Office of Science
Notice 03-16

Catalysis Science

Department of Energy

Office of Science Financial Assistance Program Notice 03-16: Catalysis Science

AGENCY: U.S. Department of Energy

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), hereby announces its interest in receiving grant applications 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 combined experimental and theoretical approaches to enable molecular-level understanding of catalytic reaction mechanisms, ultimately enabling the prediction of catalytic reactivity at multiple time and length scales. Strongly encouraged are: (a) applications containing synergistic integration of physical, chemical, and/or biochemical experimentation with solid state and molecular reactivity theories; (b) applications 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) applications 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) applications to understand and manage catalyst complexity arising from the combination of diverse functionalities, namely chemical, biological, electronic, optical, magnetic, mechanical, thermal, etc. DOE National Laboratory investigators should refer to the complementary request for proposals announced under: http://www.sc.doe.gov/production/grants/grants.html.

DATES: Letters of intent are required and must include the information specified under Application Guidelines, and must be submitted by 4:30 p.m., E.S.T., February 5, 2003. Full applications 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 applications referencing Program Notice 03-16 must be sent electronically by an authorized institutional business official through DOE's Industry Interactive Procurement System (IIPS) at: http://e-center.doe.gov (see also http://www.sc.doe.gov/production/grants/grants.html.)

IIPS provides for the posting of solicitations and receipt of applications in a paperless environment via the Internet. In order to submit applications through IIPS your business official will need to register at the IIPS website. The Office of Science will include attachments as part of this notice that provide the appropriate forms in PDF fillable format that are to be submitted through IIPS. Color images should be submitted in IIPS as a separate file in PDF format and identified as such. These images should be kept to a minimum due to the limitations of reproducing them. They should be numbered and referred to in the body of the technical scientific application as Color image 1, Color image 2, etc. Questions regarding the operation of IIPS may be E-mailed to the IIPS Help Desk at: HelpDesk@pr.doe.gov or you may call the help desk at: (800) 683-0751. Further information on the use of IIPS by the Office of Science is available at: http://www.sc.doe.gov/production/grants/grants.html.

If you are unable to submit the application through IIPS, please contact the Grants and Contracts Division, Office of Science at: (301) 903-5212, in order to gain assistance for submission through IIPS or to receive special approval and instruction on how to submit printed applications.

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 Notice

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 Notice

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 an application in response to the goals stated in this notice should contact an appropriate program manager in the Office of Basic Energy Sciences. See above for contact information.

Applications are sought from multi-investigator teams that focus on the creation of new approaches to research in catalysis. Thus, applications that present novel approaches to integrating or coordinating the various aspects of catalysis (heterogeneous, homogeneous and biological) are particularly encouraged, as are applications 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 notice 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 application should describe how that coordination may lead to a predictive science of catalysis.

Applicants 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. Applications 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 Application Guidelines for detailed instructions.)

In multi-institutional applications, only the leading institution must submit the original application, including separate and detailed budgets from each institution. Research collaboration with DOE FFRDCs is welcome, but funds will be provided to these organizations under a separate notice (http://www.sc.doe.gov/production/grants/grants.html.) A guide for submitting a collaborative application with a national laboratory 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 notice. 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 6 new grant awards during Fiscal Year 2003, contingent upon the availability of appropriated funds. For this initial funding period, three-year grants are expected, also contingent upon the availability of appropriated funds, progress of the research, and continuing program need.

Merit Review

Applications will be subjected to scientific merit review (peer review) and will be evaluated against the following criteria listed in descending order of importance as codified at 10 CFR Part 605.10(d) (http://www.sc.doe.gov/production/grants/605index.html):

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

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

Application Guidelines

Note: Each university investigator is limited to only one application as either principal investigator/project director or co-principal investigator.

Information about the development and submission of applications, eligibility, limitations, evaluation, selection process, and other policies and procedures 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 available via the World Wide Web at:

http://www.sc.doe.gov/production/grants/grants.html. The application Face Page, form DOE F 4650.2, must contain the principal investigator/project director's name, institution, phone number, fax number, and E-mail address. Requests for three-year grants are expected. For multi-institutional applications, see further instructions below.

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 application shall contain a research description limited to a maximum of 40 pages per application, including figures, tables, and previous results. It must also contain a research management and coordination plan, limited to 10 pages. The application 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 applications.

The application must have the following ordered format:

01- Face page (DOE F 4650.2)
02- Table of contents
03- Project abstract (400 word maximum)
04- Executive summary (3 page maximum)
05- Budget for each year and cumulative budget (DOE F 4620.1)
06- Budget explanation
07- Cover page(s) with project title, names of project director and co-principal investigators and their affiliations. For multi-institutional applications, list the investigator names, their institutions, the yearly amount request from each institution and the yearly total request.
08- Research description (40 page maximum, including goals, background, research plan, previous results (if any), and research methodology)
09- Research management and coordination plan (10 page maximum)
10- References (including full titles)
11- Biographical sketches (3 page maximum per principal investigator and external collaborator)
12- Description of main facilities to be used in the research
13- Current and pending support for each investigator listed in the budget(s)
14- Letters of commitment from external collaborators
15- Federal certification pages for the submitting institution

16- Appendix 1 (For multi-institutional applications only): original signed pages
17- Appendix 2 (For multi-institutional applications only): combined budget sheets

Specific instructions for multi-institutional applications:

The leading institution project director/principal investigator is responsible for the management and coordination of the overall effort and for submitting the application. If the application were funded, each institution would receive a separate grant or contract and there would be no subcontracts. Therefore, each institution must prepare and sign its own face page (item 1 listed above), budget sheets and explanation (items 5-6 above) and federal certification pages (item 15 above). On the face page, each institution should identify its principal investigator and specify its amount request. The project director/principal investigator of the leading institution must electronically or otherwise submit the application using the following format: (item 1) leading institution face page citing the amount requested by the leading institution; (items 2-15) body of the application including the leading institution's budget and explanation (items 5-6); (item 16) Appendix 1, containing all original budgets, explanations and federal certification pages from the other institutions; and (item 17) Appendix 2, containing a spreadsheet that combines the budgets from the multiple institutions in an easily readable format.

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

John Rodney Clark
Associate Director of Science
for Resource Management

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