Program Announcement
To DOE National Laboratories
LAB 06-17

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 mission to assist in strengthening the Nation's scientific research enterprise through the support of fundamental science and the experimental tools to perform basic research, announces its interest in receiving proposals for basic research for the Hydrogen Fuel Initiative (HFI). Areas of focus include: Novel Materials for Hydrogen Storage; Functional Membranes; and Nanoscale Catalysts. We seek to support outstanding research programs that will lead to key discoveries to make hydrogen a feasible fuel for the future. Research funded under this initiative will pursue breakthroughs in materials, chemical and physical understandings, and interdisciplinary theory-modeling-simulation-experimentation approaches in order to surpass the existing scientific and technical barriers. More information on these focus areas is provided in the SUPPLEMENTARY INFORMATION section below.

DATES: Potential researchers are **REQUIRED** to submit a brief preproposal through appropriate Laboratory channels. Preproposals referencing Program Announcement LAB 06-17 must be received by DOE by 4:30 p.m., Eastern Time, **July 6, 2006**. Preproposals will be reviewed for conformance with the guidelines presented in this notice and suitability in the technical areas specified in this notice. A response to the preproposals encouraging or discouraging formal proposals will be communicated to the applicants by **September 12, 2006. Complete guidance on the content and format of the preproposal is provided in the SUPPLEMENTARY INFORMATION section below.**

Only those researchers that receive notification from DOE encouraging a formal proposal may submit a full proposal. **No other formal proposals will be considered.** Formal proposals in response to this notice must be received by **December 12, 2006, 8:00p.m. Eastern Time.**

NUMBER OF PREPROPOSALS: each FFRDC may submit up to four preproposals as lead institution. The first four 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 the full proposal submissions of those encouraged.

ADDRESSES: Preproposals referencing Program Announcement LAB 06-17 should be sent as PDF file attachments via e-mail to: hydrogen@science.doe.gov with Subject line specifying "Program Announcement LAB 06-17" and the primary submission category, i.e., "Novel Materials for Hydrogen Storage," "Functional Membranes," or "Nanoscale Catalysts." No FAX or mail submission of preproposals will be accepted.

Formal Proposals

This section pertains only to those proposers that have been encouraged to submit a full proposal. A complete formal FWP in a single Portable Document Format (PDF) file must be submitted through the DOE ePMA system (https://epma.doe.gov) as an attachment. To identify that the FWP is responding to this program announcement, please fill in the following fields in the "ePMA Create Proposal Admin Information" screen as shown:

Proposal Short Name:
Fiscal Year:
Proposal Reason:
Program Announcement Number: Lab 06-17 *
Program announcement Title: Basic Research for the Hydrogen Fuel Initiative, DOE Research Program Announcement *
Proposal Purpose:
Estimated Proposal Begin Date:
HQ Program Manager Organization:

* Please use the wording shown when filling in these fields to identify that the FWP is responding to this Program Announcement.

In order to expedite the review process, please submit a CD and two copies of the proposal using the following, by U.S. Postal Service Express Mail, any commercial mail delivery service, or when hand-carried to:

U.S. Department of Energy
Office of Science
Office of Basic Energy Sciences, SC-22
19901 Germantown Road
Germantown, MD 20874-1290
ATTN: Program Announcement LAB 06-17

FOR FURTHER INFORMATION CONTACT: Dr. Jane Zhu, Materials Sciences and Engineering Division, E-Mail: Jane.Zhu@science.doe.gov, Phone: (301) 903-3811; or Dr. Raul Miranda, Chemical Sciences, Geosciences, and Biosciences Division, E-Mail: Raul.Miranda@science.doe.gov, Phone: (301) 903-8014. Postal Address: Office of Basic Energy Sciences, SC-22/Germantown Building, U.S. Department of Energy, 1000 Independence Avenue, SW, Washington, D.C. 20585-1290.

SUPPLEMENTARY INFORMATION: Since President Bush in his 2003 State of the Union address announced the Hydrogen Fuel Initiative for a clean and secure energy future, the U.S. DOE has sponsored new research to attend to the initiative goals [http://www.science.doe.gov/bes/hydrogen.html]. The U.S. DOE Hydrogen Program, through the participation of science and technology offices, supports both basic and applied research and development toward realizing the national hydrogen vision to produce and deliver hydrogen energy in an affordable, safe, and convenient manner. Information for applied R&D in hydrogen production, delivery, storage, fuel cell technologies, technology validation, safety, codes and standards can be found at http://www.hydrogen.energy.gov.

A workshop was sponsored in May 2003 by the Office of Basic Energy Sciences (OBES) 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 depicted the vast gap between present-day scientific knowledge/technology capabilities and what would be required for the practical realization of a hydrogen economy. The workshop report is still a current source of information and summarizes the interests of the OBES.

In supporting the President's Hydrogen Fuel Initiative (HFI), the OBES issued its first request for proposals in 2004 under the "Basic Research for the Hydrogen Fuel Initiative," over 70 new awards were funded in 2005 and 2006 at universities and national laboratories covering the priority areas identified in the 2003 workshop report [http://www.science.doe.gov/bes/hydrogen.html]. This initial set of awards contributes to important areas addressing hydrogen production and storage and hydrogen utilization in fuel cells. To tackle the challenges presented by the HFI, the basic research effort needs to be increased both in intensity and scope, particularly in regards to materials functionalities and structures, synthesis methods, and instrumental characterization methods, as well as with regards to new theoretical methods and simulation approaches. This Notice solicits innovative basic research proposals to significantly strengthen the scientific basis that will allow comprehensive understanding of the physical and chemical processes that lead to the extraction of hydrogen from its natural environments, storage and distribution of hydrogen, and the efficient energy conversion, all in a safe as well as economically and environmentally sustainable manner. We seek to support outstanding fundamental research programs potentially leading to discoveries and breakthroughs, focused on primarily three broad areas:

1. **Novel Materials for Hydrogen Storage**
2. **Functional Membranes**
3. **Nanoscale Catalysts**

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

Novel Materials for Hydrogen Storage

On-board hydrogen storage is considered to be one of the most challenging barriers to the widespread use of hydrogen because the performance of current hydrogen storage materials and technologies falls far short of vehicle requirements. Hydrogen storage is also needed for off-board uses such as for stationary power generation and for hydrogen delivery and refueling infrastructure. Enormous improvements in hydrogen storage capacity and in hydrogen uptake and release kinetics and cycling durability are needed to meet the storage demands for a future hydrogen economy. Incremental improvements in current technologies will not be sufficient to meet the stated practical goals (see for example, http://www.eere.energy.gov/hydrogenandfuelcells/mypp/). As indicated in the BES hydrogen workshop report, basic research is essential for identifying novel materials and processes that can provide the 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 interfaces of these classes of materials or may come from "outside-the-box" concepts. Innovative basic research in the following high priority areas is needed:

- ***Novel materials***. Research is needed to develop and examine new materials and obtain an atomic- and molecular-level understanding of the physical and chemical processes involved in hydrogen storage and release. These novel storage materials may fall outside of the hydrogen-storage materials that are currently under investigation. The innovative design and synthesis of tailored materials with high storage capacity as well as fast release times will need (a) reliable information about the structure, thermodynamic, physical, and chemical properties of novel storage materials and (b) an understanding of the interaction of hydrogen in solid- state materials.
- ***Complex hydrides***. A basic understanding of the structure, physical, chemical, and mechanical properties of metal hydrides and complex chemical hydrides is still needed. Specifically, the fundamental factors that control bond strength, atomic processes associated with hydrogen uptake 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. Innovative synthesis and processing routes need to be developed. The effect of dopants in achieving reasonable kinetics and reversibility needs to be understood at the atomic 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.
- ***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. Examples of research areas include: hydrogen interactions with surface, interface, grain boundaries and bulk defects of a particular storage material. 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 and characterization techniques are needed to meet the high sensitivity requirements associated with characterizing hydrogen-materials interactions, especially for nanostructured materials, while maintaining high specificity in characterization. The structure and surface properties of high-performance nanomaterials need to be identified

to facilitate the modeling and provide an understanding of structure- property relationship. *in-situ* studies are needed to characterize site-specific hydrogen adsorption and release processes at the molecular level.

Functional Membranes

Novel membranes optimized with respect to ionic conductivity, thermal stability, cost, and durability are needed to significantly improve the performance of fuel cell systems for hydrogen energy conversion. A detailed understanding of interactions between chemical species and membranes, or among species confined within membranes, is needed to develop new separation processes. The molecular design and synthesis of new membranes to selectively transport hydrogen, oxygen and other species is vital to the purification of fuel streams, transport of species between electrodes, and separation of 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. Often they must function in water environment at temperatures below the boiling point of water. These membranes may lack selectivity to prevent cross-over between electrodes or to separate selected species efficiently. Currently available oxide membranes, which are critical for ionic transport in higher-temperature fuel cells, are also inefficient. For all types of membranes, the fundamental physical and chemical processes that determine transport and separation efficiency need better understanding. Overcoming the barriers described above 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. The following are some of the high priority research directions.

- ***Integrated nanoscale architectures***. The nanoscale dimensions of catalyst particles, support materials, and ion-conducting membranes make it possible to design compact structures that facilitate transport of ions, electrons, and gases. Self-assembly or other approaches to synthesize integrated structures pose significant technical challenges but have the potential to improve catalyst uniformity and perhaps enhance endurance and overall performance. Synthesis and characterization of radically new nanoscale and porous materials are required, including but not restricted to microporous oxides, metal-organic frameworks, bioinspired structures, carbons that remove sulfur and carbon monoxide from hydrogen, etc. New approaches to the design and fabrication of integrated nanoscale architectures may enable ultra-pure hydrogen to be produced from fossil, solar, thermochemical and bioinspired processes.
- ***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 and other technologies that depend on ionic transport. Polymeric membranes that conduct protons and remain hydrated up to high temperatures are needed. Membranes that do not even require hydration yet meet the conductivity, durability and cost requirements are also desired. Novel oxide-ion membranes that operate at lower temperatures while maintaining selectivity and permeability, as well as membranes that are stable and durable under harshly corrosive environments are needed for efficient thermal cycles. Achieving these goals will require discovery of novel

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 polymeric as well as oxide membranes is emerging. The diversity of transport mechanisms and their dependence on structure over a wide temperature range requires extensive theory, modeling and simulation to discover the basic principles and develop design strategies for improved membrane performance. Significant emphasis is placed on understanding the nature of proton transport in 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.
- ***Characterization of electrochemical and buried interfaces***. Innovative techniques are needed to study the microstructure and reactivity of buried interfaces under chemical or electrical potentials. This is relevant to such applications as electrocatalyst/electrolyte interfaces in membrane-electrode assemblies, or membrane-ceramic interfaces in separation media. Understanding and controlling the structure and morphology of the membranes and their evolution during operation is crucial to maximizing performance. Therefore, in- situ characterization methods become particularly important.

Nanoscale Catalysts

Catalysis impacts many of the technologies for which breakthroughs are needed, ranging from production of hydrogen from traditional sources such as oil and gas, as well as underexploited sources such as coal, biomass, and water, to the low-activation-energy storage or removal of hydrogen, and to the production of electricity from fuel cells or photocells. Catalysts in many cases make possible hydrogen-related transformations that are unfeasible or impractical otherwise, by providing new reaction pathways. In other cases, catalysts increase the efficiency of hydrogen-related processes such as production, uptake and release of stored hydrogen by reduction of the energy of 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 or low-temperature combustion catalysts are based on noble metals. From a fundamental point of view, it is of interest to expand our understanding and use of non-noble metals in fuel cells, reforming and other processes. The following are some of the high-priority research directions.

- ***Synthesis-structure-function relationships of nanoscale catalysts***. The control of chemical selectivity and activity is the key to the discovery of new or more efficient hydrogen-related activation and conversion pathways. The selectivity and activity properties that arise with matter at nanometer dimensions are mostly unknown or need to be better understood. The relationship between the electronic structure of the catalyst or electrocatalyst and the support, and the catalytic activity needs to be better known. Thus, single-site catalysts with predictable chemical functionalities need to be developed. The chemical conversion of hydrogen-containing molecules with well-defined and stable clusters of metals, oxides and other compounds needs to be understood. Such need for deeper understanding is particularly crucial for catalysts based on non-noble metals.

- ***Structural dynamics of catalysts***. It is desirable to synthesize and operate catalysts with predictable structures and compositions under reaction conditions. Catalytic structure, particularly at the atomic and electronic levels, is dynamic, and current catalyst design activities must be advanced beyond the static configurations of atomic and electronic structures. Structural changes at surfaces and interfaces are particularly of interest in addition to changing crystal phases, agglomeration, dissolution and reprecipitation. Such research should unravel the many chemical and physical events that influence catalytic behavior. It is of interest to consider fast transients, for example cationic or anionic segregation that occurs during redox cycles and leads to the formation and re-annealing of defect planes, or metal surface diffusion that is driven by chemical, thermal or electric gradients and leads to restructuring. It is also of interest to consider slow transient phenomena, for example nanoparticle sintering in electrodes, solid phase separation in mixed oxides, polymerization and phase separation of oxide species on surfaces, solid state reactions and deactivation or promotion, etc.
- ***Dynamic behavior of catalytic reactions***. Catalytic reactions of oxygen- or hydrogen-containing molecules proceed with mechanisms that can be described with classical kinetics or microkinetics models, which primarily explain the statistical behavior of reacting species. It is of interest, however, to uncover the dynamics of single events, such as bond formation and scission on surfaces or at single sites, or elemental transfer between adsorbed species, or energy transfer between reactants, products, catalytic sites and outgoing or incoming electrons, etc., by means of advanced experiments and theory. At the longer timescales corresponding to a full catalytic turnover, it is of interest to understand how macroscopic mechanisms or statistical molecular behavior correlate with the catalytic structural dynamics described in the previous bullet.
- ***Innovative synthesis techniques***. A basic challenge for catalysis in hydrogen production, storage and fuel cells is the synthesis of well-defined catalysts. Approaches are needed to tailor the molecular precursors and building blocks to yield stable quasi-equilibrium structures that retain excellent catalytic performance and robustness at extreme conditions of temperature, pressure, and potential cycling while exposed to the reaction medium. Synthesis with atomic- scale precision is necessary to produce tailored structures of catalysts on supports with controlled size, shape and surface characteristics. New, high-throughput innovative synthesis methods must be combined 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.
- ***Bio-inspired catalysts***. A fundamental understanding is needed of bio-inspired complexes that are able to perform activation of hydrogen-containing molecules. New opportunities for hydrogen reactions are sought from the discovery of synthetic analogues that operate at the high potential required for water oxidation and are able to perform a four-electron reduction, or proton-coupled redox reactions, and avoid the production of corrosive intermediates. In analogy to natural systems, bio-inspired catalysts should be able to self-repair and provide robust resilience to defects.
- ***Techniques for in-situ characterization under reaction***. Fundamental understanding of complex catalytic mechanisms in hydrogen processes requires identification of the nature

of the active sites under actual reaction conditions; the interaction of the reactants, intermediates and products with the active sites; detection of intermediate species; and quantification of the dynamics of atomic, electronic and energetic exchanges. There is a special need for ultrafast and high- resolution imaging and spectroscopic techniques to determine the interatomic arrangements, interactions and transformations in model catalysts during reaction. Such methods, in combination with advances in theory and simulation, should lead to fundamental understanding of catalytic mechanisms.

- ***Theory, modeling, and simulation of catalytic pathways***. This initiative seeks to support innovative methods to produce predictive models of catalytic reactivity relevant to hydrogen energy processes. Theoretical methods have now been developed to the point that entire reaction pathways and reactivity trends can be predicted and understood. Close coupling between experimental observations and theory, modeling, and simulation will provide unprecedented capabilities to design more selective, robust, and defect-tolerant catalysts for hydrogen production, storage, and fuel cells. 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 nano-, meso- and macroscopic scales.

Solar-energy related research, specifically solar production of hydrogen and photocatalytic formation of fuels, is covered under a separate notice. Please see the Office of Science Financial Assistance Program Notice DE-FG02-06ER06-15, Basic Research for Solar Energy Utilization, http://www.science.doe.gov/grants/FAPN06-15.html.

Program Funding

It is anticipated that up to $12 million annually starting in Fiscal Year 2007 (subject to appropriations) will be available for multiple awards for this notice. Proposers may request project support for up to three years. All awards are contingent on the availability of funds and programmatic needs.

Preproposal

Each FFRDC may submit up to four preproposals as lead institution. The preproposal should consist of a description of the research proposed to be undertaken by the proposer and a clear explanation of its importance to the advancement of basic hydrogen research and its relevance to the HFI. The preproposal must be submitted electronically to hydrogen@science.doe.gov as two files:

(1) A cover page in Excel format downloadable from: http://www.science.doe.gov/bes/hydrogen_preapp_cover.xls. The information to be entered on the cover page worksheet includes: Program Announcement Number; Lead Principal Investigator name, address, email address, telephone number, and fax number; project title; selection of one submission category (see below); budget request for each project year; and total budget request for the project. On the worksheet named coPIs enter the names and institutions of all co-Principal Investigators and/or senior collaborators (excluding postdocs and graduate students). Please do not alter the overall format of the

cover- page Excel file, i.e., do not move or merge cells, as this will significantly slow the processing of the preproposal.

(2) A PDF file containing a narrative section not to exceed 3 pages (including text and figures) describing the research objectives, approaches to be taken, the institutional setting, and a description of any research partnership if appropriate. In addition, include brief, one-page, vitae from each Principal Investigator. As noted above, the preproposal must also identify the primary submission topic: (1) Novel Materials for Hydrogen Storage; or (2) Functional Membranes; or (3) Nanoscale Catalysts. The purpose of this self-identification into a research topic is solely for the purposes of grouping similar proposals for peer review.

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. 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 are to be prepared and submitted consistent with policies of the investigator's laboratory and the local DOE Operations Office. The instructions and format described below should be closely followed. Laboratories may submit proposals directly to the SC Program Office listed above. A copy should also be provided to the appropriate DOE Operations Office. Program Announcement LAB 06-17 must be referenced 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 evaluation criteria listed below 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 President'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. Federal and 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

3.1 Field Work Proposal (FWP) Format (Reference DOE O 412.1A) (DOE ONLY)
3.2 Proposal Cover Page
3.3 Proposal Abstract
3.4 Table of Contents
3.5 Management Plan

Sections 3.6-3.13 are to be completed for each subtask in the proposal.
Up to 4 tightly integrated subtasks are allowed in each proposal.
Multiple subtasks should be presented as follows:
First Subtask: Sections 3.6.1, 3.7.1,..., 3.12.1, 3.13.1
Second Subtask: Sections 3.6.2, 3.7.2, ..., 3.12.2, 3.13.2
.
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3.6 Subtask Title and Abstract
3.7 Budget and Budget Explanation
3.8 Narrative
3.9 Literature Cited
3.10 Other Support of Investigators and Collaborations
3.11 Biographical Sketches
3.12 Description of Facilities and Resources
3.13 Appendix (All appended material must be separate from the proposal, e.g., in electronic folders containing multiple PDF files of publications.)

2.1 How to Submit

A complete formal FWP in a single Portable Document Format (PDF) file must be submitted through the DOE ePMA system (https://epma.doe.gov) as an attachment. To identify that the FWP is responding to this program announcement, please fill in the following fields in the "ePMA Create Proposal Admin Information" screen as shown:

Proposal Short Name:
Fiscal Year:

Proposal Reason:
Program Announcement Number: Lab 06-17 *
Program announcement Title: Basic Research for the Hydrogen Fuel Initiative, DOE Research Program Announcement *
Proposal Purpose:
Estimated Proposal Begin Date:
HQ Program Manager Organization:

* Please use the wording shown when filling in these fields to identify that the FWP is responding to this Program Announcement.

In order to expedite the review process, please submit a CD and two copies of the proposal using the following, by U.S. Postal Service Express Mail, any commercial mail delivery service, or when hand-carried to:

U.S. Department of Energy
Office of Science
Office of Basic Energy Sciences, SC-22
19901 Germantown Road
Germantown, MD 20874-1290
ATTN: Program Announcement LAB 06-17

3. Detailed Contents of the Proposal

Proposals must be readily legible, when printed and must conform to the following 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.

Number pages consecutively at the bottom of each page throughout the document. Start each major section at the top of a new page with the section number and title, for example, "2.0 Table of Contents." Do not use unnumbered pages.

3.1 Field Work Proposal Format (Reference DOE O 412.1A) (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. The format described below should be closely followed. 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 (No special form is required.

Title of proposed project
FWP Number(s) corresponding to the proposed project (if available for new proposals)
BES Program announcement title: Basic Research for the Hydrogen Fuel Initiative
Name of laboratory
Name of principal investigator (PI) (one Lead PI only)
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

If other institutions are participating in the project, include a table listing institutions, lead investigator at each institution, and requested funding for each institution at this point on the cover page.

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 Proposal Abstract

Provide an abstract to convey an overall vision and the long-term goals and objectives of the proposed research. Describe what the specific research proposed is intended to accomplish, the approach to be taken, and the integration and synergy of the various subtasks. Discuss the potential scientific impact and significance of the proposed research. Indicate how the proposed research addresses the scientific/technical areas specifically described in the call. The maximum length for the abstract is one page.

3.4 Table of Contents

Provide the initial page number for each of the sections of the proposal.

3.5 Management Plan

The plan, up to 5 pages, needs to describe the overall strategy in developing and managing the proposed research program. Describe the overarching scientific goals that link the groups and researchers together. Include an overview of the functions and responsibilities of key personnel and the relationships among the subtasks. Clearly illustrate the integration, synergy, and coordination among the subtasks.

Describe any distinguishing strengths of conducting this particular research at your DOE laboratory, such as the synergisms among the investigators of a large interdisciplinary team; the ability to utilize unique DOE facilities at the laboratory; the benefits of collocation with researchers from other DOE programs; the ability to rapidly reconfigure your research thrust to respond to new challenges; and your successes at working with other research performers on transferring results to targeted research and development. Cite specific examples to illustrate such distinguishing strengths.

As appropriate for the research described in the proposal, describe the role of any advisory committee, executive committee, program committee, or their equivalent. Identify any plans for administering educational programs and outreach activities associated with the proposed research. Plans for administering shared facilities should be described under Section 3.12, Description of Facilities and Resources.

If the proposal consists of multiple subtasks, an overall budget summary should be provided here, which sums to the individual budgets for each subtask (see Section 3.7 for details)

Sections 3.6-3.13 are to be completed for each subtask in the proposal.
Up to 4 tightly coordinated subtasks are allowed in a proposal.
Multiple subtasks should be presented as follows:
First Subtask: Sections 3.6.1, 3.7.1,..., 3.12.1, 3.13.1
Second Subtask: Sections 3.6.2, 3.7.2, ..., 3.12.2, 3.13.2
.

3.6 Subtask Title and Abstract

Provide an abstract for the subtask that is no more than 250 words. No more than 4 subtasks are allowed in the proposal. Give the broad, long-term objectives and what the specific research proposed is intended to accomplish. Indicate how the proposed research addresses the BES scientific/technical area specifically described in the announcement.

3.7 Budget and Budget Explanation

A budget, conforming to the guidelines given below, is required for the entire project period, which normally will be three years, and for each Fiscal Year. You optionally may utilize DOE's budget page, Form 4620.1, for providing the equivalent budget information (Form 4620.1 is available at the following web site: http://www.science.doe.gov/grants/budgetform.pdf). Modifications of this form are permissible to comply with institutional practices. A written justification of each subtask 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 justification of the need for each item of permanent equipment. Budgets should also be provided for each research partner from a different institution who is funded under the FWP. Any other significant support received should be shown in Section 3.10.

> *Total Budget and Level of Effort*: Provide the total budget for the project, not counting equipment requests. List the names of the principal investigator and other key personnel and the estimated number of person-months or percentage of time for which DOE funding is requested. Proposers should list the number of postdoctoral associates and other professional positions included in the proposed work and indicate the number of full-time-equivalent (FTE) person-months. 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 their level of effort. The budget explanation should define concisely the role of each position in the overall project.

> *Equipment*: Provide the total equipment budget requested. 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 that 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.

3.8 Narrative

The narrative comprises the research plan for the FWP subtask. Each proposal is allowed up to four tightly coordinated subtasks. The narrative for each subtask should not exceed 15 pages. The majority of the narrative should address the *Proposed Work*. At the beginning of each subtask section, name the senior personnel who will participate, and state the proposed number of postdoctoral and undergraduate and graduate student participants. The narrative 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 that 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 BES. The section must 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_Performance_Measures.pdf. Describe the role and intellectual contribution of each senior researcher in the subtask, and briefly outline the resources available or planned to accomplish the research goals. The need for a collaborative/laboratory approach involving several investigators and the means of achieving this should be clearly established. Include references to relevant published literature, both to work of the investigators and to work done by other researchers.

***Preliminary Studies (Optional)*:** 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. Copies of such publications or manuscripts may be included in the Appendix (Section 3.13).

***Proposed Work*:** This section should constitute the major portion of the narrative, and should reflect a well-integrated vision for the project. A clear statement of the work to be undertaken is needed and must include: objectives for the period of the proposed work and expected significance; relation to longer-term goals of the project; and relation to the present state of knowledge in the field, to work in progress by the PIs under other support and to work in progress elsewhere. The Proposed Work should outline the general plan of the proposed work, including the broad design of activities to be undertaken, and, where appropriate, provide a clear description of experimental methods and procedures needed to accomplish the Proposed Work. In addition, it should describe new techniques and methodologies and explain their advantages over what currently exists.

***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."

3.9 Literature Cited

List all references cited in the narrative, including titles. 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.

3.10 Other Support of Investigators and Collaborations

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 significant levels of active and pending other support is required for all 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, level of effort devoted to the project, and a one paragraph scope statement for each such project.

Describe any proposed interactions and collaborations with other institutions and sectors, such as universities, other national laboratories, and industrial institutions. Define the goals of the collaboration, and describe the planned activities. Describe the roles of the senior participants, the mechanisms planned to stimulate and facilitate knowledge transfer, and the potential long-term impact of the collaborations.

3.11 Biographical Sketches

This information is required for each senior personnel at the laboratory submitting the proposal and at all subcontracting institutions. Provide concise vitae, listing professional and academic essentials and complete contact information. List up to ten publications most pertinent to the research. Reference to the information already provided in Section 3.9 may be appropriate. This portion of the biographical sketches is limited to a maximum of two pages for each investigator.

Each biographical sketch should also include the following information on collaborators and other affiliations to help identify potential conflicts or bias in the selection of reviewers:

> ***Collaborators*:** A list of all persons in alphabetical order (including their current organizational affiliations) who are currently or who have been collaborators or co-authors with the individual on a project, book, article, report, abstract or paper during the 48 months preceding the submission of this proposal. Include collaborators on this proposal. If there are no collaborators, this should be so indicated.
>
> ***Graduate and Postdoctoral Advisors*:** A list of the names of the individual's own graduate advisor(s) and principal postdoctoral sponsor(s), and their current organizational affiliations.
>
> ***Thesis Advisor and Postgraduate-Scholar Sponsor*:** A list of all persons (including their organizational affiliations), over the last five years with whom the individual has had an association as thesis advisor or postgraduate-scholar sponsor. The total number of graduate students advised and postdoctoral scholars sponsored also must be identified.

3.12 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. Describe any shared facilities and infrastructure to be established, including specific major instrumentation, and plans for the development of instrumentation. Describe plans for maintaining and operating new facilities, including staffing, and plans for ensuring access to outside users. Distinguish clearly between existing facilities and those still to be acquired or developed.

3.13 Appendix

All appended material must be submitted as separate PDF files from the proposal PDF file, e.g., in electronic folders containing multiple PDF files of publications. However, reviewers are not required to consider information in the Appendix. Do not use the appendix to circumvent the page limitations of the proposal. Reviewers may not have time to read extensive appendix materials with the same care as they will read the proposal proper. Only information that may not be easily accessible to a reviewer should be included, such as publications in print or manuscripts accepted for publication. The appendix may also include letters from investigators at other institutions stating their agreement to *participate* in the project. Do not include letters of endorsement of the project.

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. Travel funds to attend this meeting must be appropriately budgeted.