<u>The First Five Years of the Materials Genome Initiative:</u>
<u>Accomplishments and Technical Highlights</u>

August 2, 2016

"To help businesses discover, develop, and deploy new materials twice as fast, we're launching what we call the Materials Genome Initiative."
President Obama's remarks at
Carnegie Mellon University
June 24, 2011

On June 24, 2011, President Obama announced the Materials Genome Initiative (MGI), a multi-agency initiative designed to create a new era of policy, resources, and infrastructure that support U.S. institutions in the effort to discover, manufacture, and deploy advanced materials twice as fast and at a fraction of the cost than it's taken in the past. Over the past five years, Federal agencies, including the Departments of Energy (DOE) and Defense (DoD), the National Science Foundation (NSF), the National Institute of Standards and Technology (NIST), and the National Aeronautics and Space Administration (NASA), have invested more than $500 million in resources and infrastructure in support of this initiative.

Federal agencies have been working closely together and with collaborators from the public and private sectors to cultivate a cultural paradigm shift and make technical progress towards the initiative's ambitious goals. Agencies have established or supplemented an array of research and development programs. An expanding set of materials databases are being accessed by thousands of users to mine the properties of hundreds of thousands of materials. And, interdisciplinary research centers at universities and government laboratories around the country are discovering and developing new materials, working with industrial collaborators to deploy those materials, and educating the future materials workforce.

This document provides a selection of accomplishments and technical highlights illustrating the progress made during the first five years of the initiative. The examples are organized under the following four key challenges as set out in the [2014 MGI Strategic Plan] (note that many examples contribute to more than one challenge):

- Lead a culture shift in materials research to encourage and facilitate an integrated team approach;
- Integrate experiment, computation, and theory and equip the materials community with advanced tools and techniques;
- Make digital data accessible; and
- Create a world-class materials workforce that is trained for careers in academia or industry.

LEAD A CULTURE SHIFT IN MATERIALS RESEARCH

1. NIST and the National Renewable Energy Laboratory (NREL) are launching a virtual high-throughput experimentation facility with the goal of accelerating the generation of the huge volumes of additional data needed to validate existing materials models and to develop new, more sophisticated models with more powerful predictive capabilities. The virtual facility will consist of a national network of high-throughput synthesis and characterization tools integrated into the MGI materials data infrastructure. The facility will foster coordination and data integration across high-throughput experimentation programs. The result will be a widely accessible, growing resource open to all researchers in pursuit of novel materials. Read more.

2. NIST launched and funds *the Center for Hierarchical Materials Design*, a collaboration between NIST, Northwestern University, University of Chicago, and Argonne National Laboratory (ANL) to develop key components of the materials innovation infrastructure, including databases of materials properties and materials simulation software, while simultaneously using these tools to design new materials with targeted applications such as aerospace, electronics, and health care. Read more and more.

3. A team sponsored by the DoD Air Force Research Laboratory (AFRL) and led by GE-Aviation and Lockheed Martin demonstrated that by coupling process modeling with mechanical analysis, engineers can design better, more innovative components while reducing the time needed and cost for design. Composite materials can provide tremendous improvements in aircraft fuel efficiency, but are very complex to make and use in aircraft design. The methods produced by the team are becoming standard work within both companies and will enable them to design new aircraft components with higher confidence at less cost. Read more and more.

4. The DoD Army Research Laboratory (ARL) established the *Enterprise for Multiscale Research of Materials* to enable the design of materials for future Army Systems. This enterprise is comprised of ARL researchers and a broad range of academic and industrial collaborators. Two Collaborative Research Alliances have been formalized, one for *Materials in Extreme Dynamic Environments* led by Johns Hopkins University that focuses on protection materials, and one for *Multi-Scale Modeling of Electronic Materials* led by the University of Utah that focuses on battery and electronic applications. These alliances are focused on developing materials to meet future Army needs, while also building the future workforce. Read more and more.

5. The DoD's Office of Naval Research (ONR) established the *Lightweight Innovations for Tomorrow* (LIFT) Manufacturing Innovation Institute for metals processing and

structural design to provide lighter weight products, systems, and vehicles. LIFT is providing the facilities and expertise to mitigate risk for businesses of all sizes in adopting advanced manufacturing technology. The institute is also working to strengthen the skills of a diverse workforce through programs targeting returning veterans, at risk youth, university students pursuing graduate degrees, and current manufacturing workforce. Read more and more.

6. NASA, in close collaboration with NIST, established the *MaterialsLab* program on the International Space Station. This program is accelerating the development of higher-performing materials and processes for use both in space and on Earth, offering unique insights into how materials develop and behave in the microgravity environment. By sharing the results through NASA's open Physical Sciences Informatics data repository, researchers—including students—can easily access data from station experiments and build on each other's work. Read more.

INTEGRATE EXPERIMENT, COMPUTATION, AND THEORY

7. NSF established the interdisciplinary program *Designing Materials to Revolutionize and Engineer our Future* (DMREF), which is funding small academic teams to discover, design, and make materials with specific and desired functions or properties from first principles. (Also see item 28.) Since its inception in 2012, the DMREF program has awarded 258 grants to teams at 80 academic institutions in 30 states. Read more.

8. Successful iteration between experiment and computation led a NSF and DOE-funded team from University of Wisconsin-Madison to discover and design the first-of-its-kind, multifunctional material that is both metallic and polar—contradictory properties in one material that can be exploited in future devices to perform simultaneous electrical, magnetic, and optical functions. Read more and more.

9. An NSF-funded team from the University of California, Santa Barbara, in collaboration with General Electric and others, has designed and built a custom microscope that combines electron, ion, and laser beams to analyze new materials for defects at the nanometer scale in three dimensions. The addition of the laser is critical to speeding up the process of gathering the information, so what used to take six to nine months now takes only a couple of days. The microscope is key to the team's development of new multilayered materials designed for high performance in extreme environments. In addition to developing new measurement methods, the team is pioneering the use of new modeling tools to speed up the development process and using advanced computer algorithms and "big data" analysis to hone designs before testing them. Read more and more.

10. NSF has launched the *Materials Innovation Platforms* program that aims to significantly accelerate materials research and development. (Also see item 30.) Funded institutions are serving as "platforms" to develop new bulk and thin film crystalline hard materials through state-of-the-art instrumentation, and fostering an environment that combines multidisciplinary expertise with the best tools available, providing access to the instrumentation, data, and new materials created. Read more.

11. The DOE Energy Frontier Research Center (EFRC) *Next Generation Materials by Design*, led by NREL, has used the DOE's *Materials Project* database to identify and test promising, non-toxic alternatives to perovskite solar materials. (Also see item 22.) The team had previously identified defect tolerance and long carrier lifetime as the key properties of lead-based perovskite solar materials, which have achieved efficiencies of more than 20% in only a few years. Applying the newly discovered criteria and theoretical calculations, the database enabled the team to evaluate 27,000 compounds and identify nine additional classes of promising non-toxic alternatives. In collaboration with the *Center for Excitonics* EFRC at the Massachusetts Institute of Technology, six candidate materials were synthesized and characterized, with two showing promising properties. Read more and more.

12. Through a tight integration of predictive theory and modeling with experimental synthesis and characterization, the DOE-funded *Nanoporous Materials Genome Center* has discovered and explored microporous and mesoporous metal-organic frameworks and zeolites for energy-relevant processes. (Also see item 24.) The Center is developing and implementing theoretical and computational approaches ranging from high-level electronic structure calculations combined with advanced molecular dynamics and Monte Carlo sampling approaches to graph theoretical analysis of pore structures. These approaches are assembled in a hierarchical screening workflow to discover and advance understanding of novel functional nanoporous materials for gas storage, carbon capture, gas- and solution-phase separation, and catalysis. Read more.

13. The DOE *Critical Materials Institute* (CMI) relies on the integrated MGI approach to accelerate the discovery and development of rare-earth replacements, such as new phosphors for high-efficiency lighting. The CMI, one of DOE's Energy Innovation Hubs, is a collaboration of researchers from universities, four DOE national laboratories, and members of industry working together to assure the supply chains for materials critical to clean energy technologies. Read more and more.

14. At the *Manufacturing Demonstration Facility*, a collaborative manufacturing community established at DOE's Oak Ridge National Laboratory, modeling and simulation are tightly integrated with materials characterization and *in-situ* process

monitoring to help industry adopt new manufacturing technologies. Such integration is key to the success of additive manufacturing and to the commercialization of low-cost carbon fiber composite materials for energy-efficient vehicles. Read more.

15. Researchers from AFRL, ANL, Lawrence Livermore National Laboratory (LLNL), Carnegie Mellon University, Petra III (Germany), PulseRay, and Cornell University have developed a revolutionary way of using high-intensity x-rays to measure the detailed structure of a material while it is being bent, compressed, or stretched. The measurement method provides new insights into how materials fail—insights that are critical for creating more accurate models needed to rapidly optimize, predict and improve the performance of light-weight, high-strength materials for aircraft and automobiles. Read more and more.

16. Researchers at AFRL have invented an automated system that can create a material under controlled conditions, measure the resulting properties, evaluate the results, and then determine and perform the best next experiment—all without a scientist involved. Materials research is a complex business, unraveling the reasons why materials behave like they do is time consuming and expensive, and can also be tedious. This automated system is now being used to dramatically speed the pace of research in understanding how to make better carbon nanotubes for use in high performance materials for aircraft. Read more and more.

17. A DoD ONR Multidisciplinary University Research Initiative team led by the University of Connecticut has combined high-throughput computational screening, informatics, and experimental synthesis and testing to develop a set of new organic polymer dielectrics with enhanced properties compared to materials now in use. Their success is an excellent example of how the MGI is being harnessed to collaboratively design new materials—in this case including an entirely new class of metal-based polymer—through an informatics-driven approach. Read more.

18. Researchers AFRL and Blue Quartz Software have developed a new, open-source suite of tools for managing the information that links how a material is made to how it performs in service. The new tools, the *Spatial Informational Management Protocol Library* and *Digital Representation Environment for the Analysis of Microstructure in 3D*, not only manage complex data in space, time, and material variables, but provide software tools to rapidly analyze materials information in new ways. The capabilities provided by these tools allow materials scientists and engineers to quickly gain new insights into the way in which materials work. Read more and more.

19. NASA has announced plans to fund a university-led institute to develop ultra-high strength, lightweight structural materials needed for the journey to Mars using an MGI-inspired approach. Extending human presence to Mars and deeper into the solar system requires high performance materials and structures to enable a safe and affordable space infrastructure. Although carbon nanotubes offer potentially transformative mechanical, electrical, and thermal properties, manufacturing products that live up to that potential has been difficult. A computationally guided approach that integrates advanced modeling throughout the entire materials development lifecycle will be used to overcome this challenge. Read more and more.

MAKE DIGITAL DATA ACCESSIBLE

20. NIST created the *Materials Data Repository* (MDR) to answer the question, "Where do I put my data, so that others can use it?" The MDR now hosts approximately 50 gigabytes of highly heterogeneous data (with several terabytes of additional data in the pipeline) spanning 80 individual research communities, with participation of 123 distinct organizations across academia, government, and industry. The MDR hosts materials data for public access, but also allows additional metadata describing the data to be specified, provides a persistent identifier allowing for long term citation and discovery, and assignment of a distribution license, giving data publishers control over the rights to the information. Read more.

21. NIST is developing the *Materials Resource Registry* as a materials information "yellow pages," enabling world-wide discovery of available resources (modeled after the Virtual Astronomical Observatory's registry). With more than a hundred listings today, and an international team working under the framework of the Research Data Alliance, searches over thousands of material resources are now within reach. Read more.

22. The DOE established and funds *The Materials Project* at the University of California, Berkeley, where the properties of new and predicted materials determined through high performance computing and state-of-the-art theoretical tools are archived in a publicly available database that now has more than 20,000 users. (Also see item 11.) The database includes more than 66,000 crystalline compounds, 500,000 nanoporous materials, 70,000 electrochemical phase diagrams, 43,000 electronic band structures, and 2,900 full elastic tensors (important for understanding mechanical behavior). This data is being used by hundreds of researchers each day to identify and design new materials for clean energy applications. Read more.

23. The DOE Battery Hub *Joint Center for Energy Storage Research* released two major sets of battery data to the public through the *Materials Project* in May 2016. One set encompasses data calculated for nearly 1,500 compounds investigated as potential electrodes for batteries with the potential of doubling the battery's power compared with current lithium ion batteries. The other set contains data on more than 21,000 organic molecules relevant for liquid electrolytes for grid storage batteries as well as a host of other research applications. The release also included two new web apps—the *Molecules Explorer* and the *Redox Flow Battery Dashboard*—plus an add-on to the *Battery Explorer* web app that enables researchers to investigate other ions in addition to lithium. The *Redox Flow Battery* app generates both scientific parameters as well as techno-economic ones, so battery designers can quickly rule out a molecule that might perform well but be prohibitively expensive to manufacture. Read more and more.

24. The extensive computational and experimental data generated by the DOE-funded *Nanoporous Materials Genome Center* can now be easily explored using the *Nanoporous Materials Explorer* web app available through the *Materials Project*. (Also see items 12 and 22.) The app provides an interactive platform for the aggregation and presentation of data related to nanoporous materials in a way that was not previously possible, enabling rapid identification of promising materials based on their performance and properties. Read more.

25. DOE has established and is funding the *Center for PRedictive Integrated Structural Materials Science,* which has created a unique scientific framework for accelerated predictive materials science for structural metals that integrates advanced experiments, theory, and simulation. The Center has released four high performance computational tools for simulating microstructures and mechanical behavior of metals and alloys, with the open source codes made available to the public. On August 1, 2016, the Center inaugurated the *Materials Commons*, a unique, collaborative approach for storing and disseminating scientific information. This data repository is designed to seamlessly capture and store up to 400 TB of publically accessible information. Read more and more.

26. DOE launched the *Energy Materials Network*, a growing network of consortia allowing industry ready access to its national laboratories' capabilities, tools, and expertise in order to accelerate the materials development cycle for U.S. manufacturers. The initial consortia include *LightMAT*, a network of ten national laboratories with technical capabilities that are relevant to lightweight materials development and use; *ElectroCat*, dedicated to finding new ways to replace rare and costly platinum group metals used in hydrogen fuel cells with more abundant and inexpensive substitutes; and *CaloriCool*, dedicated to the discovery of high-

performance energy conversion materials that can be economically adopted by industry for a new generation of energy efficient solid-state cooling and refrigeration devices. Read more and more.

27. The DOE *High Performance Computing for Manufacturing Program* is coupling U.S. manufacturers with the DOE national laboratories' world-class computational research and development expertise, and advanced computing resources to address key challenges in U.S. manufacturing whose solutions will have broad industry and national impact. Under this program, LLNL and Lawrence Berkeley National Laboratory, in collaboration with Agenda 2020, are developing scalable models for the pulp and paper industry to help reduce energy use in paper-making. LLNL is also working with collaborators to dramatically cut the lead time and expense of producing gallium nitride wafers needed for solid-state lighting and power switching devices. Read more, more, and more.

CREATE A WORLD-CLASS MATERIALS WORKFORCE

28. Workforce development is a major objective of NSF's DMREF program, and it is providing graduate students and post-doctoral researchers with a broad education through co-advising and student exchange within multi-disciplinary teams. New courses have been developed on methods that promote accelerated materials development. (Also see item 7.) Symposia have been organized at national conferences in order to educate the community on MGI strategies. Ongoing, coordinated outreach activities aimed at underrepresented groups, K-12 students, and the general public are sharing the excitement of new materials discovery and development. Since the inception of the program in 2012, 110 post-doctoral researchers, 730 graduate students, and 100 undergraduate students have been trained in research applying the MGI-approach. Read more.

29. The NSF Research Traineeship program, designed to encourage the development of bold, new, potentially transformative, and scalable models for graduate training, has awarded nearly $6 million to develop training in data-enabled materials science and engineering. Programs at Pennsylvania State University and the University of Southern Mississippi are developing new ways to train students on how to bridge *ab initio* methods and applications, and on methods to understand complex interfaces, respectively. These awards will help ensure that graduate students develop the skills, knowledge, and competencies needed to pursue a range of MGI-related careers. Read more and more.

30. A new summer school is one of many educational and outreach activities being conducted under NSF's *Materials Innovation Platforms* to accelerate materials discovery and development. (Also see item 10). At the *PARADIM Bulk Crystal*

Summer School, a week-long workshop held at John Hopkins University in July 2016, graduate students, postdocs, and young faculty learned about the synthesis, characterization, and theory of crystal growth through a combination of hands-on experience and lectures by internationally recognized crystal growth specialists. Read more.

31. To address the need to educate and develop materials scientists capable of applying and/or developing computational tools, NSF is funding the *Summer School for Integrated Computational Materials Education*. The summer school, held annually starting in 2011, is accelerating the incorporation of computational materials science at universities that lack the resources to implement them on their own, training instructors to teach computational materials science and engineering (CMSE) to undergraduate students. This program also provides a stepping-stone towards more intensive CMSE education and its wider adoption by developing the needed human resources. Read more.

32. The *Informatics Skunkworks,* launched under an NSF grant for "A Computational Materials Data and Design Environment" at University of Wisconsin, Madison, is helping undergraduates develop informatics for science and engineering applications, learn advanced data science and machine learning skills, expand their domain-specific knowledge, and grow their experience of working with teams, faculty, and industry. The group has developed a scalable approach for exposing undergraduates to the potential of informatics for materials science and engineering. Read more and more.