Office of Science
Notice 99-13

Complex and Collective Phenomena

Department of Energy
Office of Science

Office of Science Financial Assistance Program Notice 99-13; Complex and Collective Phenomena

Agency: U.S. Department of Energy

Action: Notice inviting research 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 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.

DATES: Potential applicants are strongly encouraged to submit a brief preapplication. All preapplications, referencing Program Notice 99-13, should be received by DOE by 4:30 P.M., E.S.T., March 2, 1999. A response to the preapplications encouraging or discouraging a formal application generally will be communicated to the applicant within 21 days of receipt.

The deadline for receipt of formal applications is 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 preapplications, referencing Program Notice 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 applications referencing Program Notice 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 Notice 99-13. This address must also be used when submitting applications 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).

SUPPLEMENTARY INFORMATION:

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.

Program Funding

It is anticipated that an estimated $1.5 million will be available for grant awards during FY 1999, contingent upon the availability of appropriated funds. Multiple year funding of grant awards is expected, also contingent upon the availability of appropriated funds, progress of the research and continuing program need. Applications received by the Office of Science, Office of Basic Energy Sciences, under its current competitive application mechanisms may be deemed appropriate for consideration under this notice and may be funded under this program.

Preapplications

A brief preapplication may be submitted. The preapplication 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 preapplication 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.

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

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 605.10(d).

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.

The evaluation will include program policy factors such as the relevance of the proposed research to the terms of the announcement and an agency's programmatic needs. Note, 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.

Applicants are encouraged to collaborate with researchers in other institutions, such as universities, industry, non-profit organizations, federal laboratories and Federally Funded Research and Development Centers (FFRDCs), including the DOE National Laboratories. A parallel announcement with a similar potential total amount of funds will be issued to DOE FFRDCs. All projects will be evaluated using the same criteria, regardless of the submitting institution.

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.er.doe.gov/production/grants/grants.html. On the grant face page, form DOE F 4650.2, block 15, provide the principal investigator's phone number, fax number and e-mail address. The research description must be 20 pages or less, exclusive of figure illustrations, and must contain an abstract or summary of the proposed research. Attachments include curriculum vitae, a listing of all current and pending federal support, and letters of intent when collaborations are part of the proposed research.

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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