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**Consensus Study Report**
Highlights

NSF Efforts to Achieve the Nation's Vision for the Materials Genome Initiative: Designing Materials to Revolutionize and Engineer Our Future (DMREF)

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NSF Efforts to Achieve the Nation's Vision for the Materials Genome Initiative

Designing Materials to Revolutionize and Engineer Our Future (DMREF)

Consensus Study Report

Advanced materials are essential to address challenges in clean energy, national security, and health and human welfare, yet it can take decades to move a material from initial discovery to the market. The nation's Materials Genome Initiative (MGI) is focused on achieving more rapid development, manufacturing, and deployment of materials at a fraction of the cost. The National Science Foundation's (NSF's) Designing Materials to Revolutionize and Engineer Our Future (DMREF) program is part of this effort through its support of the development of fundamental science, the workforce, and computational and experimental tools for materials development.

At the request of NSF, the National Academies of Sciences, Engineering, and Medicine convened an expert committee to examine the impact that the DMREF program is having as it is progressing and adapting to achieve the nation's vision for the MGI. *NSF Efforts to Achieve the Nation's Vision for the Materials Genome Initiative* evaluates the DMREF program's goals, progress, and scientific accomplishments within the context of similar efforts both within the United States and abroad. This document highlights some of the committee's recommendations for aligning DMREF to take full advantage of existing and future opportunities to accelerate materials research from fundamentals to deployment. The complete report and recommendations can be read or downloaded at https://nap.nationalacademies.org/catalog/26723.

IDENTIFYING OPPORTUNITIES FOR THE FUTURE
Since the launch of the MGI in 2011, significant advances have been realized in computational materials science, data science,
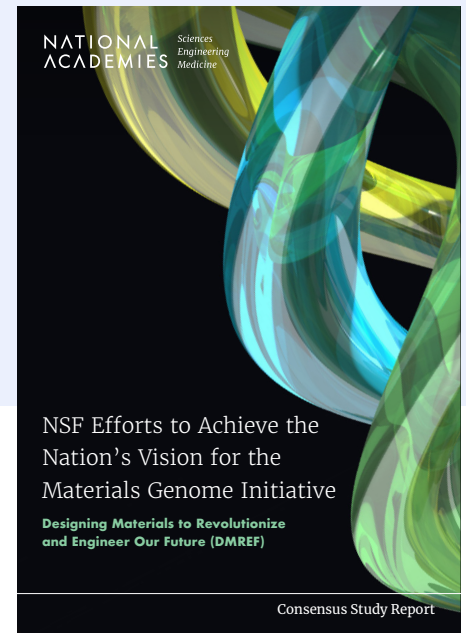
and materials informatics. The development of data-driven methods such as machine learning and artificial intelligence approaches, and their direct integration with computational or experimental discovery platforms, creates an urgency for more centralized gathering of the data produced during research. At present, the data are distributed among a number of servers and repositories.

Although the National Institute of Standards and Technology (NIST) maintains a Materials Data Repository, DMREF is uniquely situated to promote the integration of theory, modeling, experimentation, data science, robotics, and other novel areas in materials research. To that end, the report recommends **NSF and DMREF should take a leadership role to support the development of a national plan for a platform that creates interoperable systems that allow for comprehensive collection, dissemination, and use of computational and experimental materials data.**

COORDINATING AND COLLABORATING WITH AGENCIES

The fundamental science research supported by DMREF needs to be connected to the needs for advanced materials development and deployment work, including the future MGI national grand challenges, being done in other parts of the initiative. Because multiple federal agencies are supporting fundamental science efforts and technology development toward identified needs in the service of the MGI, opportunities exist at several levels, from collaboration at the level of individual researchers to partnership in joint programs. **DMREF should continue to encourage partnership and collaboration between grantees and researchers in government laboratories to provide diverse perspectives on the fundamental scientific challenges most relevant to the MGI.**

Many of these MGI mission-oriented agencies conduct in-depth investigations and detailed workshops to identify scientific and technical gaps for various functional areas and to develop roadmaps for these areas that are valuable for guiding efforts in fundamental research. The report recommends **DMREF should engage with mission-oriented agencies to obtain input on identified fundamental science gaps that most critically** **need to be closed to address the nation's needs as demonstrated in the MGI's national grand challenges.**

ATTRACTING AND DEVELOPING THE WORKFORCE

The development of the advanced materials workforce has been central to the MGI. DMREF has played a key role in the development of a new culture in advanced materials, integrating computation and experiment, and engaging disciplines such as computer science and data science. The program provides early exposure to integrated theoretical-experimental research to students and postdoctoral researchers.

However, the level to which students are educated about the broader context and goals of the MGI, and the degree of integration and interdisciplinarity of their training, is very uneven among different DMREF projects. The report recommends **students, postdoctoral associates, and other junior scientists associated with DMREF projects should develop substantial understanding of all aspects of the project, beyond those aspects that are the primary focus of their work. DMREF should encourage and help principal investigators to develop and implement the interdisciplinary training that this entails.**

ACCELERATING RESEARCH TOWARD DEPLOYMENT

The DMREF program's efforts primarily focus on basic science and naturally find their place at the lowest technology readiness level: in the discovery of new materials for various functional applications and the development of new tools, techniques, and methodologies related to theory, simulations, and data science as well as developing experimental tools that allow for high-throughput synthesis and high-throughput characterization of various functional properties.

NSF could amplify the impacts of the DMREF program by easing the transition of successful basic science research to higher technology readiness levels. **NSF should create new opportunities for translational funding, potentially through a supplemental mechanism, to provide timely support during DMREF projects that are at the cusp of deployment, with the potential**

for generating intellectual property or commercial spinoffs. The report recommends partnerships with groups including NSF's new Directorate for Technology, Innovation and Partnerships, and others such as NSF's Grant Opportunities for Academic Liaison with Industry program, the Innovation Corps program, and the Partnerships for Innovation program.

EVALUATION OF DMREF

As the primary NSF program dedicated to fostering the goals of the MGI, DMREF is leading a culture shift in materials research that emphasizes the integration of experimentation, theory, computation, and data, as well as workforce development straddling these areas. DMREF's focus on fundamental science and theoretical–experimental integration in a "bottom–up" framework has produced groundbreaking research on many fronts that has been critical to the progress of the MGI.

As DMREF matures, it should continue to increase its engagement with industry and federal agencies to identify key questions and transition the results from its fundamental science efforts to rapidly deploy advanced materials that meet national priorities.

COMMITTEE ON ADVISING NSF ON ITS EFFORTS TO ACHIEVE THE NATION'S VISION FOR THE MATERIALS GENOME INITIATIVE

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