Program Announcement
To DOE National Laboratories
LAB 04-20

Basic Research
for the Hydrogen Fuel Initiative

SUMMARY: The Office of Basic Energy Sciences (BES) of the Office of Science (SC), U.S. Department of Energy (DOE), in keeping with its energy-related mission to assist in strengthening the Nation's scientific research enterprise through the support of basic science, announces its interest in receiving proposals for projects on basic research for the Hydrogen Fuel Initiative (HFI). Areas of focus include: Novel Materials for Hydrogen Storage; Membranes for Separation, Purification, and Ion Transport; Design of Catalysts at the Nanoscale; Solar Hydrogen Production; and Bio-Inspired Materials and Processes. More information on these focus areas is provided in the SUPPLEMENTARY INFORMATION section below.

DATES: Potential researchers are required to submit a brief preproposal. All preproposals must be received by DOE by 4:30 p.m., Eastern Time, **July 15, 2004**. Preproposals will be reviewed for conformance with the guidelines presented in this announcement and suitability in the technical areas specified in this announcement. A response to the preproposals encouraging or discouraging formal proposals will be communicated to the researchers within approximately forty-five days of receipt.

Only those preproposals that receive notification from DOE encouraging a formal proposal may submit full proposals. **No other formal proposals will be considered**. Formal proposals in response to this announcement must be received by **January 4, 2005**.

ADDRESSES: Preproposals referencing Program Announcement LAB 04-20 should be sent as **PDF file** attachments via e-mail to: hydrogen@science.doe.gov with "Program Announcement LAB 04-20" and the submission category (e.g., Novel Materials for Hydrogen Storage) in the Subject line. No FAX or mail submission of preproposals will be accepted.

NOTE: Each FFRDC may submit up to six preproposals as lead institution; the first six preproposals received from an FFRDC as lead institution will be considered to be that institution's official submission. BES reserves the right to encourage, in whole or in part, any, all, or none of the preproposals submitted, and may issue further guidance on the scope of full proposal submissions of those encouraged.

Formal proposals referencing Program Announcement LAB 04-20 must be submitted as PDF files on a CD accompanying a printed original and seven copies of the proposal by U.S. Postal Service Express Mail, any commercial mail delivery service, or when hand carried by the researcher to: U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, SC-13, 19901 Germantown Road, Germantown, MD 20874-1290, ATTN: Program Announcement LAB 04-20.

FOR FURTHER INFORMATION CONTACT: Harriet Kung, Ph.D., Office of Basic Energy Sciences, Materials Sciences and Engineering Division, SC-131, telephone: (301)903-1330, E-mail: harriet.kung@science.doe.gov.

SUPPLEMENTARY INFORMATION: President Bush, in his 2003 State of the Union address, announced a $1.2 billion hydrogen initiative to reverse America's growing dependence on foreign oil and reduce greenhouse gas emissions. DOE Office of Energy Efficiency and Renewable Energy (EERE) coordinates the DOE Hydrogen Program; efforts include R&D of hydrogen production, delivery, storage, and fuel cell technologies; technology validation; safety, codes and standards; and education [http://www.eere.energy.gov/hydrogenandfuelcells/].

The President's 2005 Budget proposed that fundamental research within DOE Office of Science be enhanced, focused, and included in the HFI. The basic research will help overcome key technology hurdles in hydrogen production, storage, and conversion by seeking revolutionary scientific breakthroughs [http://www.ostp.gov/html/budget/2005/FY05HydrogenFuelInitiative1-pager.pdf].

In the fall of 2002, the National Academies' National Research Council appointed a Committee on Alternatives and Strategies for Future Hydrogen Production and Use. While addressing the topic on "Research and Development Priorities," the Committee concludes that "There are major hurdles on the path to achieving the vision of the hydrogen economy; the path will not be simple or straightforward." Specifically, the Academies' report recommends significant exploratory research in some areas with a focus on interdisciplinary scientific approaches [http://www.nap.edu/books/0309091632/html/].

In May 2003, a workshop was sponsored by BES to identify basic research needs for hydrogen production, storage and use. The workshop report, entitled *Basic Research Needs for the Hydrogen Economy* [http://www.science.doe.gov/bes/Hydrogen.pdf], detailed a broad array of basic research challenges. These challenges depict the gap between present-day scientific knowledge/technology capabilities and what would be required for the practical realization of a hydrogen economy. This Announcement solicits innovative basic research proposals to establish the scientific basis that underpins the physical, chemical, and biological processes governing the interaction of hydrogen with materials. We seek to support outstanding fundamental research programs to ensure that discoveries and related conceptual breakthroughs from basic research will provide a solid foundation for the innovative design of materials and processes to usher in hydrogen as the clean and sustainable fuel of the future. Five high-priority research directions, encompassing both short-term showstoppers and long-term grand challenges, will be the focus of this solicitation. They are:

1. Novel Materials for Hydrogen Storage
2. Membranes for Separation, Purification, and Ion Transport
3. Design of Catalysts at the Nanoscale
4. Solar Hydrogen Production
5. Bio-Inspired Materials and Processes

The following provides further information under each of the five focus areas to illustrate the scope of proposals solicited under this Announcement.

Novel Materials for Hydrogen Storage

On-board hydrogen storage is considered to be the most challenging aspect for the successful transition to a hydrogen economy, because the performance of current hydrogen storage materials and technologies falls far short of vehicle requirements. A factor of two to three improvement in hydrogen storage capacity and energy density, and considerable improvements in hydrogen uptake and release kinetics and cycling durability are needed to achieve performance targets within the next decade. Improvements in current technologies will not be sufficient to meet the goals. The Hydrogen Storage Grand Challenge solicitation, issued by the DOE Office of Energy Efficiency and Renewable Energy (EERE) in June 2003, aims at addressing these critical performance gaps by supporting innovative R&D efforts in the areas of metal hydrides, chemical hydrides, carbon-based materials, and new materials or technologies (http://www.eere.energy.gov/hydrogenandfuelcells/2003_storage_solicitation.html).

As indicated in the BES hydrogen workshop report, basic research is essential for identifying novel materials and processes that can provide important breakthroughs needed to meet the HFI goals. These breakthroughs may result from research at the nanoscale facilitated by new understanding derived from both theory and experiment. The advances may not necessarily come from within the boundaries of metal hydrides, chemical hydrides or carbon-based materials; instead success may well be found at the interstices of these classes of materials or may come from "out-of-the-box" concepts. Innovative basic research in the following high priority areas is needed:

- ***Complex hydrides.*** A basic understanding of the physical, chemical, and mechanical properties of metal hydrides and chemical hydrides is needed. Specifically, the fundamental factors that control bond strength, atomic processes associated with hydrogen update and release kinetics, the role of surface structure and chemistry in affecting hydrogen-material interactions, hydrogen-promoted mass transport, degradation due to cycling, reversibility in metal hydrides, and regeneration of chemical hydrides must be understood. Specific emphasis is also placed on innovative synthesis and processing routes (e.g., solvent-free synthetic approaches), and on the exploration of multi-component complex hydrides. The effect of dopants in achieving reasonable kinetics and reversibility needs to be understood at the molecular level.
- ***Nanostructured materials.*** Nanophase materials offer promise for superior hydrogen storage due to short diffusion distances, new phases with better capacity, reduced heats of adsorption/desorption, faster kinetics, and surface states capable of catalyzing hydrogen dissociation. Improved bonding and kinetic properties may permit good reversibility at lower desorption temperatures. Tailored nanostructures based on light metal hydrides, carbon-based nano-materials, and other non-traditional storage approaches need to be explored with the focus on understanding the unique surfaces and interfaces of nanostructured materials and how they affect the energetics, kinetics, and thermodynamics of hydrogen storage.
- ***Other materials.*** Research is needed to explore other novel storage materials, e.g., those based on nitrides, imides, and other materials that fall outside of metal hydrides, chemical

hydrides, and carbon-based hydrogen storage materials as identified by EERE's "Grand Challenge" for Basic and Applied Research in Hydrogen Storage Solicitation.

- ***Theory, modeling, and simulation.*** Theory, modeling, and simulation will enable (1) understanding the physics and chemistry of hydrogen interactions at the appropriate size scale and (2) the ability to simulate, predict, and design materials performance in service. Examples of research areas include: hydrogen interactions with surface and bulk microstructures, hydrogen bonding, role of nanoscale, surface interactions, multiscale hydrogen interactions, and functionalized nanocarbons. The emphasis will be to establish the fundamental understanding of hydrogen-materials interactions so that completely new and revolutionary hydrogen storage media can be identified and designed.
- ***Novel analytical and characterization tools.*** Sophisticated analytical techniques are needed to meet the high sensitivity requirements associated with characterizing hydrogen-materials interactions, especially for nanostructured materials (e.g., individual carbon nanotubes), while maintaining high specificity in characterization. In-situ studies are needed to characterize site-specific hydrogen adsorption and release processes at the molecular level.

Membranes for Separation, Purification, and Ion Transport

Membranes that selectively transport atomic, molecular, or ionic hydrogen and oxygen are vital to the hydrogen economy: they purify hydrogen fuel streams, transport hydrogen or oxygen ions between electrochemical half-reactions, and separate hydrogen in electrochemical, photochemical, or thermochemical production routes. Often these membrane functions are closely coupled with catalytic functions such as dissociation, ionization, or oxidation/reduction. Successful integration of membranes with nanocatalysts may improve the efficiency in reforming, shift chemistry and hydrogen separation utilizing different feedstocks by combining one or more of these steps.

Current membrane materials often lack sufficient selectivity to eliminate critical contaminants or to prevent leakage transport between fuel cell compartments that robs efficiency. The Nafion*TM* membrane, which is presently the best available for separating low temperature fuel cell chambers, is expensive and allows enough gas transport to reduce efficiency. Currently available oxide membranes, which are critical for ionic transport in higher-temperature fuel cells, are inefficient and fail to operate at the lower temperatures needed for use in transportation. Separation membranes that could operate in the rigorous chemical environment of a thermal cycle hydrogen generator would be of substantial value but are unknown at present. Overcoming these barriers will require an integrated, basic research effort to enable discovery of new membrane materials, improvement in membrane performance, and integration of membrane and catalytic functions. High priority research directions include:

- ***Integrated nanoscale architectures.*** The similar nanoscale dimensions of catalyst particles and of pores that transport fuel, ions, and oxygen hold promises to enable gas diffusion layers, catalyst support networks, and electrolytic membranes in fuel cells to be integrated into a single network for ion, electron, and gas transport. Chemical self-assembly of this integrated network would dramatically reduce cost and improve uniformity. Synthesis and characterization of radically new nanoscale and porous materials are required, including microporous oxides, metal-organic frameworks, and carbons that remove sulfur and carbon monoxide from hydrogen. This new approach to the design and fabrication of integrated nanoscale architectures would enable ultra-pure hydrogen to be produced from fossil, solar, thermochemical and bio-based processes. It might also revolutionize fuel cell designs.

- ***Fuel cell membranes.*** Novel membranes with higher ionic conductivity, better mechanical strength, lower cost, and longer life are critical to the success of fuel cell technologies. Polymeric membranes that conduct protons and remain hydrated to 120-150°C are needed to reduce the purity requirements and enable the use of non-noble-metal catalysts. Solid oxide fuel cells need lower-temperature oxide-ion membranes to minimize corrosion and differential thermal expansion, while maintaining selectivity and permeability. Many thermal water-splitting cycles subject materials to harshly corrosive, high temperature environments. Sorbents and membranes that are stable and durable in such environments are needed for efficient thermal cycles. Achieving these goals will require discovery of better, more durable materials, as well as better understanding and control of the electrochemical processes at the electrodes and membrane electrolyte interfaces.
- ***Theory, modeling, and simulation of membranes and fuel cells.*** Fundamental understanding of the selective transport of molecules, atoms, and ions in membranes is in its infancy. The diversity of transport mechanisms and their dependence on local defect structure requires extensive theory, modeling and simulation to establish the basic principles and design strategies for improved membrane materials. The emphasis is to understand the nature of proton transport in polymer electrolyte membranes; the interaction of complex aqueous, gaseous, and solid interfaces in gas diffusion electrode assemblies; the nature of corrosion processes under applied electrochemical potentials and in oxidative media; and the origin of the performance robbing overpotential for fuel cell cathodes.

Design of Catalysts at the Nanoscale

Catalysis is vital to the success of the HFI owing to its roles in converting solar energy to chemical energy, producing hydrogen from water or carbon-containing fuels such as coal and biomass, and producing electricity from hydrogen in fuel cells. Catalysts can also increase the efficiency of the uptake and release of stored hydrogen with reduced need for thermal activation. Breakthroughs in catalytic research would impact the thermodynamic efficiency of hydrogen production, storage, and use, and thus improve the economic efficiency with which the primary energy sources - fossil, biomass, solar, or nuclear - serve our energy needs. Most fuel-cell and low-temperature reforming catalysts are based on expensive noble metals (e.g., platinum), and their limited reserves threaten the long-term sustainability of a hydrogen economy. High priority research directions include:

- ***Nanoscale catalysts.*** Nanostructured materials - with high surface areas and large numbers of controllable sites that serve as active catalytic regions - open new opportunities for significantly enhancing catalytic activity and specificity. The concepts, technologies, and synthetic capabilities derived from research at the nanoscale now provide new approaches for the controlled production of catalysts. Specific emphasis is on elucidating the atomic and molecular processes involved in catalytic activity, selectivity, deactivation mechanisms, and on understanding the special properties that emerge at the nanoscale.

- ***Innovative synthetic techniques.*** Emerging technologies that allow synthesis at the nanoscale with atomic-scale precision will open new opportunities for producing tailored structures of catalysts on supports with controlled size, shape and surface characteristics. New, high- throughput innovative synthesis methods can be exploited in combination with theory and advanced measurement capabilities to accelerate the development of designed catalysts. In addition, novel, cost-effective fabrication methods need to be developed for the practical application of these new designer catalysts. The interplay between theory and experiment forms a recursive process that will accelerate the development of predictive models to support the development of optimized catalysts for specific steps in hydrogen energy processing.
- ***Novel characterization techniques.*** To fully understand complex catalytic mechanisms will require detailed characterization of the active sites; identification of the interaction of the reactants, intermediates and products with the active sites; conceptualization and, possibly, detection of the transition states; and quantification of the dynamics of the entire catalytic process. This will entail the production of well-defined materials that can be characterized at the atomic level. Special focus is placed on developing new analytical tools to permit the determination of the interatomic arrangements, interactions and transformations *in situ*, i.e., during reaction, in order to reveal details about reaction mechanisms and catalyst dynamics.
- ***Theory, modeling, and simulation of catalytic pathways.*** Computational methods have now developed to the point that entire reaction pathways can be identified and these advances will allow trends in reactivity to be understood. Close coupling between experimental observations and theory, modeling, and simulation will provide unprecedented capabilities to design more selective, robust, and impurity-tolerant catalysts for hydrogen production, storage, and use. This approach will enable the design and control of the chemical and physical properties of the catalyst, its supporting structure, and the associated molecular processes at the nanoscale.

Solar Hydrogen Production The sun is Earth's most plentiful source of energy, and it has sufficient capacity to fully meet the global needs of the next century without potentially destructive environmental consequences. Efficient conversion of sunlight to hydrogen by splitting water through photovoltaic cells driving electrolysis or through direct photocatalysis at energy costs competitive with fossil fuels is a major enabling milestone for a viable hydrogen economy. Basic strategies for cost effective solar hydrogen production are rooted in fundamental scientific breakthroughs in chemical synthesis, self-assembly, charge transfer at nanoparticle interfaces, and photocatalysis. High priority research directions for solar hydrogen include:

- ***Nanoscale structures.*** The sequential processes of light collection, charge separation, and transport in photovoltaic and photocatalytic devices require nanoscale architectural control and manipulation. Nanoscale assemblies of multiple wavelength absorbers (e.g., semiconductor quantum dots), nanoscale polymer or molecular diodes that prevent recombination, and employing short collection lengths between the excitation and collection points have the potential to dramatically improve efficiencies. Semiconductor-metal nanocomposites show promise for improved light-harvesting and charge-separation efficiency. Incorporation of multielectron redox catalysts for direct water splitting greatly simplify the water splitting process and offer new horizons for improved photocatalytic hydrogen production.

- ***Light harvesting and novel photoconversion concepts.*** New strategies are needed to efficiently use the entire solar spectrum. These strategies could involve molecular photon antennas, junctions containing multiple absorbers, and up- and down-conversion of light to the appropriate wavelengths. Dye-sensitized TiO2 nanocrystalline solar cells have emerged as a potential, cost effective alternative to silicon solar cells. New photochemical sensitizers are needed (e.g. bi- and trimetallic transition metal complexes) that absorb in the visible and near-infrared and that are efficient injectors of electrons into semiconductor nanoparticles. Solid-state molecule-based solar photochemical conversion, however, offers distinct advantages over liquid junction dye-sensitized nanocrystalline solar cells. Multicomponent molecular architectures are envisioned in which bioinspired multiredox catalysts are incorporated within durable polymer, zeolite, or membrane organizing environments for vectorial electron transfer. The exploitation of higher energy radiation to produce charge carriers would enable the use of corrosion-resistant wide band-gap semiconductors without sensitizers for hydrogen production.
- ***Organic semiconductors and other high performance materials.*** The organic semiconductors offer an inexpensive alternative to traditional semiconductors for photovoltaic and photocatalytic devices. Basic research on the fundamental charge excitation, separation, and collection processes in organics and their dependence on nanoscale structure is needed to bring their efficiency from the current 3% to 10% or more, which is needed for economically competitive photovoltaic and photocatalytic hydrogen production. In addition, novel materials for transparent conductors, electrocatalysts, electron- and hole-conducting polymers, and for charge promoting separation in liquid crystals and organic thin films are needed for novel photovoltaic and photocatalytic solar hydrogen production.
- ***Theory, modeling, and simulation of photochemical processes.*** Theory and modeling are needed to develop a predictive framework for the dynamic behavior of molecules, complex photoredox systems, interfaces, and photoelectrochemical cells. As new physical effects are discovered and exploited, particularly those involving semiconductor nanoparticles and supramolecular assemblies, challenges emerge for theory to accurately model the behavior of complex systems over a range of time and length scales.

Bio-inspired Materials and Processes Direct production of hydrogen from water and other carbon neutral sources using sunlight (solar radiation) offers real promises in realizing a clean and sustainable energy future, but there are many obstacles to efficient and cost-effective technologies. Fortunately, plants and some bacteria are endowed with enzymes and catalysts that can produce hydrogen while powered by sun light or fermentation-derived energy at operating temperatures ranging from 0°C to 100°C. While inherent biological inefficiencies and public sensitivity to genetically engineered organisms may need to be overcome for biological production of hydrogen to become competitive and viable, a fundamental understanding of the molecular machinery of biological systems could provide the knowledge that is needed to design artificial, bio-inspired materials that make solar photochemical production of hydrogen a reality. Our current knowledge of many of the basic aspects of these biological processes is limited.

Fundamental research into the molecular mechanisms underlying biological hydrogen production is the essential key to our ability to adapt, exploit, and extend what nature has accomplished for our own renewable energy needs. Important research directions include:

- ***Enzyme catalysts.*** A fundamental understanding is needed of the structure and chemical mechanism of enzyme complexes that support hydrogen generation. For example, photochemical hydrogen production requires biology-inspired catalysts that (1) can operate at the very high potential required for water oxidation, (2) can perform a four-electron reaction to maximize energetic efficiency and avoid limiting cathode overpotentials, and (3) can avoid production of corrosive intermediates (such as hydroxyl radicals), and mediate proton- coupled redox reactions. Research approaches would likely include novel analytical technologies and would merge aspects of disparate biological and physical techniques.
- ***Bio-hybrid energy coupled systems.*** As more is understood about biocatalytic hydrogen production, there is the possibility that critical enzymes that are synthesized and employed by biological systems can be harvested and combined with synthetic materials to construct robust, efficient hybrid systems that are scalable to hydrogen production facilities. Before we can efficiently apply biological catalysts to hydrogen generation, we need to understand how these catalysts are assembled with their cofactors into integrated systems. How are these multi-component systems organized, continually refreshed, and maintained, while remaining functional in the face of damaging side reactions or changing external environmental conditions? Can the natural enzymes be reduced in size and complexity to contain the essential catalytic activity while removing the complex regulation and signaling components that are required for integration into functioning biological species?
- ***Theory, modeling, and nanostructure design.*** Taking cues from these various natural processes, computational approaches may be employed for rational redesign of enzymes for improved hydrogen production, reduced sensitivity to inhibitors, and improved stability. Emerging capabilities in nanoscale science hold particular promise for harnessing the chemical processes inherent in bio-inspired hydrogen production. For example, nanoscale structures can be designed to spatially separate oxygen and hydrogen formation during photochemical water splitting for a biomimetic or biohybrid system that circumvents problems with inactivation of catalytic sites. Research at the nanoscale is challenging, but offers the promise of inexpensive materials for overcoming current kinetic constraints in hydrogen energy systems.

Program Funding

It is anticipated that up to $12 million annually will be available for multiple awards for this announcement. Initial awards will be in Fiscal Year 2005, and proposals may request project support for up to three years. All awards are contingent on the availability of funds and programmatic needs.

Preproposal

The preproposal should consist of a description of the research proposed to be undertaken by the researcher including a clear explanation of its importance to the advancement of basic hydrogen research and its relevance to the HFI. The preproposal must include a cover sheet downloadable at: http://www.science.doe.gov/bes/HFI_preapp_cover_lab.pdf to identify the institution, Principal Investigator name(s), address(es), telephone and fax number(s) and E-mail address(es), the title of the project, the submission category, and the yearly breakdown of the total budget request. A brief (one-page) vitae should be provided for each Principal Investigator. The preproposal should consist of a maximum of 3 pages of narrative (including text and figures) describing the research objectives, approaches to be taken, the institutional setting, and a description of any research partnership if appropriate.

Full Proposal

The Department of Energy will accept Full Proposals by invitation only, based upon the evaluation of the preproposals. After receiving notification from DOE concerning successful preproposals, researchers may prepare formal proposals. The Project Description must not exceed 20 pages, including tables and figures, but exclusive of attachments. The proposal must contain an abstract or project summary, short vitae, and letters of intent from collaborators if appropriate. The proposal should also contain one paragraph addressing how the proposed research will address one or more of the four BES long-term program measures used by the Office of Management and Budget to rate the BES program annually; these measures may be found at [http://www.sc.doe.gov/bes/BES_PART_Long_Term_Measures_FEB04.pdf]. DOE is under no obligation to pay for any costs associated with the preparation or submission of proposals.

Full proposals adhering to DOE Field Work Proposal format (Reference DOE Order 412.1) are to be prepared and submitted consistent with policies of the investigator's laboratory and the local DOE Operations Office. Laboratories may submit proposals directly to the SC Program Office listed above. A copy should also be provided to the appropriate DOE Operations Office.

Coordination and Integration with the DOE Offices of Energy Efficiency and Renewable Energy (EERE), Fossil Energy (FE), and Nuclear Energy Science and Technology (NE) Hydrogen Program

The proposal solicitation and selection processes will be coordinated with EERE, FE, and NE's program to ensure successful integration of the basic research components with the applied technology program. Specifically, input from EERE, FE and NE have been incorporated in the formulation of this announcement, and further input will be solicited in the review of preproposals. There will also be an annual Contractors' Meeting for all participants in the BES program to help coordinate and integrate research efforts related to hydrogen research. The Annual Contractors' Meeting of BES principal investigators will be coordinated with EERE, FE and NE, and will include presentations on applied research and development needs from researchers inside and outside of the Contractors' group.

The instructions and format described below should be followed. Reference Program Announcement LAB 04-20 on all submissions and inquiries about this program.

OFFICE OF SCIENCE
GUIDE FOR PREPARATION OF SCIENTIFIC/TECHNICAL PROPOSALS
TO BE SUBMITTED BY NATIONAL LABORATORIES

Proposals from National Laboratories submitted to the Office of Science (SC) as a result of this program announcement will follow the Department of Energy Field Work Proposal process with additional information requested to allow for scientific/technical merit review. The following guidelines for content and format are intended to facilitate an understanding of the requirements necessary for SC to conduct a merit review of a proposal. Please follow the guidelines carefully, as deviations could be cause for declination of a proposal without merit review.

1. Evaluation Criteria

Proposals will be subjected to formal merit review (peer review) and will be evaluated against the following criteria which are listed in descending order of importance:

Scientific and/or technical merit of the project

Appropriateness of the proposed method or approach

Competency of the personnel and adequacy of the proposed resources

Reasonableness and appropriateness of the proposed budget

Basic research that is relevant to the Administration's Hydrogen Fuel Initiative

The external peer reviewers are selected with regard to both their scientific expertise and the absence of conflict-of-interest issues. Non-federal reviewers may be used, and submission of a proposal constitutes agreement that this is acceptable to the investigator(s) and the submitting institution.

2. Summary of Proposal Contents

Field Work Proposal (FWP) Format (Reference DOE Order 5700.7C) (DOE ONLY)
Proposal Cover Page
Table of Contents
Abstract
Narrative
Literature Cited
Budget and Budget Explanation
Other support of investigators
Biographical Sketches
Description of facilities and resources
Appendix

2.1 Number of Copies to Submit

Formal proposals referencing Program Announcement LAB 04-20 must be submitted as PDF files on a CD accompanying a printed original and seven copies of the proposal by U.S. Postal Service Express Mail, any commercial mail delivery service, or when hand carried by the researcher to: U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, SC-13, 19901 Germantown Road, Germantown, MD 20874-1290, ATTN: Program Announcement LAB 04-20.

3. Detailed Contents of the Proposal

Proposals must be readily legible, when photocopied, and must conform to the following three requirements: the height of the letters must be no smaller than 10 point with at least 2 points of spacing between lines (leading); the type density must average no more than 17 characters per inch; the margins must be at least one-half inch on all sides. Figures, charts, tables, figure legends, etc., may include type smaller than these requirements so long as they are still fully legible.

3.1 Field Work Proposal Format (Reference DOE Order 5700.7C) (DOE ONLY)

The Field Work Proposal (FWP) is to be prepared and submitted consistent with policies of the investigator's laboratory and the local DOE Operations Office. Additional information is also requested to allow for scientific/technical merit review.

Laboratories may submit proposals directly to the SC Program office listed above. A copy should also be provided to the appropriate DOE operations office.

3.2 Proposal Cover Page

The following proposal cover page information may be placed on plain paper. No form is required.

Title of proposed project
SC Program announcement title
Name of laboratory
Name of principal investigator (PI)
Position title of PI
Mailing address of PI
Telephone of PI
Fax number of PI
Electronic mail address of PI
Name of official signing for laboratory*
Title of official
Fax number of official
Telephone of official
Electronic mail address of official
Requested funding for each year; total request
Use of human subjects in proposed project:

If activities involving human subjects are not planned at any time during the proposed project period, state "No"; otherwise state "Yes", provide the IRB Approval date and Assurance of Compliance Number and include all necessary information with the proposal should human subjects be involved.

Use of vertebrate animals in proposed project:

If activities involving vertebrate animals are not planned at any time during this project, state "No"; otherwise state "Yes" and provide the IACUC Approval date and Animal Welfare Assurance number from NIH and include all necessary information with the proposal.

Signature of PI, date of signature

Signature of official, date of signature*

*The signature certifies that personnel and facilities are available as stated in the proposal, if the project is funded.

3.3 Table of Contents

Provide the initial page number for each of the sections of the proposal. Number pages consecutively at the bottom of each page throughout the proposal. Start each major section at the top of a new page. Do not use unnumbered pages and do not use suffices, such as 5a, 5b.

3.4 Abstract

Provide an abstract of no more than 250 words. Give the broad, long-term objectives and what the specific research proposed is intended to accomplish. State the hypotheses to be tested. Indicate how the proposed research addresses the SC scientific/technical area specifically described in this announcement.

3.5 Narrative

The narrative comprises the research plan for the project and is limited to 5 pages per task. It should contain the following subsections:

Background and Significance: Briefly sketch the background leading to the present proposal, critically evaluate existing knowledge, and specifically identify the gaps which the project is intended to fill. State concisely the importance of the research described in the proposal. Explain the relevance of the project to the research needs identified by the Office of Science. Include references to relevant published literature, both to work of the investigators and to work done by other researchers.

Preliminary Studies: Use this section to provide an account of any preliminary studies that may be pertinent to the proposal. Include any other information that will help to establish the experience and competence of the investigators to pursue the proposed project. References to appropriate publications and manuscripts submitted or accepted for publication may be included.

Research Design and Methods: Describe the research design and the procedures to be used to accomplish the specific aims of the project. Describe new techniques and methodologies and explain the advantages over existing techniques and methodologies. As part of this section, provide a tentative sequence or timetable for the project.

Subcontract or Consortium Arrangements: If any portion of the project described under "Research Design and Methods" is to be done in collaboration with another institution, provide information on the institution and why it is to do the specific component of the project. Further information on any such arrangements is to be given in the sections "Budget and Budget Explanation", "Biographical Sketches", and "Description of Facilities and Resources".

3.6 Literature Cited

List all references cited in the narrative. Limit citations to current literature relevant to the proposed research. Information about each reference should be sufficient for it to be located by a reviewer of the proposal.

3.7 Budget and Budget Explanation

A detailed budget is required for the entire project period, which normally will be three years, and for each fiscal year. It is preferred that DOE's budget page, Form 4620.1 be used for providing budget information*. Modifications of categories are permissible to comply with institutional practices, for example with regard to overhead costs.

A written justification of each budget item is to follow the budget pages. For personnel this should take the form of a one-sentence statement of the role of the person in the project. Provide a detailed justification of the need for each item of permanent equipment. Explain each of the other direct costs in sufficient detail for reviewers to be able to judge the appropriateness of the amount requested.

Further instructions regarding the budget are given in section 4 of this guide.

* Form 4620.1 is available at web site: http://www.sc.doe.gov/production/grants/Forms-E.html

3.8 Other Support of Investigators

Other support is defined as all financial resources, whether Federal, non-Federal, commercial or institutional, available in direct support of an individual's research endeavors. Information on active and pending other support is required for all senior personnel, including investigators at collaborating institutions to be funded by a subcontract. For each item of other support, give the organization or agency, inclusive dates of the project or proposed project, annual funding, and level of effort devoted to the project.

3.9 Biographical Sketches

This information is required for senior personnel at the laboratory submitting the proposal and at all subcontracting institutions. The biographical sketch is limited to a maximum of two pages for each investigator.

3.10 Description of Facilities and Resources

Describe briefly the facilities to be used for the conduct of the proposed research. Indicate the performance sites and describe pertinent capabilities, including support facilities (such as machine shops) that will be used during the project. List the most important equipment items already available for the project and their pertinent capabilities. Include this information for each subcontracting institution, if any.

3.11 Appendix

Include collated sets of all appendix materials with each copy of the proposal. Do not use the appendix to circumvent the page limitations of the proposal. Information should be included that may not be easily accessible to a reviewer.

Reviewers are not required to consider information in the Appendix, only that in the body of the proposal. Reviewers may not have time to read extensive appendix materials with the same care as they will read the proposal proper.

The appendix may contain the following items: up to five publications, manuscripts (accepted for publication), abstracts, patents, or other printed materials directly relevant to this project, but not generally available to the scientific community; and letters from investigators at other institutions stating their agreement to participate in the project (do not include letters of endorsement of the project).

4. Detailed Instructions for the Budget

(DOE Form 4620.1 "Budget Page" may be used)

4.1 Salaries and Wages

List the names of the principal investigator and other key personnel and the estimated number of person-months for which DOE funding is requested. Proposers should list the number of postdoctoral associates and other professional positions included in the proposal and indicate the number of full-time-equivalent (FTE) person-months and rate of pay (hourly, monthly or annually). For graduate and undergraduate students and all other personnel categories such as secretarial, clerical, technical, etc., show the total number of people needed in each job title and total salaries needed. Salaries requested must be consistent with the institution's regular practices. The budget explanation should define concisely the role of each position in the overall project.

4.2 Equipment

DOE defines equipment as "an item of tangible personal property that has a useful life of more than two years and an acquisition cost of $25,000 or more." Special purpose equipment means equipment which is used only for research, scientific or other technical activities. Items of needed equipment should be individually listed by description and estimated cost, including tax, and adequately justified. Allowable items ordinarily will be limited to scientific equipment that is not already available for the conduct of the work. General purpose office equipment normally will not be considered eligible for support.

4.3 Domestic Travel

The type and extent of travel and its relation to the research should be specified. Funds may be requested for attendance at meetings and conferences, other travel associated with the work and subsistence. In order to qualify for support, attendance at meetings or conferences must enhance the investigator's capability to perform the research, plan extensions of it, or disseminate its results. Consultant's travel costs also may be requested.

4.4 Foreign Travel

Foreign travel is any travel outside Canada and the United States and its territories and possessions. Foreign travel may be approved only if it is directly related to project objectives.

4.5 Other Direct Costs

The budget should itemize other anticipated direct costs not included under the headings above, including materials and supplies, publication costs, computer services, and consultant services (which are discussed below). Other examples are: aircraft rental, space rental at research establishments away from the institution, minor building alterations, service charges, and fabrication of equipment or systems not available off- the-shelf. Reference books and periodicals may be charged to the project only if they are specifically related to the research.

a. Materials and Supplies

The budget should indicate in general terms the type of required expendable materials and supplies with their estimated costs. The breakdown should be more detailed when the cost is substantial.

b. Publication Costs/Page Charges

The budget may request funds for the costs of preparing and publishing the results of research, including costs of reports, reprints page charges, or other journal costs (except costs for prior or early publication), and necessary illustrations.

c. Consultant Services

Anticipated consultant services should be justified and information furnished on each individual's expertise, primary organizational affiliation, daily compensation rate and number of days expected service. Consultant's travel costs should be listed separately under travel in the budget.

d. Computer Services

The cost of computer services, including computer-based retrieval of scientific and technical information, may be requested. A justification based on the established computer service rates should be included.

e. Subcontracts

Subcontracts should be listed so that they can be properly evaluated. There should be an anticipated cost and an explanation of that cost for each subcontract. The total amount of each subcontract should also appear as a budget item.

4.6 Indirect Costs

Explain the basis for each overhead and indirect cost. Include the current rates.