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 the sponsors of this solicitation. Through support from DOE's Office of Fossil Energy and Carbon Management (FECM), and the Office of Energy Efficiency and Renewable Energy's (EERE) Industrial Efficiency and Decarbonization Office (IEDO), 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 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. 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. 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 lab supercomputers to decarbonize U.S. industry 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 and community colleges; including Historically Black Colleges and Universities (HBCUs) and Minority Serving Institutes (MSIs), and non-profit organizations, especially those located in disadvantaged and underserved communities, to ensure HPC National Laboratory resources and technologies promote equitable access, use, and benefits.

DOE's FECM and IEDO support and encourage the advancement of diversity, equity, inclusion, and accessibility (DEIA) in the context of HPC National Laboratory applicant submissions. Selected projects will be awarded up to $400,000 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 $400,000 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 20% 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 November 2023. 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: HPC4Mtls

The Hydrogen with Carbon Management and Point Source Carbon Capture programs under DOE's Office of Fossil Energy and Carbon Management (FECM) are the primary sponsors for this call of the High Performance Computing for Materials Program. FECM minimizes environmental and climate impacts of fossil fuels and industrial processes while working to achieve net-zero emissions across the U.S economy. 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 largest sources of carbon emissions today.

Under FECM's Hydrogen with Carbon Management program, 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's Point Source Carbon Capture program works to accelerate the deployment of technologies that capture carbon dioxide (CO_2) emissions from natural gas and industrial sources over the next decade, with the goal of creating highly efficient, transformational carbon capture technologies. These technologies will be capable of operation under flexible duty cycles and foster creation of regional power generation that can achieve greater than 95% carbon capture.

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 the industrial sector such as cement and steel producers, power plants, or clean hydrogen producers/users).

Of particular interest to FECM's Advanced Energy Materials program in this solicitation are:

Advanced Structural Materials for Hydrogen Applications

- Computationally understanding critical welded joints using novel austenitic materials under hydrogen environment at high temperatures and their use in various applications, such as fuel cells, gasifiers and turbines.
- Improving the understanding of the material impacts including hydrogen embrittlement effects of blends of natural gas and hydrogen on materials in BOP (balance of plant) components for technologies in hydrogen environments, such as fuel cells, gasifiers and turbines.
- Use of computational databases and machine learning for development of ceramic metal composites (TBC and CMC) for use in components of combustion turbines firing natural gas- hydrogen blends or 100% hydrogen.
- Comparative assessment of additive manufacturing pathways for CMC production for hydrogen Turbines versus traditional wrought-based manufacturing pathways. The

project will identify the best improved, automated and innovative, low-cost CMC manufacturing pathways.

Advanced Functional Materials for Hydrogen Applications

- Computationally understanding and improving degradation 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 R-SOFCs for the oxygen-ion conducting R-SOFCs.

Topic areas of interest for FECM's Point Source Capture program are:

Reactive Carbon Capture

- Development of tools for identifying optimal deployment locations for reactive carbon capture approaches, with consideration of CO_2 sources (exhaust streams at electric generation facilities, industrial facilities or directly from the atmosphere), availability of required energy sources and co-reactants (e.g., carbon-free electricity, green hydrogen), process operating requirements, and integration of product(s) generated into existing supply chains and markets.

- Development of modeling and optimization approaches to increase operational flexibility of reactive carbon capture systems to adapt to fluctuations in CO_2-containing gas streams and intermittent renewable energy supply.

Emissions

- Development of dynamic process control models that can be integrated with online measurements, engineering controls and machine learning tools, to manage and mitigate non-CO_2 emissions from installing carbon capture on industrial and electricity generation sources.

    (i) Elucidation of the chemical degradation mechanisms of sorbents and solvents for point source capture for industrial applications;
    (ii) Use of computational databases and machine learning for development of novel CO_2 binding sorbent materials / membrane materials to achieve over 99% capture efficiency with low concentration CO_2 point source capture streams (NGCC);
    (iii) Use of computational databases and machine learning for development of novel reactive capture materials;
    (iv) Development of monitoring, reporting and verification tools (e.g., sampling algorithms, databases, models etc.) for non-CO_2 emissions from installing carbon capture systems on industrial and electricity generation sources;
    (v) Development of atmospheric chemistry models for non-CO_2 emissions from installing carbon capture systems on industrial and electricity generation sources;

(vi) Development of process models for modular design carbon capture systems to improve process flexibility.

Area 2: HPC4Mfg

The primary goals of the HPC4Mfg Program are to 1) improve manufacturing performance to lower the cost and improve the functionality of clean energy technologies, 2) improve the efficiency and productivity of U.S. manufacturing, and 3) accelerate the development of technologies that eliminate industrial greenhouse gas emissions. The program solicits proposals that require HPC modeling and simulation to overcome impactful manufacturing process challenges resulting in improved performance, reduced lifecycle energy consumption, greenhouse gas emissions, and/or increased productivity. Proposals should provide a realistic assessment of the carbon emissions reduction, energy impact, 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.

The Industrial Efficiency and Decarbonization Office (IEDO) provides funding, management, and the strategic direction necessary for a balanced national program of research, development, and demonstration (RD&D), as well as technical assistance and workforce development, to drive improvements in energy, materials, and production efficiency and to accelerate decarbonization across the industrial sector. IEDO and its programs are critical to putting the nation on a pathway to achieve net-zero carbon emissions by 2050.

The industrial sector is considered one of the most difficult to decarbonize due to the diversity and complexity of energy inputs, processes, and operations. Achieving net-zero emissions across the U.S. economy by 2050 will require an aggressive, multidimensional approach to eliminating industrial emissions. Based on analysis in DOE's Pathways to Commercial Liftoff Reports, while some technologies are ready to deploy today, it's estimated that addressing over 60% of emissions reductions needed in heavy industry currently costs more than $50 per metric ton CO_2, making those solutions unlikely to be deployed on an economic basis. Additional RD&D is essential to reduce these costs and to unlock new pathways to reduce emissions. HPC can play a key role in accelerating the advancements needed to realize these goals.

This topic aims to advance the strategies identified in DOE's Industrial Decarbonization Roadmap and support the goals of the Industrial Heat Shot. IEDO seeks to advance highly innovative and impactful technologies through HPC4Mfg. The potential GHG impacts of projects will be a major consideration in the evaluation of proposals. Technologies with only marginal impacts on GHG emissions or energy use are unlikely to be of interest.

For this topic, the following types of applications are of particular interest:

- Development, optimization, and/or integration of equipment and processes that contribute to DOE's Industrial Heat Shot by significantly reducing emissions from industrial process heating.

a. Electrified heating technologies, such as electric resistance, induction, electric arc/plasma, electromagnetic, and hybrid technologies. For example, application-specific optimization of energy-material interactions is a critical barrier to development of electromagnetic heating technologies.

b. Industrial heat pumps, including components and integrated systems that can deliver heat at or above 200°C. For example, compressor operation at high temperatures and pressures is limited by lubricant performance.

c. Utilization of alternative fuels and energy sources, such as clean hydrogen, biofuels, and solar thermal. For example, hydrogen combustion characteristics are different from natural gas, requiring new optimization of components and overall combustion systems.

d. Processes that significantly reduce or eliminate the heat needed for industrial processes, such as membrane separations, nonthermal drying, and electrochemical processes.

e. Thermal energy storage technologies, including sensible, latent, and thermochemical systems.

- Advancements in technologies that significantly reduce emissions from energy- and emissions-intensive industries such as chemicals, iron & steel, cement & concrete, food & beverage, forest products, aluminum, and glass. Reductions in core process emissions as well as reductions in lifecycle emissions (e.g., improving material circularity or enabling use of alternative feedstocks) are both of interest.

- Advancements in technologies that enable flexible industrial energy use and grid edge capabilities (i.e., interaction with the electric grid).

- Improvements in energy efficiency and/or emissions reductions for water and wastewater treatment, including for industrial and agricultural wastewaters.

For this topic, the following types of applications are specifically *not of interest*:

- Applications focused on electricity generation systems or components, including combined heat and power (CHP) and waste heat to power (WHP) technologies.
- Applications focused on production of fuels (e.g., hydrogen, biofuels, synthetic fuels).
- Applications focused on CO_2 capture and/or storage.

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 Concept Paper and one Full Application. 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 $400,000. 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 20% 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 $500K)

TASK	DOE Funds	Industry Partner Cash Contribution	Industry Partner In-kind
Total Project Funding = $500K	**$400K**		**$100K**

Follow-on Project (Uses results from a previously funded project; total project funding of $500K)

TASK	DOE Funds	Industry Partner Cash Contribution	Industry Partner In-kind
Total Project Funding = $500K	**$400K**	**$50K**	**$50K**

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 seven-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 or cancelation 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. Event dates are subject to change.

Event	Dates (2024)
Call for Proposal	April 15, 2024
Concept Paper Due	May 13, 2024
Request for Full Proposal	July 2024
Full Proposal Due	August 2024
Finalists Notified	October 2024

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 and the electronic proposal system. This 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. The following is a description of the concept paper template.

- **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:** *Describe how this specific HPC effort will result in national-scale, long-term energy, 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/carbon improvements, performance increases, cost savings, and/or time reductions. Describe additional impacts this work will have on manufacturing and HPC communities. Include plans for any publications, improvements to open-source software, public databases that will be released or improved, and training provided for students or postdocs, industry staff, etc.*

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: Energy/CO_2 Savings Estimates (not included in page count)** *The Proposal must include numerical estimates for annual energy and carbon savings. Energy/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. Concept paper template will include format for providing savings estimate and justifications.*

- **Appendix B: Changes from Previous Submissions (Reapplications) (not included in page count)** *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.*

- **Appendix C: 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. PDT 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 DOE 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. This template should be used to prepare your submission. Proposals should not exceed seven (7) 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 nine (9) single-spaced pages using 12-point 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, company name, and National Laboratory PI contact information.*

- **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 Phase I 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 by each participant. Include description of work activities performed by the industry partner, national laboratory partner, and/or university or non-profit. 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. Summarize how your project plan will address the following key proposal review criteria: advances to the state of the art in the industrial section, technical feasibility, and relevance to high performance computing.*

- **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:** *Describe how this specific HPC effort will result in national-scale, long-term energy 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/carbon improvements, performance increases, cost savings, and/or time reductions. Describe additional impacts this work will have on manufacturing and HPC communities. Include plans for any publications, improvements to open-source software, public databases that will be released or improved, and training provided for students or postdocs, industry staff, etc.

- **Energy Savings Estimates:** *Proposals must include numerical estimates for annual energy and carbon (equivalent) savings. 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. If a new or modified material is developed, can the team provide preliminary techno-economic analysis by the close of the project?*

- **Other Impacts:** *Describe other impacts this work will have on manufacturing and HPC communities. Describe plans for any publications, improvements to open-source software, public databases that will be released or improved, and training provided for students or postdocs, etc.*

Appendices

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 funding will 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. Industry partner cash contributions are made to either the laboratory or a university or non-profit. Total DOE funds must not exceed $400K. DOE funding to the university must not exceed 50% of the total DOE*

funds. Total industry contributions (including in kind and cash) must be at least 20% of the total project funding. Industry contributions for Phase I projects may be 100% in-kind contributions, whereas Phase II projects require at least 50% of the industry contribution to be in cash. Total project funding must not exceed $500K.

Appendix D: Computational Resources (not included in page count) *In paragraph form, describe the computational approach, the performance of the codes, and the resources requested (platform and number of core hours). Platforms are listed on the HPC4EI Computing Resource web page, please indicate a preference and why that system is preferred. Provide information about whether the code can run efficiently on a GPU platform or requires a CPU platform. Also describe how the results are to be disseminated to the end users. If you plan to use a GPU based machine, please indicate the machine name and provide your compute time in node hours, otherwise please provide your compute time in core hours.* ***For requests over 10 Million core-hours on a CPU resource or equivalent on a GPU resource, describe how you plan to gain access to this level of resources, and tell us who your contact is at the computing facility where you will be accessing those resources.***

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) *Provide resumes of project team to include industry partner PI(s), national laboratory PI(s), and/or university or non-profit organization.*

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. PDT 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 drawn from participating 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 significant 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 additional impacts for the community such as publications, improvements to open-source software, public databases that will be released or improved, and training provided for students or postdocs, etc.?

Point of Contact

During the period of the call for proposals, all questions relating to this announcement can 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 Cooperative Research and Development Agreement (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, the 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 sample posted on the HPC4EI solicitation website. CRADA forms for different National Laboratories will vary, but the terms are substantively similar.

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.