

Program Announcement To DOE National Laboratories LAB 03-16

Catalysis Science

SUMMARY: The Office of Basic Energy Sciences (BES) of the Office of Science (SC), U. S. Department of Energy (DOE), hereby announces its interest in receiving proposals for high-risk, long-term, multi-investigator, multidisciplinary research on the science of catalysis. See Supplementary Information below for specific guidelines. The goal of the Catalysis Science research effort is to develop multidisciplinary approaches to enable molecular-level understanding of catalytic reaction mechanisms, ultimately enabling the prediction of catalytic reactivity spanning multiple time and length scales. Strongly encouraged are: (a) proposals containing synergistic integration of physical, chemical, and/or biochemical experimentation with solid state and molecular reactivity theories; (b) proposals that integrate atomistic design of catalytically active sites; molecular, supramolecular or solid-state synthesis; and in-situ, time- and space-resolved, spectroscopy and microscopy; (c) proposals to identify mechanisms and principles common to homogeneous, heterogeneous, and bio catalysis for the purpose of advancing the understanding of catalysis and developing novel chemical or physical functionalities; and (d) proposals to understand and manage catalyst complexity arising from the combination of diverse functionalities, namely chemical, biological, electronic, optical, magnetic, mechanical, thermal, etc. University investigators collaborating with FFRDC investigators should refer to the complementary request for applications announced under: <http://www.sc.doe.gov/production/grants/Fr03-16.html>.

DATES: Letters of intent are required and must include the information specified under Proposal Guidelines, and must be submitted by 4:30 p.m., E.S.T., February 5, 2003.

Full proposals must be preceded by the letters of intent and must be submitted by 4:30 p.m., E.S.T., March 26, 2003, in order to be accepted for merit review and consideration for award during Fiscal Year 2003.

ADDRESSES: Letters of intent must be sent as email attachment in PDF format to Drs. Raul Miranda (raul.miranda@science.doe.gov) and William Millman (william.millman@science.doe.gov).

Formal proposals, referencing Program Announcement LAB 03-16, must be submitted as PDF files on a CD accompanying a printed original of the proposal and seven copies and sent to: U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, Chemical Sciences, Geosciences, and Biosciences Division, SC-14/Germantown Building, 1000 Independence Avenue, SW, Washington, D.C. 20585-1290, ATTN: Program Announcement LAB 03-16.

When submitting proposals by U.S. Postal Service Express Mail, any commercial mail delivery service, or when hand carried by the researcher, the following address must be used: U.S.

Department of Energy, Office of Science, Office of Basic Energy Sciences, Chemical Sciences, Geosciences, and Biosciences Division, SC-14, 19901 Germantown Road, Germantown, MD 20874-1290, ATTN: Program Announcement LAB 03-16.

FOR FURTHER INFORMATION CONTACT: Dr. Raul Miranda by telephone at: (301) 903-8014, or Dr. William Millman at: (301) 903-5805, or at the E-mail addresses mentioned above, or by mail at U.S. Department of Energy, Office of Science, SC-14/Germantown Building, 1000 Independence Avenue, S.W., Washington, DC 20585-1290.

SUPPLEMENTARY INFORMATION:

General and Particular Goals of this Announcement

The general goals of the Catalysis Science research effort at the Office of Basic Energy Sciences are the following: (1) attain a fundamental scientific understanding of catalytic reactivity of molecular, supramolecular or nanoscale, and condensed matter; (2) acquire basic knowledge of the structural, dynamic, and electronic aspects of multi-atom assemblies that are associated with materials undergoing chemical transformations and converting or transferring energy or mass; and (3) develop the methodology and tools to design and synthesize hard, soft (macromolecular and biological), and hybrid materials at the atomic level to achieve controlled reactivity, multi- functionality, and time-dependent behavior.

The particular goal of the Catalysis Science effort is to dramatically accelerate the development of a predictive science of chemical catalysis by means of appropriate theoretical and experimental collaborations. To that end, focused and joint activities among complementary scientists and engineers will be supported to discover structure-property relationships and set the foundations for comprehensive theories of catalyst reactivity and time-dependent behavior. Consequently, support will be given for the use of advanced experimental and theoretical tools, as well as the development of new synthetic, spectroscopic, structural, theoretical and information management tools, for achieving systematic probing and exacting control of structure-reactivity relationships.

Expected Long-Term Impact of the Research Funded under this Announcement

The fundamental understanding sought with this research should, in the long term, lead to novel molecular or nanoscale constructs endowed with designed chemical reactivity. As catalysts, such materials should possess, by definition, the ability to direct chemical transformations quickly, selectively, and repeatedly, toward desired sets of products, without themselves suffering degradation. To convert selected species that may be components of complex mixtures, future catalysts will also possess enzyme-like reactant specificity and chemo-, regio- and stereo- selectivity. Acting in environments with various types of heterogeneity, future synthetic catalysts will be self-adaptive or externally controllable, by incorporating both sensing and acting functionalities in the same structure. Future catalysts will have self-healing capabilities in order to reverse degradation and prevent deactivation. They might be tunable to absorb energy in specific spectral ranges and deliver such energy to selected chemical bonds. These complex structures will efficiently convert currently intractable fossil and renewable feedstocks into clean fuels, chemical commodities, fine chemicals

and special materials. They will also dramatically purify our environment, protect our security, balance our body chemistry, and impact a number of industries: power, food, transportation, electronics, housing, etc. The objective of this research effort is to develop fundamental scientific understanding of the physicochemical mechanisms and discovery of the principles that will allow the design and controlled synthesis of the catalysts that will achieve this vision.

Emphasis on Research Teams

Note: Single investigators wishing to submit a proposal in response to the goals stated in this announcement should contact an appropriate program manager in the Office of Basic Energy Sciences. See above for contact information.

Proposals are sought from multi-investigator teams that focus on the creation of new approaches to research in catalysis. Thus, proposals that present novel approaches to integrating or coordinating the various aspects of catalysis (heterogeneous, homogeneous and biological) are particularly encouraged, as are proposals that integrate advanced experimental techniques, synthetic methodology, and theory and modeling. Participation by investigators who are new to catalysis science research is strongly encouraged.

In particular, this announcement targets imaginative multidisciplinary research efforts coordinating some or all of the following disciplines: chemistry, biology, physics, materials science, engineering; molecular and solid state synthesis, structural and spectroscopic instrumentation, reaction mechanisms and dynamics; chemical and materials theory, applied mathematics, information science and computation. The proposal should describe how that coordination may lead to a predictive science of catalysis.

Researchers are invited, but not required, to partner with multiple institutions: universities, DOE National Laboratories (FFRDCs) and Nanoscale Science Research Centers, when appropriate and necessary for the intellectual and operational benefit of the collaboration. Proposals must include a management plan describing the intellectual responsibility of each investigator and how each of them is essential to achieving the overall project milestones (see Proposal Guidelines for detailed instructions.)

In FFRDC-led multi-institutional proposals, the leading FFRDC must submit the original proposal, including separate and detailed budgets from each institution. A guide for submitting a collaborative proposal with researchers in other institutions, such as universities, non-profit organizations, for-profit commercial organizations, Federal agencies and DOE National Laboratories (FFRDCs) can be accessed via the web at: <http://www.sc.doe.gov/production/grants/Colab.html>. International collaborations are also welcome, but the international partner will not receive funding under this announcement. Use of national and international user facilities is encouraged but not required. All projects will be evaluated using the same criteria, regardless of the submitting institution.

Program Funding

It is anticipated that up to \$4 million will be available for up to 4 new FWP awards during Fiscal

Year 2003, contingent upon the availability of appropriated funds. The FWP will be renewed yearly for up to three year, contingent upon the availability of appropriated funds, progress of the research, and continuing program needs. A new proposal will be peer-reviewed during the third year of the FWP and may result in either issuance of a renewed FWP award or complete termination of the FWP.

Merit Review

Proposals will be subjected to scientific merit review (peer review) and will be evaluated against the following criteria listed in descending order of importance (as specified under BES Merit Review Procedures for Projects at DOE Laboratories: <http://www.sc.doe.gov/production/bes/labreviews.pdf>):

1. Scientific and/or technical merit of the project;
2. Appropriateness of the proposed method or approach;
3. competency of researcher's personnel and adequacy of proposed resources; and
4. Reasonableness and appropriateness of the proposed budget.

In addition, proposals will be evaluated in terms of the organizational plan and the research coordination. The evaluation will also include program policy factors such as the relevance of the proposed research to the terms of the announcement and programmatic needs.

External peer reviewers will be selected with regard to both their scientific expertise and the absence of conflict of interest. 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.

Proposal Guidelines

Note: Each FFRDC is limited to only one proposal as leading institution. FFRDC investigators may appear as lead or co-investigator on only one university or FFRDC led proposal.

General information about the development and submission of proposals, limitations, evaluation, selection process, and other policies and procedures may be found in "Office of Basic Energy Sciences Guide for Preparation of Review Documents", with electronic access at http://www.sc.doe.gov/production/bes/Guide_for_Lab_Rev_Docs.pdf. The following special requirements also apply and supersede the general instructions.

The letter of intent should be brief and contain a project title, principal investigator/ project director, co-principal investigators, external collaborators not included in the budget, institutions involved, estimated total budget, purpose and innovative aspects of the research, and primary role of each principal investigator. The letters of intent are not binding and will be used by program managers exclusively for preliminary identification of potential peer reviewers, conflicts of interest, and duplications of effort.

The full proposal shall contain a research description limited to a maximum of 40 pages per proposal, including figures, tables, and previous results. It must also contain a research management and

coordination plan, limited to 10 pages. The proposal must have a short abstract focusing on the goals of the research and an executive summary that includes research methodology and coordination plan for the research team. Attachments must include a brief biography for each investigator and external collaborator; a listing of all current and pending federal, state, and private support for each investigator listed in the budget; and letters of commitment from external collaborators not included in the budget. The required page and font format are: 8.5 inch x 11 inch page size; 1 inch top, bottom and right margins; 1.25 inch left margin; single, 1.5 or double line spacing; 12 pt font size for text and appropriate fonts for equations and symbolic notation. DOE is under no obligation to pay for any costs associated with the preparation or submission of proposals.

The proposal must have the following ordered format:

- 01-** Cover page(s) with project title, names of project director and co-principal investigators and their affiliations. For Multi-institutional proposals, list the investigator names, their institutions, the yearly amount requested from each institution and the yearly total request.
- 02-** Table of contents
- 03-** Project abstract (400 word maximum)
- 04-** Executive summary (3 page maximum)
- 05-** Budget for each year and cumulative budget for three years (use form DOE F 4620.1) for the submitting institution.
- 06-** Budget explanation
- 07-** Research description (40 page maximum, including goals, background, research plan, previous results (if any), and research methodology)
- 08-** Research management and coordination plan (10 page maximum)
- 09-** References (including full titles)
- 10-** Biographical sketches (3 page maximum per principal investigator and external collaborator)
- 11-** Description of main facilities to be used in the research
- 12-** Current and pending support for each investigator listed in the budget(s)
- 13-** Letters of commitment from external collaborators
- 14-** Appendix 1 (For multi-institutional proposals see below): Field Work Proposal Format (DOE Order 5700.7C)
- 15-** Appendix 2 (For multi-institutional proposals only): combined budget sheets

Specific instructions for multi-institutional proposals led by a FFRDC:

The leading FFRDC project director/principal investigator is responsible for the management and coordination of the overall effort and for submitting the proposal. If the proposal were funded, each institution would receive a separate award and there would be no subcontracts. Therefore, each FFRDC must prepare and sign its own FWP Format (DOE Order 5700.7C), budget sheets and explanations (items 5-6 above) and/or each university must provide its own face page (DOE F 4650.2(10-92)), budget sheets, budget explanation and federal certification pages. On the FWP Format or face page, each institution should identify its principal investigator and specify its amount requested. The project director/principal investigator of the leading institution must submit the proposal using the following format: (item 1) cover page as described above; (items 2-15) body of the proposal including the leading institution's budget and explanation (items 5-6); (item 14)

Appendix 1, containing all original budgets, explanations and federal certification pages from the other institutions; and (item 15) Appendix 2, containing a spreadsheet that combines the budgets from the multiple institutions in an easily readable format.

Reference Program Announcement LAB 03-16 on all submissions and inquiries about this program. Formal proposals must be submitted as PDF files on a CD accompanying a printed original of the proposal and seven copies, and must be sent to the address provided above.