Office of Science
Financial Assistance
Funding Opportunity Announcement
DE-PS02-07ER07-04

Basic Research
for Advanced Nuclear Energy Systems

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 strengthen 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 grant applications for basic research for Advanced Nuclear Energy Systems. Areas of focus include understanding of nanoscale interactions under extreme conditions, mastering the behavior of actinides and of fission products, solution behavior under extreme conditions of radiation and temperature, and interfacial behavior under extreme environmental conditions. Research funded under this initiative will pursue breakthroughs in scientific understanding that will advance materials design, will improve characterization of materials and processes, will enhance chemical processes under the extreme conditions present in nuclear energy systems, and will extend interdisciplinary theory-modeling-simulation-experimentation methodology to surmount the existing scientific and technical barriers for nuclear energy systems of the future. More information on these focus areas is provided in the Supplementary Information section below.

Preapplications Required: November 22, 2006, 8:00 pm Eastern Time.

Preapplication. Potential applicants are **REQUIRED** to submit a brief preapplication containing the information specified below. Preapplications referencing Program Solicitation DE-PS02-07ER07-04, must be received by DOE by 8:00 pm, Eastern Time, November 22, 2006. An electronic acknowledgement of preapplication receipt will be sent to all preapplicants by December 4, 2006. If you receive no such acknowledgement, contact us after that date through nuclear@science.doe.gov. Preapplications will be reviewed for conformance with the guidelines presented and suitability in the technical areas specified in this solicitation. A response to the preapplications encouraging or discouraging formal applications will be communicated to the applicants by January 4, 2007.

Although lead principal investigators may submit more than one preapplication, no more than one formal application will be accepted per lead principal investigator. Only those preapplicants who receive notification from DOE encouraging a full application may submit a formal application. **No other formal applications will be considered.**

Formal Application Due Date: March 14, 2007, 8:00 pm Eastern Time

Applications must be submitted using Grants.gov, the Funding Opportunity Announcement can be found using the CFDA Number, 81.049 or the Funding Opportunity Announcement number, DE-PS02-07ER07-04. **Applicants must follow the instructions and use the forms provided on Grants.gov.**

PREAPPLICATION REVIEW AND CRITERIA

The preapplication must consist of a description of the research proposed to be undertaken by the applicant and a clear explanation of its importance to the advancement of basic advanced nuclear energy research and its relevance to the initiative. The preapplication must be submitted electronically to nuclear@science.doe.gov as two files:

(1) A cover page in Excel format downloadable from: http://www.science.doe.gov/bes/nuclear_preapp_cover.xls. The information to be entered on the cover page worksheet includes: Program Announcement Number (DE-PS02-07ER07-04); 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; total budget request for the project; and the names and institutions of all co-Principal Investigators and/or senior collaborators (excluding postdoctoral scientists and graduate students). 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 your preapplication.

(2) A PDF file containing a narrative section not to exceed 3 pages (including text, minimum font size 11, references, and figures) describing the research objectives, approaches to be taken, the institutional setting, and a description of any research partnership if applicable. In addition, include a brief, one-page, curriculum vita from each Principal Investigator.

As noted above, the preapplication must also identify the primary submission topic:

(1) Understanding nanoscale interactions under extreme conditions
(2) Mastering the behavior of actinides and fission products
(3) Solution behavior under extreme conditions of radiation and temperature
(4) Interfacial behavior under extreme environmental conditions

The purpose of this self-identification into a research topic is primarily for the purposes of grouping similar applications for peer review.

This section pertains only to those preapplications that have been encouraged. Only one application per lead principal investigator will be accepted. The formal application should follow the preapplication with regard to scope and budget to the fullest extent possible.

Formal applications must contain a one-paragraph abstract or project summary. Each 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.science.doe.gov/bes/BES_PART_Performance_Measures.pdf.

Applications may be submitted with co-investigators from more than one academic institution; questions may be directed to one of the persons named below. If an Federally Funded Research and Development Center (FFRDC) collaboration is proposed by an applicant, the budget for personnel requested from the FFRDC should not exceed 25% of the overall budget. Budgets should include an estimate for travel to one contractors' meeting each year.

For Further Information Contact:
Dr. Lester Morss, Chemical Sciences, Geosciences and Biosciences Division, SC-22.1, telephone: 301-903-9311, e-mail: lester.morss@science.doe.gov or Dr. Tim Fitzsimmons, Materials Sciences and Engineering Division, SC-22.2, telephone: 301-903-9830, e-mail: tim.fitzsimmons@science.doe.gov.

Supplementary Information:
A workshop was held July 31-August 3, 2006 by the Office of Basic Energy Sciences to identify basic research needs for advanced nuclear energy systems. The workshop report, entitled *Basic Research Needs for Advanced Nuclear Energy Systems* http://www.science.doe.gov/bes/reports/files/ANES_rpt.pdf, detailed scientific grand challenges and a broad array of priority research directions. These challenges depicted the gap between present- day scientific knowledge/technology capabilities and what would be required for the practical realization of advanced closed-cycle nuclear reactors. The workshop report is a current source of information and summarizes the interests of BES.

This Notice solicits innovative basic research applications to significantly strengthen the scientific basis that will allow comprehensive understanding of the physical and chemical processes that lead to reliable, affordable and clean nuclear energy, 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 these broad areas:

(1) Understanding nanoscale interactions under extreme conditions
(2) Mastering the behavior of actinides and of fission products
(3) Solution behavior under extreme conditions of radiation and temperature
(4) Interfacial behavior under extreme environmental conditions

The following topics exemplify, but do not provide an exclusive listing of, areas where advances in fundamental understanding are required.

1. Understanding nanoscale interactions under extreme conditions

Nanoscale design of materials and interfaces that radically extend performance limits in extreme radiation environments

Understanding the interaction of defects with nanostructures, and controlling defect behavior, can facilitate the design of materials and interfaces that mitigate radiation damage. New research is needed in the design and synthesis of tailored nanostructured materials. Nanoscale

characterization and time-resolved study of interactions are needed to control behavior such as defect production and trapping under extreme conditions.

Developing and verifying a first-principles, multiscale description of properties in complex materials under extreme conditions

The predictive understanding of microstructural evolution and property changes under extreme conditions is essential for the design of structural materials, nuclear fuels, and wasteforms. A first-principles understanding of the relationship of defect properties and microstructural evolution to mechanical behavior and phase stability must be developed. This will require a closely coupled approach of *in situ* studies of nanoscale and mechanical behavior with multiscale theory.

2. Mastering the behavior of actinides and fission products

Behavior of actinide-bearing materials

A robust theory of the electronic structure of actinides will provide an improved understanding of their physical and chemical properties and behavior, leading to opportunities for advances in fuels and waste forms. Advances are needed in the application of new electronic structure methods for f-element-containing molecules and solids to calculate the properties of defects in multi-component systems, and in the fundamental understanding of related chemical and physical properties at high temperature. Advances in basic science of 4f- and 5f-electron systems in solutions will extend understanding of reaction chemistry in order to improve separations technologies.

Understanding and designing new molecular systems to gain unprecedented control of chemical selectivity during reprocessing

Innovations in chemical selectivity in multicomponent separations matrices require the design, synthesis, and optimization of molecular systems to trap and release target molecules and ions efficiently and economically. The bonding, reactivity, and mechanisms of molecular and nanophase separations systems must be modeled by computation and characterized by macroscopic thermodynamic and kinetics measurements and by microscopic techniques such as electronic and X-ray spectroscopy.

Mastering actinide and fission product chemistry under all conditions

A more accurate understanding of the electronic structure of the complexes of actinide and fission products will expand our ability to predict their behavior quantitatively under conditions relevant to all stages in fuel reprocessing (separations, dissolution, and stabilization of waste forms) and in new media that are proposed for advanced processing systems. This knowledge must be supplemented by accurate prediction and manipulation of solvent properties and chemical reactivities in nontraditional separation systems such as modern "tunable" solvent systems. This will require quantitative, fundamental understanding of the mechanisms of solvent tunability, the factors limiting control over solvent properties, the forces driving chemical speciation, and modes of controlling reactions.

Exploiting organization to achieve selectivity at multiple length scales

Harnessing the complexity of organization that occurs at the mesoscale in solution will lead to new separation systems that provide for greatly increased selectivity in recovery of target species and reduce formation of secondary waste streams through ligand degradation. Research directions include design of ligands and other selectivity agents, expanding the range of selection/release mechanisms, fundamental understanding of phase phenomena and self-assembly in separations, and aqueous separations systems.

Understanding fundamental thermodynamics and kinetic processes in multi-component systems

The behavior of the minor actinides is a significant challenge that requires a fundamental understanding of the thermodynamics, transport, and chemical behavior of complex materials. Global thermochemical models of complex phases that are informed by ab initio calculations of materials properties and high-throughput predictive models of complex transport and phase segregation will be required for full fuel fabrication calculations. These models, when coupled with appropriate experimental efforts, will lead to significantly improved fuel performance by creating novel tailored fuel forms.

3. Solution behavior under extreme conditions of radiation and temperature

Fundamental effects of radiation and radiolysis in chemical processes

The reprocessing of nuclear fuel and the storage of nuclear waste present an environment that includes substantial radiation fields. A predictive understanding of the chemical processes resulting from intense radiation, high temperatures, and extremes of acidity and redox potential on chemical speciation is required to enhance efficient, targeted separations processes and effective storage of nuclear waste. In particular, the effect of radiation on the chemistries of ligands, ionic liquids, polymers, and molten salts is poorly understood. There is a need for an improved understanding of the fundamental processes that affect the formation of radicals and ultimately control the accumulation of radiation-induced damage to separation systems.

4. Interfacial behavior under extreme environmental conditions

Exploiting organization to achieve selectivity at multiple length scales

Control of mesoscale complexity in solution or at interfaces will lead to new separation systems that provide for greatly increased selectivity in recovery of target species and reduce formation of secondary waste streams through ligand degradation. Research directions include design of ligands and other selectivity agents, expanding the range of selection/release mechanisms, fundamental understanding of phase phenomena and self-assembly in separations, and aqueous separations systems.

Adaptive material-environment interfaces for extreme conditions

Revolutionary advances in the understanding of interfacial behavior through new modeling and *in situ* experimental techniques are needed to support the control of interfaces that can provide dynamic stability over a wide range of conditions and with much greater "self-healing"

capabilities. Achieving the necessary scientific advances will require moving beyond interfacial chemistry and physics in ultra high vacuum environments to the development of *in situ* techniques to monitor the processes at fluid/solid and solid/solid interfaces under conditions of high pressure and temperature, and harsh environments.

Predictive multiscale modeling of materials and chemical phenomena in multi-component systems under extreme conditions

The advent of large-scale simulations will significantly enhance the prospect of probing important molecular-level mechanisms underlying the macroscopic phenomena of solution and interfacial behavior in actinide-bearing systems and structural components, performance and failure under extreme conditions. There is an urgent need to develop multiscale algorithms capable of efficiently treating systems whose time evolution is controlled by activated processes and rare events.

The workshop report provides further information under each of the focus areas to illustrate the scope of proposals that are solicited under this Notice. In particular, section II of the workshop describes scientific grand challenges and section IV lists priority research directions and scientific challenges.

Posted on the Office of Science Grants and Contracts Web Site
October 12, 2006.