

Program Announcement To DOE National Laboratories LAB 99-13

Complex and Collective Phenomena

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 innovative research on the topic of complex and collective phenomena. Opportunities exist for research covering the entire range of disciplines supported by the BES program, including research in the materials sciences, chemical sciences, engineering sciences, geosciences and energy biosciences.

Much of the research supported by the BES program and its predecessor organizations during the past 50 years has been devoted to solving very difficult problems in idealized, simple systems. The challenge now is to use that knowledge to understand complex systems. This program will support work at the frontiers of basic research. Work is intended to be revolutionary rather than evolutionary, and it is expected that it may involve multidisciplinary and/or interdisciplinary efforts. Further it is expected to strengthen the basis for understanding complex and collective phenomena currently viewed from a single domain such as the atomic level (reductionist view) or continuum mechanics (classical view). The program is open to the entire range of disciplines supported by the BES program. Additional information on the BES Research Program is available at the following web site address:
<http://www.er.doe.gov/production/bes/bes.html>.

Some important categories of studies that might be included within the initiative in Complex and Collective Phenomena are:

Materials that are beyond binary; that lack stoichiometry; that are far from equilibrium; that have little or no symmetry or low dimensionality. Often desired properties and behaviors exist only in "non-ideal compounds," i.e., those that are made from more than a few elements, made in non-stoichiometric combinations, made far from equilibrium; or made in one or two dimensions. As examples, high-temperature superconductors are complex compounds of four or more elements that are not stoichiometric with respect to oxygen; the glassy metal state, which has many desirable properties, has no long range order or symmetry; and many interesting and useful properties exist in atomic and molecular arrangements that have only one or two dimensions, such as is found in thin films, membranes, and quantum dots. These classes of materials, which will dominate the next generation of energy technologies, pose new challenges and opportunities because of their complexity.

Functional synthesis. Although chemists routinely synthesize molecules to desired elemental composition and structure, the ability to predict structure/function relationships remains elusive. Because function can be exquisitely sensitive to even minor changes in both composition and structure and because the number of combinations is virtually boundless, we are unable to predict what combinations of elements and arrangements of atoms give rise to desired properties such as superconductivity, magnetism, ductility, toughness, strength, resistance, catalytic function, or enzymatic function.

The control of entropy. To a scientist, entropy has a precise mathematical definition; however, to a nonscientist, entropy can be viewed as synonymous with disorder. A standard maxim in physics is that "the entropy of the universe tends to increase," i.e., things become increasingly disordered with time. Interestingly, most of our energy now comes from fossil fuels that were derived from photosynthesis -- the ability of plants to reduce entropy locally by absorbing sunlight and converting carbon dioxide to lower-entropy hydrocarbons, polysaccharides, and other compounds. However, even though photosynthesis has been studied for decades, we still do not completely understand it nor have we been able to duplicate or improve on it. This one example of the control of entropy -- the ability to mimic the functions of plants -- remains one of the outstanding challenges in the natural sciences.

Phenomena beyond the independent particle approximation. Phenomena beyond the independent particle model -- that by their nature are collective -- challenge our understanding of the natural world and require major advances in theory, modeling, computing, and experiment. Collective phenomena include widely diverse phenomena in the gas and condensed phases, including Bose-Einstein condensation, high-temperature superconductivity, and electron correlation.

Scaling in space and time. Research in chemistry, materials, engineering, geosciences, and biosciences covers lengths from the atomic scale to the cellular scale to the hundreds of kilometers scale and times from femtoseconds to millennia. We understand single atoms, molecules, and pure crystals fairly well; but, when we go beyond these simple systems to larger more complex systems, our understanding is limited. The relationships between constituent and collective properties and behavior of systems over a wide range of spatial scales, and their response to processes operating over a wide range of time scales, are not well understood. Improving our understanding of phenomena over wide time scales -- from femtoseconds in spectroscopy to decades in the regulatory system of plants to thousands of years in radioactive waste disposal--and over spatial scales from atomic to geologic is important.

DATES: Proposers are strongly encouraged to submit a brief preproposal. All preproposals, referencing Program Announcement LAB 99-13, should be received by DOE by 4:30 P.M., E.S.T., March 2, 1999. A response to the preproposals encouraging or discouraging a formal proposal generally will be communicated to the proposer within 21 days of receipt.

The deadline for receipt of formal proposals submitted in response to this announcement must be received by 4:30 P.M., E.S.T., April 21, 1999, in order to be accepted for merit review and to permit timely consideration for award in Fiscal Year 1999.

ADDRESSES: All preproposals, referencing Program Announcement LAB 99-13, should be sent to Dr. Jerry J. Smith, Division of Materials Sciences, SC-13, Office of Science, U.S. Department of Energy, 19901 Germantown Road, Germantown MD 20874-1290.

Formal proposals referencing Program Announcement LAB 99-13 should be forwarded to: U.S. Department of Energy, Office of Science, Grants and Contracts Division, SC-64, 19901 Germantown Road, Germantown, Maryland 20874-1290, ATTN: Program Announcement LAB 99-13. This address must also be used when submitting proposals by U.S. Postal Service Express, any commercial mail delivery service, or when hand carried by the applicant.

FOR FURTHER INFORMATION CONTACT: For questions concerning research topics in specific technical areas, contact the following individuals in the appropriate division of interest:

Dr. Jerry J. Smith, Division of Materials Sciences, SC-13, Office of Science, U.S. Department of Energy, 19901 Germantown Road, Germantown, MD 20874-1290, telephone (301) 903-4269, e-mail: (jerry.smith@oer.doe.gov).

Dr. William S. Millman, Division of Chemical Sciences, SC-14, Office of Science, U.S. Department of Energy, 19901 Germantown Road, Germantown, MD 20874-1290, telephone (301) 903-5805, e-mail: (william.millman@oer.doe.gov).

Dr. James Tavares, Division of Energy Biosciences, SC-17, Office of Science, U.S. Department of Energy, 19901 Germantown Road, Germantown, MD 20874-1290, telephone (301) 903-6190, e-mail: (jim.tavares@oer.doe.gov).

Dr. Robert Price, Division of Engineering, SC-15, Office of Science, U.S. Department of Energy, 19901 Germantown Road, Germantown, MD 20874-1290, telephone (301) 903-3565, e-mail: (bob.price@oer.doe.gov).

Dr. Nick Woodward, Division of Geosciences, SC-15, Office of Science, U.S. Department of Energy, 19901 Germantown Road, Germantown, MD 20874-1290, telephone (301) 903-4061, e-mail: (nick.woodward@oer.doe.gov).

Program Funding

It is anticipated that an estimated \$1.5 million will be available for awards during FY 1999, contingent upon the availability of appropriated funds. Multiple year funding of awards is expected, also contingent upon the availability of appropriated funds, progress of the research and continuing program need.

Preproposals

A brief preproposal may be submitted. The preproposal should identify, on the cover sheet, the institution, principal investigator name, address, telephone, fax and e-mail address, title of the project, and the field of scientific research. The preproposal should consist of no more than a three page narrative describing the research project objectives and methods of accomplishment. These will be reviewed relative to the scope and research needs of the Complex and Collective Phenomena initiative.

Preproposals are strongly encouraged but not required prior to submission of a formal proposal. Please note that notification of a successful preproposal is not an indication that an award will be made in response to the formal proposal.

The instructions and format described below should be followed. Reference Program Announcement LAB 99-13 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 criteria which are listed 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

The evaluation will include program policy factors such as the relevance of the proposed research to the terms of the announcement, the uniqueness of the proposer's capabilities, and demonstrated usefulness of the research for proposals in other DOE Program Offices as evidenced by a history of programmatic support directly related to the proposed work.

2. Summary of Proposal Contents

- Field Work Proposal Format (Reference DOE Order 5700.7C) (DOE ONLY)
- Proposal Cover Page
- Table of Contents
- Abstract
- Narrative
- Literature Cited
- Budget and Budget Explanation
- Other support of investigators
- Biographical Sketches
- Description of facilities and resources
- Appendix

2.1 Number of Copies to Submit

An original and seven copies of the formal proposal/FWP must be submitted.

3. Detailed Contents of the Proposal

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

3.1 Field Work Proposal Format (Reference DOE Order 5700.7C) (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. 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

The following proposal cover page information may be placed on plain paper. No form is required.

Title of proposed project
SC Program announcement title
Name of laboratory
Name of principal investigator (PI)
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

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 Table of Contents

Provide the initial page number for each of the sections of the proposal. Number pages consecutively at the bottom of each page throughout the proposal. Start each major section at the top of a new page. Do not use unnumbered pages and do not use suffices, such as 5a, 5b.

3.4 Abstract

Provide an abstract of no more than 250 words. Give the broad, long-term objectives and what the specific research proposed is intended to accomplish. State the hypotheses to be tested. Indicate how the proposed research addresses the SC scientific/technical area specifically described in this announcement.

3.5 Narrative

The narrative comprises the research plan for the project and is limited to 25 pages. It 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 which 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 the Office of Science. Include references to relevant published literature, both to work of the investigators and to work done by other researchers.

Preliminary Studies: 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.

Research Design and Methods: Describe the research design and the procedures to be used to accomplish the specific aims of the project. Describe new techniques and methodologies and explain the advantages over existing techniques and methodologies. As part of this section, provide a tentative sequence or timetable for the project.

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".

3.6 Literature Cited

List all references cited in the narrative. 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.

3.7 Budget and Budget Explanation

A detailed budget is required for the entire project period, which normally will be three years, and for each fiscal year. It is preferred that DOE's budget page, Form 4620.1 be used for providing budget information*. Modifications of categories are permissible to comply with institutional practices, for example with regard to overhead costs.

A written justification of each budget item 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 detailed justification of the need for each item of permanent equipment. Explain each of the other direct costs in sufficient detail for reviewers to be able to judge the appropriateness of the amount requested.

Further instructions regarding the budget are given in section 4 of this guide.

* Form 4620.1 is available at web site:
<http://www.er.doe.gov/production/grants/forms.html>

3.8 Other Support of Investigators

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 active and pending other support is required for all senior 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, and level of effort devoted to the project.

3.9 Biographical Sketches

This information is required for senior personnel at the laboratory submitting the proposal and at all subcontracting institutions. The biographical sketch is limited to a maximum of two pages for each investigator.

3.10 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.

3.11 Appendix

Include collated sets of all appendix materials with each copy of the proposal. Do not use the appendix to circumvent the page limitations of the proposal. Information should be included that may not be easily accessible to a reviewer.

Reviewers are not required to consider information in the Appendix, only that in the body of the proposal. Reviewers may not have time to read extensive appendix materials with the same care as they will read the proposal proper.

The appendix may contain the following items: up to five publications, manuscripts (accepted for publication), abstracts, patents, or other printed materials directly relevant to this project, but not generally available to the scientific community; and letters from investigators at other institutions stating their agreement to participate in the project (do not include letters of endorsement of the project).

4. Detailed Instructions for the Budget (DOE Form 4620.1 "Budget Page" may be used)

4.1 Salaries and Wages

List the names of the principal investigator and other key personnel and the estimated number of person-months for which DOE funding is requested. Proposers should list the number of postdoctoral associates and other professional positions included in the proposal and indicate the number of full-time-equivalent (FTE) person-months and rate of pay (hourly, monthly or annually). 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 total salaries needed. Salaries

requested must be consistent with the institution's regular practices. The budget explanation should define concisely the role of each position in the overall project.

4.2 Equipment

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 \$5000 or more." Special purpose equipment means equipment which 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. General purpose office equipment normally will not be considered eligible for support.

4.3 Domestic Travel

The type and extent of travel and its relation to the research should be specified. Funds may be requested for attendance at meetings and conferences, other travel associated with the work and subsistence. In order to qualify for support, attendance at meetings or conferences must enhance the investigator's capability to perform the research, plan extensions of it, or disseminate its results. Consultant's travel costs also may be requested.

4.4 Foreign Travel

Foreign travel is any travel outside Canada and the United States and its territories and possessions. Foreign travel may be approved only if it is directly related to project objectives.

4.5 Other Direct Costs

The budget should itemize other anticipated direct costs not included under the headings above, including materials and supplies, publication costs, computer services, and consultant services (which are discussed below). Other examples are: aircraft rental, space rental at research establishments away from the institution, minor building alterations, service charges, and fabrication of equipment or systems not available off-the-shelf. Reference books and periodicals may be charged to the project only if they are specifically related to the research.

a. Materials and Supplies

The budget should indicate in general terms the type of required expendable materials and supplies with their estimated costs. The breakdown should be more detailed when the cost is substantial.

b. Publication Costs/Page Charges

The budget may request funds for the costs of preparing and publishing the results of research, including costs of reports, reprints page charges, or other journal costs (except costs for prior or early publication), and necessary illustrations.

c. Consultant Services

Anticipated consultant services should be justified and information furnished on each individual's expertise, primary organizational affiliation, daily compensation rate and number of days expected service. Consultant's travel costs should be listed separately under travel in the budget.

d. Computer Services

The cost of computer services, including computer-based retrieval of scientific and technical information, may be requested. A justification based on the established computer service rates should be included.

e. Subcontracts

Subcontracts should be listed so that they can be properly evaluated. There should be an anticipated cost and an explanation of that cost for each subcontract. The total amount of each subcontract should also appear as a budget item.

4.6 Indirect Costs

Explain the basis for each overhead and indirect cost. Include the current rates.