

National Science Foundation 4201 Wilson Boulevard Arlington, Virginia 22230

NSF 13-036

Dear Colleague Letter: DMREF proposals to the Division of Chemistry in fiscal year 2013

Date: January 4, 2013

The Division of Chemistry (CHE) 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 Chemistry must:

- be submitted within the window 15 January 15 February 2013, inclusive;
- be submitted to CHE 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
- explore fundamental chemical science that will advance the DMREF agenda;
- describe a research plan that meets the central MGI 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 explore fundamental chemical science may fit well with other NSF divisions that

are participating in DMREF, and chemists are strongly encouraged to join any DMREF proposal that makes good use of their expertise. CHE welcomes DMREF proposals from teams of investigators. Although CHE does not require that team proposals involve separate experts from each of the areas of theory, computation, and experiment, successful proposals to CHE will offer clear evidence of the close, iterative collaboration among experts that is necessary to meet the central MGI principle on which DMREF is based.

Under the DMREF theme, the Chemistry Division is interested in research aimed at understanding fundamental chemical structure and reactivity and fundamental intermolecular interactions that underpin and will enable the future discovery and design of new materials with predetermined properties and multifunctional capabilities. Such research will involve the development and deployment of predictive algorithms for multi-scale modeling and understanding of the structure-chemical property relationships that inform such chemical systems. CHE DMREF themes also include, but are not limited to, the theory, modeling and simulation-guided development of the next-generation measurement tools for characterizing the anticipatory properties of new materials and the discovery of new chemistry-driven signal transduction systems for the dynamic regulation of manufacturing processes (such as smart chemical sensors that are capable of the automatic release of regulatory chemicals).

Participants interested in submitting proposals are strongly encouraged to first contact any of the program officers listed in the main DMREF Letter. For CHE, please confer with Timothy Patten (tpatten@nsf.gov).

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