOE National Laboratories to solve a problem that could not be solved in any other way?
  - Does it demonstrate the ability to use large fractions of the machine to solve a truly large-scale problem and provide clear estimates of the compute cycles necessary for the work to be performed?

- **Impact, Including Life-Cycle Energy Impact: (Weight 40%)**

  - Does the proposal respond to the specific topic areas listed and interests of the DOE sponsor office?
  - Does the proposal provide clear, evidence-based energy savings and carbon emissions reductions that will a *have broad (national-scale) industrial impact* through development and/or improvement of energy-efficient manufacturing technologies, as well as an impact on employment and manufacturing in the United States?
  - Does the proposal have a clearly stated plan for broad deployment of project artifacts or knowledge gained? Are specific numerical energy metrics included with a solid justification for the impact estimates?
  - Does the proposal provide clear, evidence-based improved materials performance, energy savings, carbon savings or reduced time to market that will *have broad (national-scale) industrial impact, as well as an impact on employment* in the United States?
  - Does the proposal have a clearly stated plan for broad deployment of project artifacts or knowledge gained?

Point of Contact

During the period of the call for proposals, all questions relating to this announcement should be directed to the HPC4EnergyInnovation Program at hpc4ei@llnl.gov.

Intellectual Property and Proprietary Data

The HPC4EI Program respects the importance of industry's intellectual property and datasecurity.

Industrial partner awardees are expected to enter into a DOE Model Short Form CRADA with the National Laboratory or Laboratories that will be performing the work. This CRADA contains provisions relating to proprietary information and intellectual property. Because of the need for accelerated placement and execution of the projects, terms of the CRADA will not be subject to negotiation. To review the proposed terms that make up the DOE Model Short Form CRADA, please see the example posted on the HPC4EI solicitation website.

A Non-Disclosure Agreement can be put into place during development and submission of the proposal to facilitate discussions while protecting the partner's proprietary information.

To the extent possible, it is preferred that proprietary information NOT be included in the submitted proposal. If company proprietary information is included in the proposal, the specific information should be marked as such. The HPC4EI Program officials will utilize reasonable efforts to treat the information as business sensitive.

Failure of the industry partner to finalize the CRADA within one year following receipt of the notification letter to fund the project or other significant delays in finalizing the CRADA could result in rejection/discontinuation of the proposal/project.