Office of Science
Notice DE-FG02-06ER06-15

Basic Research for Solar Energy Utilization

A change was made to this Notice on April 19, 2006. A new requirement was added, see the red text in the second Formal Application section.

U.S. Department of Energy

Office of Science Financial Assistance Program Notice
DE-FG02-06ER06-15: Basic Research for Solar Energy Utilization

AGENCY: U.S. Department of Energy
Office of Science

ACTION: Notice inviting grant applications.

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 applications for basic research in the area of solar energy utilization. This Notice solicits innovative basic research applications to establish the scientific basis that underpins the efficient *capture, conversion, and utilization* of solar energy in a cost-effective manner. We seek to support outstanding fundamental research programs that will lead to key discoveries and conceptual breakthroughs to make sunlight as the practicable solution to meet our compelling need for clean, abundant sources of energy.

DATES: Potential applicants are **REQUIRED** to submit a brief preapplication. Preapplications referencing Program Notice
DE-FG02-06ER06-15, must be received by DOE by 4:30 p.m., Eastern Time, June 5, 2006. Preapplications 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 preapplications encouraging or discouraging formal applications will be communicated to the applicants by August 11, 2006. **Complete guidance on the content and format of the preapplication is provided in the SUPPLEMENTARY INFORMATION section below.**

Only those preapplicants that receive notification from DOE encouraging a formal application may submit a formal application. **No other formal applications will be considered.** Formal applications submitted in response to this notice must be received by 8:00 p.m., Eastern Time November 14, 2006.

ADDRESSES: Preapplications referencing Program Notice
DE-FG02-06ER06-15 should be sent as an Excel and PDF file attachments via e-mail to:

solarenergy@science.doe.gov with "DE-FG02-06ER06-15" as the subject. No FAX or mail submission of preapplications will be accepted. **Do not submit preapplications via grants.gov.**

Formal Applications

This section pertains only to those applications that have been encouraged to submit a full proposal. Applications submitted to the Office of Science must be submitted electronically through Grants.Gov to be considered for award. The Funding Opportunity Number is: DE-FG02-06ER06-15 and the CFDA Number for the Office of Science is: 81.049. Instructions and forms are available on the Grants.gov website. Please see the information below and also refer to the "Funding Opportunity Announcement", Part IV - Application and Submission Information; H. Other Submission and Registration Requirements for more specific guidance on "Where to Submit" and "Registration Requirements." If you experience problems when submitting your application to Grants.gov, please visit their customer support website: http://www.grants.gov/CustomerSupport; email: support@grants.gov; or call 1-800-518-4726.

Registration Requirements: There are several one-time actions you must complete in order to submit an application through Grants.gov (e.g., obtain a Dun and Bradstreet Data Universal Numbering System (DUNS) number, register with the Central Contract Registry (CCR), register with the credential provider and register with Grants.Gov). See http://www.grants.gov/GetStarted. Use the Grants.gov Organization Registration Checklist to guide you through the process. Designating an E-Business Point of Contact (EBiz POC) and obtaining a special password called an MPIN are important steps in the CCR registration process. Applicants, who are not registered with CCR and Grants.gov, should allow at least 14 days to complete these requirements. It is suggested that the process be started as soon as possible.

VERY IMPORTANT - Download PureEdge Viewer: In order to download the application package, you will need to install PureEdge Viewer. This small, free program will allow you to access, complete, and submit applications electronically and securely. For a free version of the software, visit the following Web site: http://www.grants.gov/DownloadViewer.

FOR FURTHER INFORMATION CONTACT: Eric A. Rohlfing, Office of Basic Energy Sciences, Chemical Sciences, Geosciences and Biosciences Division, SC-22.1, telephone: (301)903-8165, E-mail: eric.rohlfing@science.doe.gov or Aravinda Kini, Office of Basic Energy Sciences, Materials Sciences and Engineering Division, SC-22.2, telephone: (301) 903-3565, E-mail: aravinda.kini@science.doe.gov.

SUPPLEMENTARY INFORMATION: In April 2005, BES sponsored a workshop to identify basic research needs for effective solar energy utilization. Over 200 workshop participants, from academia, national laboratories, government and industry in the US and abroad, critically assessed the state-of-the-art and limitations of current technologies for producing a significant fraction of our primary energy source from sunlight. The workshop report, entitled *Basic Research Needs for Solar Energy Utilization* (http://www.sc.doe.gov/bes/reports/files/SEU_rpt.pdf) detailed a broad array of key scientific challenges and research avenues to address these challenges. This Notice solicits innovative basic research proposals to establish the scientific basis that underpins the efficient *capture, conversion, and utilization* of solar energy in a cost-effective manner. We seek to support outstanding fundamental research programs that will lead to key discoveries and conceptual breakthroughs to make sunlight as the practicable solution to meet our compelling need for clean, abundant sources of energy. As in the workshop report, three broad areas that encompass many of the priority research directions will be the subject of this solicitation. They are:

1. **Solar to Electric Conversion**
2. **Solar Fuels Production**
3. **Solar Thermal Energy Utilization**

The following provides further information under each of these three areas to illustrate the scope of applications solicited under the Notice.

Solar to Electric Conversion

The challenge in converting sunlight to electricity via photovoltaic solar cells is to dramatically reduce the cost/watt of delivered solar electricity by dramatically improving the conversion efficiency. Devices that operate above the existing performance limit will require the discovery of new materials and new pathways for solar to electric conversion. Revolutionary approaches will be needed to minimize thermalization and recombination of photo-generated carriers. These breakthroughs will come from a broad range of research activities in both materials and topologies, which includes research in single- crystal, polycrystalline, amorphous, and nanostructured inorganic and organic materials; an understanding of the electronic structure of these materials; and their implementation in single and multiple junction solar cells. These cells could potentially take advantage of optical frequency shifting, multiple exciton generation, and hot carrier generation. Basic research is essential for identifying new materials and processes to make efficient solar generated electricity a reality. High priority research directions include:

- ***New concepts in solar electric conversion.*** Nano-structured architectures that can efficiently absorb the full spectrum of wavelengths in solar radiation offer the potential to revolutionize the technology used to produce solar electricity. New phenomena, such as multiple exciton generation offer the potential for photovoltaic (PV) cells to go beyond the Shockley-Queisser limit. Structures that are defect tolerant or have the capability to self repair are desired. The use of these materials in multiple junction cells can lead to dramatic advances in PV conversion efficiencies. Advances in nanoscale characterization using electron, neutron, and x-ray scattering and spectroscopy and integration of these probes with studies of photo-induced charge separation and transport will be essential to understand the structure/property relationships in these materials.
- ***Organic and hybrid organic/inorganic conversion systems.*** The current state-of- the-art organic efficiency is considerably less than inorganic based systems. Significant challenges must be overcome to introduce novel cell designs and organic components that create highly efficient and durable solar cells. In order to make advances, the fundamental problems of light absorption and charge separation and transport in organic complexes must be addressed for the organic environment of these solar cells. To increase the operational understanding of these solar cells, new experimental approaches

will be needed to correlate the chemical and physical properties of the active components and layers with their performance in operating PV devices. The combination of organic and inorganic materials could also provide new opportunities for the fabrication of high efficiency PV cells. Many, but not all, of these hybrids are materials systems that, along with organic solar cells, contain complex interfaces e.g. organic metal and organic/semiconductor. The interfaces create additional challenges that require advanced molecular design and an understanding of electronic interactions at an organic/inorganic interface.

- ***Photoelectrochemical solar cells.*** The photoelectrochemical configuration of photo-excited semiconductor with a redox medium is simple in form and fabrication, but the exploitation of photoelectrochemical cells for electrical power production awaits breakthrough advances in photoelectrode lifetimes and the employment of novel, low-cost solids and electrolytes. Breakthroughs in combinations of sensitizers and redox couples are needed to move into higher solar conversion efficiencies. Enhanced absorption in the infra-red spectrum by sensitizing dyes and quantum dots will be necessary. It is also necessary to understand the relation between the efficacy of the regenerating agent and the configuration of the mesoporous semiconductor network. Novel mesoscopic electrode designs, derived from nanostructured and nanoporous solids, are also needed. New surface chemistries and unique designs for assembling these mesoporous solids at low temperatures are sought where the electrode retains a high conductivity. Highly ordered interdigitated passageways for charge transport may be possible as are self-assembled forms of these solid networks.
- ***Novel nanoscale and self-assembled materials.*** New techniques, tools, and design principles are needed to allow optimized, photovoltaic materials and photonic structures to be fabricated over large-area substrates. Studies of nucleation and growth of novel materials can involve kinetically or thermodynamically driven self-assembly of tailored building blocks, or they may rely upon construction of the active layers and devices using carefully controlled vapor or solution-based deposition methods.
- ***Theory, modeling, and simulation.*** Solar energy systems exploit complex and multi-scale phenomena associated with molecules, materials, and their interplay with the system architecture. New theoretical, modeling, and computational tools which span many decades in space, time and structure are required to guide and interpret experiment and assist in the design of molecules, materials and systems. Improved theory and methods for electron transfer and charge separation, excited- states, their properties and their potential energy surfaces need to be developed and validated. Enhanced capabilities for excited states must enable accurately predicted band-gaps, lifetimes and band offsets generally, but especially in materials that are realistic candidates for solar energy systems.

Solar Fuels Production

Because of the day/night variation of the solar resource, the practical use of solar energy faces two overarching technological challenges: economically converting sunlight into useful energy, and storing and dispatching that converted energy to end users in an economical, convenient form. There must be a means to cost-effectively convert this energy into forms useful for transportation, residential and industrial applications. The ability to use sunlight to produce CH4 or H2 from abundant, non-toxic resources such as CO2 and water would revolutionize the economical, environmentally sound production of fuels. There are two key challenges in cost-effective formation of solar fuels. One is to replicate the essential components of the photosynthetic machinery to store chemical energy outside of a natural organism or plant. The other is to construct entirely man-made chemical components that, as an assembly, absorb sunlight and convert the energy into chemical fuels such as CH4 and H2. Examples of topical areas in which innovative research is needed include:

- ***Natural photosynthetic systems.*** The resolution of fundamental structural design principles in natural photosynthesis provides a means to accelerate the discovery of synthetic architectures that embody mechanistic principles used in biology. Design principles must be established for known and new natural photosynthetic systems in order to maximize the efficiencies of solar energy capture, conversion, and storage and enable the assembly of efficient biomimetic systems. Meeting these challenges will involve the understanding and control of the weak intermolecular forces governing molecular assembly in natural photosynthesis as well as the determination of the rules that underlie the biological mechanisms for repair and photoprotection.
- ***Bioinspired molecular assemblies.*** The challenge in bioinspired systems is to use the principles and architectures found in natural photosynthetic systems to prepare molecular assemblies that integrate light absorption, charge separation, and transport in an effective way. This innovation will involve the construction of tailored environments, composed of polymers, membranes, and gels, for organization of the antenna and donor-acceptor reaction center components (smart matrices). Bioinspired molecular systems with a pathway for fuels production must couple these single photon events to multiple redox equivalents in order to accumulate photon-initiated redox equivalents at particular molecular site. A resolution of the structural and electronic dynamics will be required over the full time scale of energy capture and conversion, which will involve the use of ultrafast spectroscopies and atomic level microscopies as well as new, emerging methods for dynamic molecular structure determination. Advanced tools and techniques that are available (or being conceived) at DOE-BES supported synchrotron and neutron facilities and Nanoscale Science Research Centers may be useful in this regard.
- ***Defect tolerant and self-repairing conversion.*** To ensure that complex biomimetic systems maintain their efficiency over long lifetimes, it is necessary to understand the repair and photoprotection mechanisms in photosynthesis and to be able to translate these mechanisms into a structure and an operating mechanism for biomimetic photosystems. Within an artificial photosynthetic system, the structural features of the protein matrix provide for redundancy as well as enhanced stability of photoreactants. A challenging and general approach to self- repair will require the design of smart molecules that seek out damage sites within a modular artificial photosynthetic system, recognize the damage site, and execute a structural repair. This approach requires building into molecules the self- autonomous features that are common in biology, but have not yet been developed for non-living systems. These investigations may also impact the development of defect-tolerant organic and inorganic PV materials.
- ***Solar hydrogen production.*** Photoelectrochemical water splitting for hydrogen production represents an advanced alternative to combining PV cells with an electrolysis system. Discovery of photoelectrodes that have appropriate light absorption

characteristics, are stable in aqueous solutions, and possess catalytic activity for multi-electron reactions is essential to produce hydrogen. Combinatorial or high-throughput methods and advanced computational methods will be useful in this regard. Emphasis must also be placed on the configuration of discovered electrodes for optimal light absorption by use of visible-absorbing dyes, carrier collection and electrocatalysis by band gap engineering, and optimizing interfaces.

- ***Photocatalytic fuels formation.*** Practical solar fuel formation requires construction of catalytic systems for the formation of energy rich fuels, such as the reduction of CO2 to CH4. The performance of the current generation of catalysts is far from that required for a solar fuels production system of the desired breakthrough efficiency goals, so that development of a new generation of fuel-forming catalysts is necessary. All methods for producing solar fuels must involve coupling of photo-driven single electron steps with fuel forming multi- electron transfer processes. A greater understanding is required, therefore, of the mechanisms of complex coupled reactions, excited-state bond making and breaking processes, and proton-coupled electron transfer reactions. These events can also occur in catalytic reactions at interfaces and surfaces. Experimental efforts must be coupled with theoretical investigations of the rates and mechanisms of multi-electron/multi-atom transfer reactions. Discovery of highly efficient, non-noble metal catalysts is also highly desirable.
- ***Theory, modeling, and simulation.*** Significant theoretical challenges are raised by the complex nature of supramolecular assemblies with their varied host architectures and their relation to light-initiated electronic and nuclear dynamics in the photosystem. New, multi-scale theoretical/computational methods are critically needed to account for the complexities of excited-state energetics applied across multiple spatial length scales relevant to supramolecular structures within complex host architectures and on the range of time scales encompassing solar-energy capture, conversion, and storage. New theoretical methods are essential for establishing predictive methods to accelerate the design of efficient systems for solar fuels production.

Solar Thermal Energy Utilization

High efficiency thermoelectric and thermophotovoltaic converters coupled to solar concentrators have the potential to generate electricity with significant increase in conversion efficiency. Currently, terrestrial thermoelectric and thermophotovoltaic systems are based on combustion heat, with the novel area of solar-based thermoelectric and thermophotovoltaic being little explored. Fundamental research is needed in the following areas:

- ***Thermoelectrics.*** Thermoelectric materials that can independently reduce phonon transport without deteriorating electronic transport offer great promise in significant enhancement in thermoelectric conversion efficiency. Bulk materials that exhibit nanoscale sub-structure and nanocomposites may offer a revolutionary approach to achieving high performance thermoelectricity. A comprehensive understanding of the role of interfaces in low-dimensional systems is needed to provide theoretical guidance on designing new generations of thermoelectric materials with significant ZT enhancement through quantum- confinement effects. Novel theory, modeling and simulation efforts are especially sought to provide the theoretical framework to assist the design of advanced thermoelectric materials that decouple electron transport from phonon transport.

- ***Thermophotovoltaics.*** One of the major challenges of spectral control for thermophotovoltaics (TPV) system is given by the high operating temperatures. Metallic and dielectric materials with low diffusion rates and evaporation rates are needed. New device concepts should be explored, such as microgap TPV. Novel materials and approaches in photonic crystals, plasmonics, phonon-polariton interactions, and coherent thermal emission are sought to exploit the spectral design and control required in TPV systems.
- ***Thermal storage.*** Thermal storage materials require high latent heat density and sufficiently high thermal conductivity for enhanced thermal energy charge and discharge processes. Present thermal storage materials are limited by the lack of reversibility of structural transformations in extended solids. The unique characteristics of solid-solid structural transformations in nanoscale materials offer great promise in overcoming the barriers. Basic research is needed to develop a comprehensive understanding governing the hysteresis and kinetics of the structural transitions in nanoscale materials with the goal of designing thermal storage materials and transitions that will perform under the appropriate conditions for solar thermal applications.

Program Funding

It is anticipated that up to $20 million annually will be available for multiple awards for this notice. Initial awards will be in Fiscal Year 2007, and applications may request project support for up to three years. All awards are contingent on the availability of funds and programmatic needs.

Preapplication

The preapplication should consist of a description of the research proposed to be undertaken by the applicant and a clear explanation of its relevance and impact on improved utilization of solar energy. The preapplication must be submitted electronically to solarenergy@science.doe.gov as two files:

(1) A cover page in Excel format downloadable from: http://www.science.doe.gov/bes/Solar_preapp_cover.xls. The information to be entered on the cover page includes: Program Announcement Number; Lead Principal Investigator name, address, email address, telephone number, and fax number; project title; name and institution of all co-Principal Investigators and/or senior collaborators (excluding postdocs and graduate students); selection of one primary and multiple secondary submission categories (see below); budget request for each project year; and total budget request for the project. 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 preapplication.

(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; and brief, one-page, vitae for each Principal Investigator.

As noted above, the preapplication must identify primary and secondary submission categories for the purposes of appropriate peer review. Applicants should identify their preapplication by indicating the number and title of the primary and secondary submission categories on the cover page. The submission categories are:

Solar Research Submission Categories:

1. **New concepts in solar electric conversion**
2. **Organic and hybrid organic/inorganic conversion systems**
3. **Photoelectrochemical solar cells**
4. **Natural photosynthetic systems**
5. **Bioinspired molecular assemblies**
6. **Defect tolerant and self-repairing conversion**
7. **Solar hydrogen production**
8. **Photocatalytic fuels formation**
9. **Solar thermal energy utilization**
10. **Novel nanoscale and self-assembled materials**
11. **Theory, modeling, and simulation**

Each preapplication must indicate a single primary research category from among this list; the applicant(s) may also check any number of secondary research areas.

The purpose of this self-identification into research categories is solely for the purposes of grouping like proposals for peer review.

Formal Application

The Department of Energy will accept Formal Applications by invitation only, based upon the evaluation of the preapplications. After receiving notification from DOE concerning successful preapplications, applicants may prepare formal applications. The Project Description must not exceed 20 pages, including tables and figures, but exclusive of attachments. The application must 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.

The application must contain an abstract or project summary, short vitae, and letters of intent from collaborators if appropriate. DOE is under no obligation to pay for any costs associated with the preparation or submission of applications.

Merit Review

Applications will be subjected to scientific merit review (peer review) and will be evaluated against the following evaluation criteria listed in descending order of importance as codified at 10 CFR Part 605.10 (d):

1. Scientific and/or Technical Merit of the Project,
2. Appropriateness of the Proposed Method of Approach,
3. Competency of Applicant's Personnel and Adequacy or Proposed Resources,
4. Reasonableness and Appropriateness of the Proposed Budget, and
5. Basic research that is relevant to improved utilization of solar energy.

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 an application constitutes agreement that this is acceptable to the investigator(s) and the submitting institution.

Submission Information

Other information about the development and submission of applications, eligibility, limitations, evaluation, selection process, and other policies and procedures including detailed procedures for submitting applications from multi-institution partnerships may be found in 10 CFR Part 605, and in the Application Guide for the Office of Science Financial Assistance Program. Electronic access to the Guide and required forms is made available at: http://www.science.doe.gov/grants/grants.html.

The Catalog of Federal Domestic Assistance (CFDA) number for this program is 81.049, and the solicitation control number is ERFAP 10 CFR Part 605.

Martin Rubinstein
Director
Grants and Contracts Division
Office of Science

Posted on the Office of Science Grants and Contracts Web Site
March 21, 2006.