Designing Materials to Revolutionize and Engineer our Future

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The Materials Genome Initiative (MGI) was announced by President Obama on June 24, 2011 with the objective of accelerating the discovery, development, and deployment of new materials.[1] It is a multi-agency initiative designed to create a new era of policy, resources, and infrastructure that supports U.S. institutions in the effort to discover, manufacture, and deploy advanced materials twice as fast at a fraction of the current cost. In December 2014, the National Science and Technology Council's Subcommittee on the Materials Genome Initiative published the strategic plan for MGI[2] that spells out four sets of goals: (1) Leading a culture shift in materials-science research to encourage and facilitate an integrated team approach; (2) Integrating experiment, computation, and theory and equipping the materials community with advanced tools and techniques; (3) Making digital data accessible; and (4) Creating a world-class materials-science and engineering workforce that is trained for careers in academia or industry. Over the past five years federal agencies have invested over $500 M in resources and infrastructure in support of this initiative. A selection of MGI accomplishments and technical successes were published[3] at MGI's fifth anniversary, illustrating the progress and future potential for this effort. As illustrated in Figure 1, the MGI is accelerating the pace at which fundamental discoveries are made and transitioned to American manufacturing by emphasizing a computationally-led and data-driven approach to research.

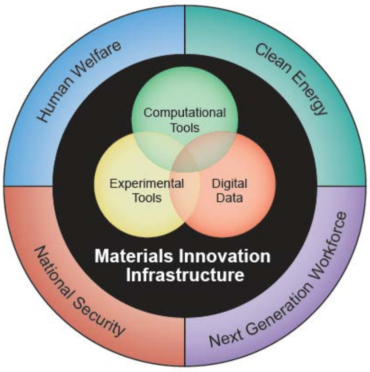

Figure 1. The Material Genome Initiative (MGI) provides a new interdisciplinary research philosophy whereby computational and experimental tools are coupled with data analytics to accelerate materials research. [1]

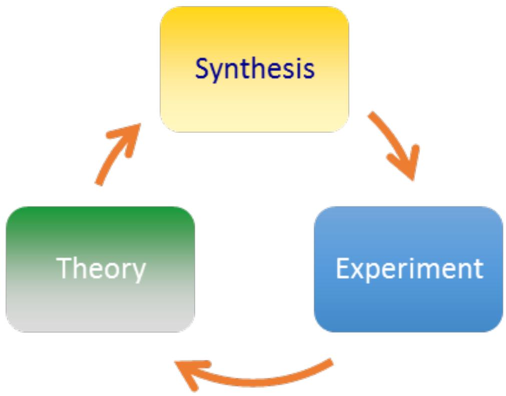

Figure 2. An iterative feedback loop among the synthesis, experiment, and theory components is the center piece of a successful DMREF project.

The Designing Materials to Revolutionize and Engineer our Future (DMREF) program represents the National Science Foundation's (NSFs) response to, and participation in, the MGI. DMREF is a multi-directorate program supported by ten divisions within the Directorates of Mathematical and Physical Sciences (MPS), Engineering (ENG), and Computer & Information Science & Engineering (CISE). The DMREF program supports efforts that span research in materials, chemistry, physics, mathematics, computer science, and engineering. NSF is interested in activities that accelerate materials discovery and deployment by building the fundamental knowledge base needed to progress toward designing and making materials with specific and desired functions or properties from first principles calculations. The goal of DMREF is to control materials properties through design. The heart of a DMREF project is the iterative feedback loop (Figure 2) whereby the materials synthesis and/or processing, characterization and/or testing, and theory and/or modeling aspects of the project strongly interact with each other to promote significant advances in each of these components in order to advance materials design. In practice, additional loops may be required for successful completion of the project.

In addition to the Intellectual Merit and Broader Impact criteria under which all NSF proposals are critiqued, DMREF proposals are also evaluated with respect to the following criteria:

- Does the proposed work help accelerate materials discovery and development by building the fundamental knowledge base needed to progress toward designing and making materials with specific, desired functions or properties?
- Does the proposed research use collaborative processes with iterative feedback between tasks? The materials synthesis /growth / processing techniques, characterization / testing methodology, theory / mathematics, data science, and computation / simulation aspects of the project must all strongly interact with each other to promote significant advances in each of these components and advance materials design.
- Does the proposed work provide training for the next generation of scientists and engineers, educated in a multidisciplinary, integrated experimental and computational approach to materials research?
- Does the proposed work provide open access to its outputs, including data, software, codes, samples, and publications?

MGI originated with an emphasis on structural materials, including alloys and ceramics. Over the past five years, DMREF has supported 114 multidisciplinary projects, involving over 400 PIs, that cover a wide range of material properties, including electronic, photonic, magnetic, catalytic, and structural. The program also supports a wide range of material classes, including molecular materials, biomaterials, polymers, ceramics, metals, alloys, and composites. DMREF is supportive of the NSF long-range transformative agenda 'Big Ideas for Future NSF Investments,'[4] and encourages proposals that align with the materials aspects of this endeavor.

While not required, DMREF encourages ties with industry and/or national laboratories. Notably, NSF supported facilities including the National High Magnetic Field Laboratory (NHMFL), ChemMatCARS, the Cornell High Energy Synchrotron Source (CHESS), and the National Institute for Standards and Technology (NIST) Center for Neutron Research (CHURNS) provide world-class tools for material characterization that can provide meaningful feedback for theoretic and synthetic efforts. Furthermore, two Material Innovation Platforms (MIPs) have recently been initiated to support materials research under the MGI framework as user facilities. These MIPs are the Platform for the Accelerated Realization, Analysis, and Discovery of Interface Materials (PARADIM) and the 2D Crystal Consortium.

This talk will introduce NSF's DMREF program and its integration within the multiagency MGI. Opportunities for a theory-guided and data-driven approach for the accelerated discovery of correlated electron materials will be discussed. The use of high magnetic fields in MGI-based research will be addressed and highlights from existing DMREF projects will be provided.

References:

[1] Materials Genome Initiative for Global Competiveness (2012), whitepaper prepared by the Group on Advanced Materials and approved by the National Science and Technology Council, Committee on Technology.
https://www.mgi.gov/sites/default/files/documents/materials_genome_initiative-final.pdf

[2] Materials Genome Initiative Strategic Plan (2014)
https://www.whitehouse.gov/sites/default/files/microsites/ostp/NSTC/mgi_strategic_plan_-_dec_2014.pdf

[3] The First Five Years of the Materials Genome Initiative: Accomplishments and Technical Highlights (2016) https://mgi.nist.gov/sites/default/files/uploads/mgi-accomplishments-at-5-years-august-2016.pdf

[4] 10 Big Ideas for Future NSF Investments (2016)
https://www.nsf.gov/about/congress/reports/nsf_big_ideas.pdf