National Science Foundation
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Arlington, Virginia 22230

NSF 13-026

Dear Colleague Letter - DMREF proposals to the Division of Mathematical Sciences in fiscal year 2013

December 3, 2012

The Division of Mathematical Sciences (DMS) of the National Science Foundation (NSF) is pleased to invite proposals in 2013 for the NSF activity Designing Materials to Revolutionize and Engineer our Future (DMREF). DMREF is part of NSF's second year of a national materials initiative entitled the Materials Genome Initiative for Global Competitiveness (MGI). (http://www.whitehouse.gov/sites/default/files/microsites/ostp/materials_genome_initiative-final.pdf) MGI recognizes the importance of materials science to the well-being and advancement of society and aims to "deploy advanced materials at least twice as fast as possible today, at a fraction of the cost." The MGI national initiative integrates all components in the continuum of materials design, including materials discovery, development, property optimization, systems design and optimization, certification, manufacturing, and deployment, with each employing the toolset that is being developed within the materials innovation infrastructure. The toolset will integrate synergistically advanced computational methods with data-enabled scientific discovery and innovative experimental techniques in such a manner as to revolutionize the approach to materials research and engineering.

DMREF comprises well-coordinated activities involving the Directorates of Mathematical and Physical Sciences, Engineering, and Computer & Information Science and Engineering. For further details and participating divisions please see the broadly aimed Dear Colleague Letter about DMREF in fiscal year 2013, posted for example on the MPS web page, NSF 13-025. As described in that Letter, success in the initiative requires a collaborative, synergistic, iterative approach that includes theory, computation, and experiments. This approach is the central principle of MGI. Consequently DMREF proposals may be reviewed jointly with divisions other than the one to which the proposal is submitted. Commonality of aims, of MGI principles, and of submission dates will facilitate joint review where appropriate. This is intended to make it easier for different disciplines to join in achieving the aims of MGI.

DMREF proposals submitted to the Division of Mathematical Sciences must:

- be submitted within the window 15 January - 15 February 2013, inclusive;
- be submitted to DMS as the division and to DMREF as the program;
- deal with problems in the range of issues described in the DMREF Dear Colleague letter, NSF 13-025
- seek new mathematical or statistical results that will advance the DMREF agenda;
- describe a research plan that meets the central Materials Genome Initiative principle of closely coupled, iterative interplay among theory, computation, and experiment.

In addition,

- the title of a DMREF proposal should begin with the word "DMREF."

Proposals that do not seek new mathematical or statistical results may nevertheless fit well with other NSF divisions that are participating in DMREF, and mathematical scientists are strongly encouraged to join any DMREF proposal that makes good use of their expertise. DMS welcomes DMREF proposals from single investigators or from teams of investigators. DMS does not require that team proposals involve at least one expert from each of the areas of theory, computation, and experiment. However, successful proposals to DMS will offer evidence of that close, iterative collaboration among experts that is necessary to meet the central MGI principle on which DMREF is based. Letters of collaboration, which say what the collaborators

will do for the proposed project and that affirm the collaborators' participation in the iterative interplay required for DMREF, are appropriate evidence.

In addition to the mathematical and statistical modeling and analysis that occurs in the interactions among experiments, models, and simulations, DMREF topics of special interest to DMS include, but are **not** limited to:

- optimization of design in complicated, high-dimensional state spaces;
- effective data mining methods to uncover relationships between e.g. microstructure and bulk properties, or relationships among composition, processing, and bulk properties;
- first-principles understanding of materials;
- and the computational challenges presented not only by multiscale issues, but also by the problem of rapidly resolving differences between theory and simulation in the face of experimental data.

The last example is similar to data assimilation and data fusion problems encountered elsewhere, but here the possibilities offered by better data and closely coupled iteration create new opportunities for theoretical and algorithmic advances, on both the mathematical and statistical sides.

Participants interested in submitting proposals are strongly encouraged to first contact any of the program officers listed in the main DMREF Letter. For DMS, please confer with Michael Steuerwalt (msteuerw@nsf.gov).

Sastry G. Pantula
Division Director
Division of Mathematical Sciences