Materials Genome Initiative
for Global Competitiveness

June 2011

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EXECUTIVE OFFICE OF THE PRESIDENT
NATIONAL SCIENCE AND TECHNOLOGY COUNCIL
WASHINGTON, D.C. 20502

June 24, 2011

Dear Colleague:

In much the same way that silicon in the 1970s led to the modern information technology industry, the development of advanced materials will fuel many of the emerging industries that will address challenges in energy, national security, healthcare, and other areas. Yet the time it takes to move a newly discovered advanced material from the laboratory to the commercial market place remains far too long. Accelerating this process could significantly improve U.S. global competitiveness and ensure that the Nation remains at the forefront of the advanced materials marketplace. This *Materials Genome Initiative for Global Competitiveness* aims to reduce development time by providing the infrastructure and training that American innovators need to discover, develop, manufacture, and deploy advanced materials in a more expeditious and economical way.

Prepared by an *ad hoc* group of the National Science and Technology Council, this initiative proposes a new national infrastructure for data sharing and analysis that will provide a greatly enhanced knowledgebase to scientists and engineers designing new materials. This effort will foster enhanced computational capabilities, data management, and an integrated engineering approach for materials deployment to better leverage and complement existing Federal investments.

The success of this initiative will require a sustained effort from the private sector, universities, and the Federal Government. I look forward to working with you to make this vision a reality.

Sincerely,

John P. Holdren
John P. Holdren
Assistant to the President for Science and Technology
Director, Office of Science and Technology Policy

Introduction

A genome is a set of information encoded in the language of DNA that serves as a blueprint for an organism's growth and development. The word genome, when applied in non-biological contexts, connotes a fundamental building block toward a larger purpose.

The Materials Genome Initiative is a new, multi-stakeholder effort to develop an infrastructure to accelerate advanced materials discovery and deployment in the United States. Over the last several decades there has been significant Federal investment in new experimental processes and techniques for designing advanced materials. This new focused initiative will better leverage existing Federal investments through the use of computational capabilities, data management, and an integrated approach to materials science and engineering.

What follows describes a vision of how the development of advanced materials can be accelerated through advances in computational techniques, more effective use of standards, and enhanced data management. Detailed benchmarks and milestones will be laid out in later documents. This document is written for all stakeholders in the materials development community — from experimental and theoretical scientists conducting basic research to industrial engineers qualifying new material products for market. These stakeholders span academic institutions, small businesses, large industrial enterprises, professional societies, and government. With the engagement of all stakeholders in the up-front planning and execution, this initiative will ensure the Nation remains competitive in the manufacturing and use of advanced materials.

Vision Statement

Advanced materials are essential to economic security and human well-being, with applications in multiple industries, including those aimed at addressing challenges in clean energy, national security, and human welfare. Accelerating the pace of discovery and deployment of advanced material systems will therefore be crucial to achieving global competitiveness in the 21st century. The Materials Genome Initiative will create a new era of materials innovation that will serve as a foundation for strengthening domestic industries in these fields. This initiative offers a unique opportunity for the United States to discover, develop, manufacture, and deploy advanced materials at least twice as fast as possible today, at a fraction of the cost.

Materials Deployment

The Challenge

In much the same way that silicon in the 1970s led to the modern information technology industry, advanced materials could fuel emerging multi-billion-dollar industries aimed at addressing challenges in energy, national security, and human welfare. Since the 1980s, technological change and economic progress have grown ever more dependent on new materials developments.[1,2] To secure its competitive advantage in global markets and succeed in the future of advanced materials development and deployment, the United States must operate both faster and at lower cost than is possible today.

At present, the time frame for incorporating new classes of materials into applications is remarkably long, typically about 10 to 20 years from initial research to first use. For example, the lithium ion battery, which is ubiquitous in today's portable electronic devices, altered the landscape of modern information technologies; however, it took 20 years to move these batteries from a laboratory concept proposed in the mid 1970s to wide market adoption and use in the late 1990s.[3,4] Even now, 40 years later, lithium ion batteries have yet to be fully incorporated in the electric car industry, where they stand to play a pivotal role in transforming our transportation infrastructure. It is clear that the pace of development of new materials has fallen far behind the speed at which product development is conducted.

As today's scientists and engineers explore a new generation of advanced materials to solve the grand challenges of the 21st century, reducing the time required to bring these discoveries to market will be a key driving force behind a more competitive domestic manufacturing sector and economic growth.[5]

The lengthy time frame for materials to move from discovery to market is due in part to the continued reliance of materials research and development programs on scientific intuition and trial and error experimentation. Much of the design and testing of materials is currently performed through time-consuming and repetitive experiment and characterization loops. Some of these experiments could potentially be performed virtually with powerful and accurate computational tools, but that level of accuracy in such simulations does not yet exist.

An additional barrier to more rapid materials deployment is the way materials currently move through their development continuum (see Figure 1), which is the series of processes that take a new material from conception to market deployment. It comprises seven discrete stages, which may be completed by different engineering or scientific teams at different institutions. This system employs experienced teams at each stage of the process, but with few opportunities for feedback between stages that could accelerate the full continuum.

In the discovery stage it is crucial that researchers have access to the largest possible data set upon which to base their models, in order to provide a more complete picture of a material's characteristics. This can be achieved through data transparency and integration. Another factor limiting a scientist's ability to model materials behavior and invent new materials is their knowledge of the underlying physical and chemical mechanisms of a material system. There is currently no standard method for researchers to share predictive algorithms and computational methods.

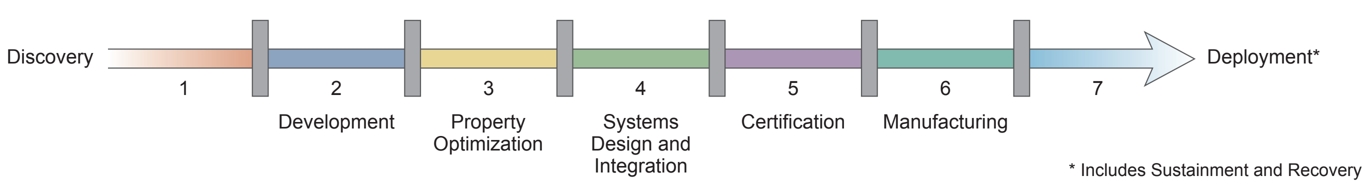


Figure 1: Materials development continuum

To achieve faster materials development, the materials community must embrace open innovation. Rapid advances in computational modeling and data exchange and more advanced algorithms for modeling materials behavior must be developed to supplement physical experiments; and a data exchange system that will allow researchers to index, search, and compare data must be implemented to allow greater integration and collaboration.

Later parts of the continuum are necessarily linear (i.e. certification cannot occur before systems design), but all stages would benefit from increased data transparency and communication. Currently, no infrastructure exists to allow different engineering teams to share data or models. Data transparency may have the largest impact after the material has been deployed, due to the fact that every industry relies on materials as components of product design. A product designer who needs a material of certain specifications may not be aware that the material has already been designed because there is no standard method to search for it. Data transparency encourages cross-industry and multidisciplinary applications.

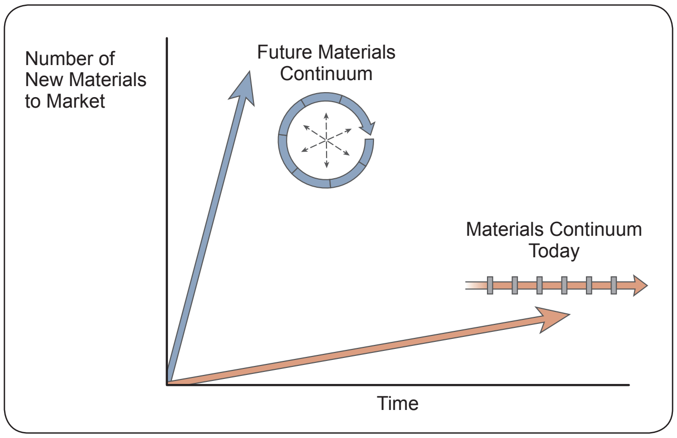


Figure 2: Initiative acceleration of the materials continuum

The life cycle of a material does not end with deployment. An issue that is coming more to the attention of industry and consumers is the recyclability and sustainability of materials. Materials engineers must design for the ever-changing parameters and uses of materials after their initial intended purpose; for example, recyclability must become a design parameter.

The Materials Genome Initiative will develop the toolsets necessary for a new research paradigm in which powerful computational analysis will decrease the reliance on physical experimentation. Improved data sharing systems and more integrated engineering teams will allow design, systems engineering, and manufacturing activities to overlap and interact (see Figure 2).

This new integrated design continuum — incorporating greater use of computing and information technologies coupled with advances in characterization and experiment — will significantly accelerate the time and number of materials deployed by replacing lengthy and costly empirical studies with mathematical models and computational simulations. Now is the ideal time to enact this initiative; the computing capacity necessary to achieve these advances exists and related technologies such as nanotechnology and bio-technology have matured to enable us to make great progress in reducing time to market at a very low cost.

Multiple international entities have recognized these issues and a number of foreign countries have already embarked on programs to address them.[6] The National Research Council of the National Academies of Sciences, in its report on Integrated Computational Materials Engineering, describes the potential outcome:

> *Integrating materials computational tools and information with sophisticated computational and analytical tools already in use in engineering fields... [promises] to shorten the materials development cycle from its current 10-20 years to 2 or 3 years.*[7]

While it is difficult to anticipate the actual reduction in development time that will result from this initiative, our goal is to achieve a time reduction of greater than 50 percent.

Accelerating the Materials Continuum

The Materials Genome Initiative would create a materials innovation infrastructure to exploit this unique opportunity. The full Initiative is captured in Figure 3.

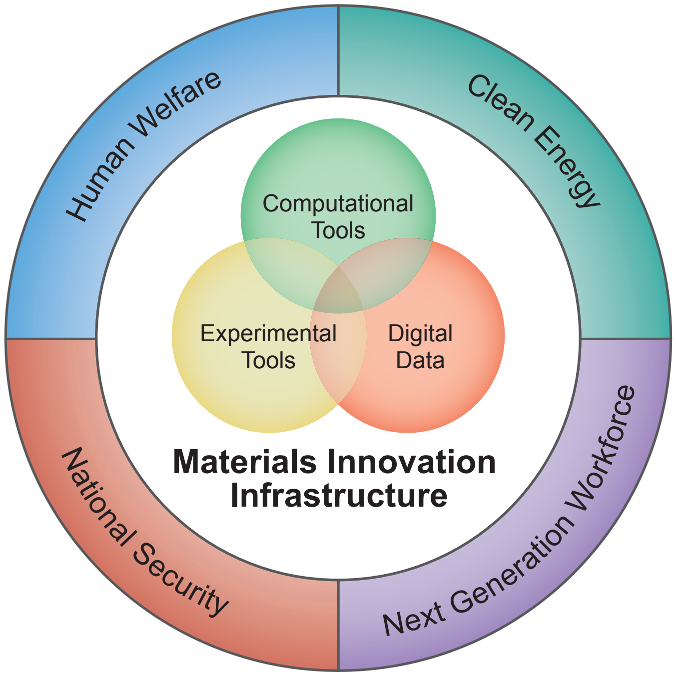


Figure 3: Initiative overview

1. Developing a Materials Innovation Infrastructure

The Materials Genome Initiative will develop new integrated computational, experimental, and data informatics tools. These software and integration tools will span the entire materials continuum, be developed using an open platform,† improve best-in-class predictive capabilities, and adhere to newly created standards for quick integration of digital information across the materials innovation infrastructure. This infrastructure will seamlessly integrate into existing product-design frameworks to enable rapid and holistic engineering design.

2. Achieving National Goals With Advanced Materials

The infrastructure created by this initiative will enable scientists and engineers to create any number of new advanced materials, many of which will help solve foundational science and engineering problems and address issues of pressing national importance. The Federal government intends to host interagency workshops with all relevant stakeholders to identify high priority material problems, which will be used to develop and coordinate the Initiative and to sustain the long-term process of accelerating materials development outlined in this vision document.

3. Equipping the Next-Generation Materials Workforce

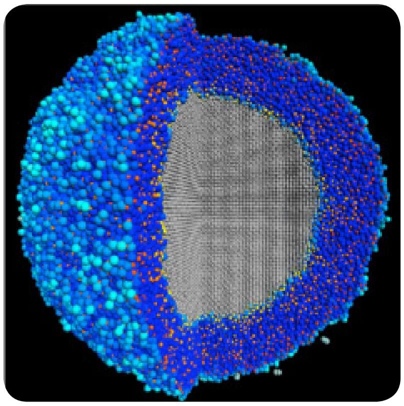
Success of this initiative cannot be measured by the tools alone, but rather by the pervasiveness of their use and the outcomes they enable. Equipping our next-generation workforce with the tools and approaches necessary to achieve our national goals will require stakeholders in government, academia, and industry to embrace the scope and contents of the materials innovation infrastructure. This will be achieved with a focus on education, workforce development, and a generational shift toward a new, more integrated approach to materials development.

† An open platform aims to accommodate open access and open source software, with mechanisms for independent software developers to retain proprietary rights.

Computational Tools

Major advances in modeling and predicting materials behavior have led to a remarkable opportunity for the use of simulation software in solving materials challenges. New computational tools have the potential to accelerate materials development at all stages of the continuum. For example, software could guide the experimental discovery of new materials by screening a large set of compounds and isolating those with desired properties. Further downstream, virtual testing via computer-aided analysis could replace some of the expensive and time-consuming physical tests currently required for validation and certification of new materials.

These computational tools are still not widely used due to industry's limited confidence in accepting non-empirically-based conclusions. Materials scientists have developed powerful computational tools to predict materials behavior, but these tools have fundamental deficiencies that limit their usefulness. The primary problem is that current predictive algorithms do not have the ability to model behavior and properties across multiple spatial and temporal scales; for example, researchers can measure the atomic vibrations of a material in picoseconds, but from that information they cannot predict how the material will wear down over the course of years. In addition, software tools that utilize the algorithms are typically written by academics for academic purposes in separate universities, and therefore lack user-friendly interfaces, documentation, robustness, and the capacity to scale to industrial-sized problems. These deficiencies inhibit efficient software maintenance and can result in software failures. Significant improvements in software and the accuracy of materials behavior models are needed.



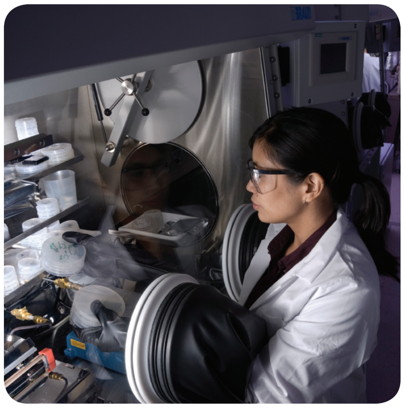
Open innovation will play a key role in accelerating the development of advanced computational tools. A system that allows researchers to share their algorithms and collaborate on creating new tools will rapidly increase the pace of innovation, which currently occurs in isolated academic settings. An existing system that is a good example of a first step toward open innovation is the nanoHUB, a National Science Foundation program run through the Network for Computational Nanotechnology.[8] By providing modeling and simulation applications that researchers can download and use on their data, nanoHUB.org supports the use of computational tools in nanotechnology research. Researchers can access state-of-the-art modeling algorithms and collaborate with colleagues via the website. To rapidly increase knowledge of first principles and advance modeling algorithms, it is essential for the materials industry to accept open innovation and design these tools on an open platform.

The ultimate goal is to generate computational tools that enable real-world materials development, that optimize or minimize traditional experimental testing, and that predict materials performance under diverse product conditions. An early benchmark will be the ability to incorporate improved predictive modeling algorithms of materials behavior into existing product design tools. For example, the crystal structure and physical properties of the materials in a product may change during the product's processing, due to varying conditions. It could be disastrous to the performance of a product if, for instance, the tensile strength of its bolts changed during manufacture. The ability to model these morphology and property changes will enable faster and better design.

Achieving these objectives will require a focus in three necessary areas: (1) creating accurate models of materials performance and validating model predictions from theories and empirical data; (2) implementing an open-platform framework to ensure that all code is easily used and maintained by all those involved in materials innovation and deployment, from academia to industry; and (3) creating software that is modular and user-friendly in order to extend the benefits to broad user communities.

Experimental Tools

The emphasis of the Initiative is on developing and improving computational capabilities, but it is essential to ensure that these new tools both complement and fully leverage existing experimental research on advanced materials. Effective models of materials behavior can only be developed from accurate and extensive sets of data on materials properties. Experimental data is required to create models as well as to validate their key results. Where computations based on theoretical frameworks fall short, empirical testing will fill in the gaps. As mentioned previously, most computational models are not yet capable of multi-scale modeling. Empirical data will help the models bridge gaps in the "material length scale" and significantly accelerate the pace of building fundamental understanding and developing new materials. Once the models are improved by incorporating new data, they will provide faster, more efficient, and more comprehensive performance data than could be generated by experiments alone.



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One advanced technique that is already implemented in industry is high throughput combinatorial processing. The General Motors Company, for example, has been working on next-generation catalysts for automobile exhaust emission control and on developing detailed kinetics and predictive physics-based models to describe the performance of these catalysts.[9] With support from the Department of Energy in 2002, General Motors used high throughput combinatorial techniques to rapidly synthesize and screen a broad range of catalyst materials, the most promising of which were tested on engines and are being considered for commercial use.[10] This type of rapid characterization technique, when complemented by computational capabilities and a highly trained workforce, will help to accelerate the discovery process.

Beyond leveraging existing experimental work, there will be specific needs for new techniques in experimentation and characterization to realize the synergy between experiments and computational methods. New experimental and characterization tools must be rooted in fundamental physics, chemistry, and materials science. Materials properties will be measured as a function of key variables, such as composition and processing history, as they relate to empirical theories and existing data. The experimental input required goes far beyond a single set of measurements. In most cases, researchers must combine and calibrate data from many experiments into a single larger data set that represents the entire system and allows the determination of complex properties. One important characterization technique is the visualization of structure in three dimensions. This is typically done by assembling and aligning a large number of two-dimensional images. The final representation may then be combined with compositional, mechanical, electronic, and optical property measurements to give quantitative and complete descriptions of a material.

The experimental piece of this initiative will implement existing and new methods and technologies to characterize relevant properties efficiently and quantitatively during synthesis and processing or over a range of operating conditions and environments. *In situ* characterization techniques to determine materials properties during processing will be paired with computational tools to enable rapid screening of materials, reactions, and processes over a wide range of length and time scales. Experimental outputs will additionally be used to provide model parameters, validate key predictions, and supplement and extend the range of validity and reliability of the models.

Digital Data

Data — whether derived from computation or experiment — are the basis of the information that drives the materials development continuum. Data inform and verify the computational models that will streamline the development process. The goal of this initiative is not only to allow researchers to easily incorporate their own data into models but additionally to enable researchers and engineers to incorporate each other's data. The sharing of data will give each research or engineer a broader set of information to work with, which will render more accurate models. A data-sharing system would also facilitate multi-disciplinary communication between scientists and engineers working on different stages of the materials development continuum. The key to accelerating the rate of innovation is streamlining how data are incorporated into models and experiments and enabling data transfer between various software systems at different institutions. Data transparency is also crucial in the later stages of the continuum, after discovery. For product designers looking for a material with certain parameters, a system that would allow them to search for advanced materials would be invaluable. Enabling cross-industry applications will be an important piece of the Initiative.

Creating this data transfer system will be a challenge, but not an unprecedented one. Various innovative data transfer methods have been developed, for example, for sharing patient information between different hospitals. As described in a 2010 President's Council of Advisors on Science and Technology report on Health Information Technology, one viable option is tagging medical information with metadata that contains the patient's identifier and can be found via a simple crawl through all the hospitals' data.[11] The advantage of a metadata system is that once the data is formatted it can be incorporated into any number of software systems at different institutions for analysis. Standard formats for the different types of materials data let researchers easily understand and incorporate their colleagues' findings into their own models. Another potentially useful technology is cloud computing, which allows for efficient remote data storage and sharing of software applications. It will be necessary to devise new approaches to data storage specific to materials data to enable effective retrieval and analysis.

Issues surrounding intellectual property naturally arise during discussions of data. There is an unavoidable tension between the scientific need for openness and the industrial concern for protection of intellectual property. Indeed, to be effective, this initiative will need to harmonize with any number of business models. In the example of metadata tagging, participants would be able to tag certain pieces of data as private so that those data would not be included in the crawl. Whatever data-sharing model is adopted, it is essential for companies working at all stages of the materials lifecycle to be free to share information when they feel disclosure would yield a net benefit, yet still keep valuable intellectual property confidential.

The digital data contribution to this initiative will establish a data-storage and transfer system for materials researchers and engineers. The system implemented would preferably allow participating institutions to retain their legacy software systems but facilitate data transfer and efficiently integrate the new data into models. The system must also allow institutions to choose which of their data sets are searchable. In addition, this initiative will emphasize accuracy and verifiability of models and experimental tools being developed and support informatics research to enable the most effective retrieval and analysis of materials data in this new paradigm. Advanced data-sharing techniques at all stages of the development continuum will be the driving force behind the Initiative and help build the scholarly record.

Achieving National Goals Using Advanced Materials

The infrastructure created by this initiative will facilitate and expedite the discovery and development of a broad spectrum of advanced materials, to the benefit of scientific inquiry and the national economy. Some of our Nation's most pressing challenges — in areas such as clean energy, national security, and human welfare — could be addressed by advanced materials. This initiative will foster cross-sector and cross-disciplinary collaboration so that scientists and engineers working on related materials for different purposes can cooperate and provide a better result. The examples that follow are problems that reflect how diverse the field of materials science is and how broad an impact this initiative may have. They are mere examples, however, of the types of problems that could be addressed.

Materials for National Security

The Department of Defense and the national defense laboratories are significantly invested in materials research. The research labs work on advances in lightweight protection materials, electronic materials, energy storage, and bio-surrogate materials to name a few. While the Department of Defense uses advanced materials to protect and arm our troops, materials also play a role in many other areas of national security. Critical minerals are a relevant example.

Material Example: Finding Substitutes for Critical Minerals

Photo courtesy of ARS

Minerals are important components of many products civilians use in daily life (e.g., cell phones, computers, and automobiles), as well as crucial military applications (e.g., avionics, radar, precision-guided munitions, and lasers). According to a National Academies study, each person in the United States consumes, on average, 25,000 pounds of non-fuel minerals each year.[12] Yet the United States does not mine or process much of that raw material. The National Academies defines a critical mineral as one whose supply chain is at risk, for which the impact of a supply restriction would be severe, or both. Currently, the American manufacturing sector is struggling to maintain adequate supplies of critical minerals at reasonable costs. As the use of critical minerals increases, this supply shortage may be amplified unless additional domestic supply is identified and captured.

Many materials are referred to as "critical" because supply is highly concentrated in either one country or by a few corporate interests, and because they are used in the production of goods that are important economically or for national security. Today, there is particular concern about materials like platinum, tellurium, and certain rare earth elements because they are essential to the manufacture of products in key high-growth sectors, including clean energy, consumer electronics, and defense, among others. The discovery and development of technology substitutes that deliver the same functionality but replace critical minerals, like the rare earth elements, with those that are more earth-abundant is one strategy that would have the dual benefit of protecting our military capabilities while also addressing the growing dependence on any mineral resource, domestic or foreign, that are unstable or subject to supply disruptions. The infrastructure created by this initiative could assist researchers and engineers to rapidly discover and develop substitutes for technologies and applications that are currently dependent on these critical minerals for which no known alternative is available today. Such applications will range from personal electronics to missile guidance systems.

Materials for Human Health and Welfare

There are many applications for advanced materials to address challenges in human health and welfare — from biocompatible materials like prostheses or artificial organs to protective materials designed to prevent injury. Advanced materials designed to prevent traumatic brain injuries are one example with potential benefits across diverse user groups including athletes and military personnel.

Material Example: Preventing Traumatic Brain Injury

Traumatic brain injuries (TBI) occur when an external force impacts the head or body, leading to a loss of consciousness, amnesia, and/or alterations in normal brain function. An estimated 360,000 military personnel have been afflicted by a TBI during the conflicts in Iraq and Afghanistan, and each year 1.7 million civilians suffer from TBI due to falls and athletic/vehicle accidents. The medical costs and lost productivity of these injuries are estimated to exceed $60 billion annually.[13,14]

Suitably designed protective gear can prevent these injuries. Designing gear that accounts for the wide range of conditions and circumstances that can lead to TBI, however, presents a challenging materials problem. For example, advanced materials might be used in a host of protective technologies for military and passenger vehicles, body armor, and sports equipment to limit the devastating effects of blasts, impacts, and collisions. But in each circumstance, understanding the response of protective gear and the subsequent manner in which impact forces are transmitted to the brain (or body) is paramount for innovative and targeted materials solutions.[15] This initiative could provide tools to assess the requirements of these different applications, optimize materials designed for specific uses, and identify potential overlapping uses for materials in the military and civilian sectors.

Materials for Clean Energy Systems

Developing sources of clean energy and reducing our dependence on oil are key national priorities. Materials research can help us find new technologies such as better catalysts for the production of biofuels, artificial photosynthesis to derive energy directly from sunlight, novel high-efficiency solar photovoltaics, and portable energy-storage devices. There are also many ways advanced materials could reduce dependence on oil in the transportation sector, as the following example points out.

Material Example: Reducing Oil Dependence for Transportation

Of the 12 million barrels of oil per day the U.S. imported from foreign sources in 2009, two-thirds was for transportation fuels.[16] Motorized road transport consumes around 19 percent of the global energy supply,[15] and aviation accounts for another 3 percent.[17,18] Improving fuel efficiency in the transportation sector is therefore an important target for decreasing oil consumption.

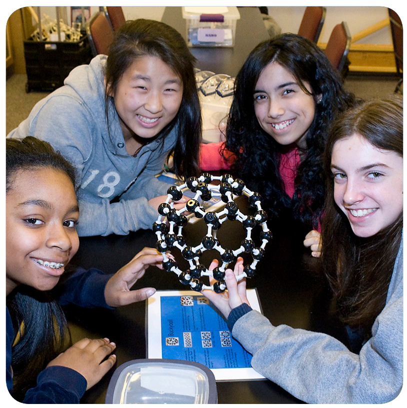
The development of new lightweight materials for vehicles could significantly improve fuel efficiency. Every 10-percent reduction in passenger vehicle weight in a conventional combustion engine car could reduce fuel use by six to eight percent.[19,20] Yet, to be successful, these lightweight materials would still need to meet the structural integrity and safety standards of more traditional materials in use today — for both commercial passenger vehicles and those designed for military deployment.

In addition, automobile companies are starting to deploy alternative vehicles such as hybrids, electric cars, and hydrogen fuel-cell-powered cars. The technologies used in these vehicles have great potential to replace conventional combustion engines, however there are unresolved issues limiting their widespread use. Current batteries have low energy density and take a long time to charge. Hydrogen fuel cells powerful enough to run a car use significant quantities of high cost metals.

This initiative could provide tools to optimize and deploy new materials such as high-performance, cost-effective, lightweight structural materials and better portable energy-storage devices that will address national economic and security challenges through the reduction of oil use in the United States.

Equipping the Next-Generation Workforce

It is clear that a new infrastructure for materials development will not solve real-world problems unless it is widely deployed. Equipping our next-generation workforce with the tools and approaches necessary to achieve our national goals will require stakeholders in government, academia, and industry to embrace and continuously expand the scope and contents of the materials innovation infrastructure. Investments must also be directed toward advancing a culture supporting the routine production and use of the tools developed, illustrating the opportunities and advantages it creates, and guiding its implementation and validation across the entire materials continuum — from education of undergraduates through the adoption of these paradigm shifts by industry.



The inherently fragmented and multidisciplinary nature of the materials community poses barriers to establishing the required networks for sharing results and information. One of the largest challenges will be encouraging scientists to think of themselves not as individual researchers but as part of a powerful network collectively analyzing and using data generated by the larger community. These barriers must be overcome. Rapid advances in materials discovery and design will be realized not merely through one-on-one interactions or pre-existing relationships, but also through multiple layers of collaboration among government agencies, academia, and industry. The Initiative will develop and support a coordinated effort to establish the infrastructure and protocols to facilitate collaborations among academic, government, and industrial participants, both by function (experimentalists, engineers, theoretical scientists, and computer scientists) and institution (academia, government research laboratories, small and medium enterprises, and large companies). New partnerships will also be stimulated between manufacturers and software developers to rapidly convert science-based materials computational tools into engineering tools.

By expanding and facilitating more integrated relationships, the Initiative will bring experimentalists, theorists, computer scientists, and engineers into closer proximity to work in the same research space. Furthermore, the digital data aspects and open platforms that call for more transparency and easy access to data will facilitate a more integrated materials community, thereby expediting the development of more accurate models, highly reproducible and validated work, and a better understanding of materials properties and product design.

Support for advanced computation and experimental tools will provide basic research opportunities that will serve to educate researchers, faculty, and students in the critical aspects of contributing to and applying the infrastructure from discovery to deployment. This includes the increased use of modeling and simulation along with understanding how these must be coupled with new experimental and characterization tools.

University involvement with the foundational science and engineering problems will further encourage materials scientists and engineers to learn how to integrate their knowledge into quantitative tools that materials and systems design engineers can use to identify, optimize, and speed product development. A natural consequence of this integrated and coordinated research approach will be the introduction of new cross-disciplinary courses in undergraduate and graduate curricula that put into practice the fundamental tenets of the Materials Genome Initiative.

An added benefit is that the computational toolsets developed through this initiative will become an integral component of all engineering programs, allowing students to explore "what if" scenarios as part of their regular coursework. This exploratory approach will instill in them the fundamental principles of integrated discovery that underlie this initiative, and ensure that the next-generation of scientists and engineers are empowered to fully exploit the power of this new infrastructure, while continuing to expand the tools and knowledgebase on which future advances will depend.

Finally, an important extension of these educational efforts into the industrial sector will be continuing education programs to enhance the skills of professionals in industry, who will have an important role as implementers of these materials innovations. Professional societies serving the materials community can utilize and leverage their existing education infrastructure, experience, and expertise to further advance this goal.

While this document does not describe specific policy actions for implementation of the Materials Genome Initiative, it does suggest next steps toward achieving the vision outlined here. The Administration will begin a "road mapping" exercise on all pieces of the materials innovation infrastructure — for example, by convening workshops between government agencies, industry, national labs, and universities to elicit suggestions for policy, infrastructure design, and the identification of high priority foundational science and engineering problems. While some government agencies have existing programs that will connect to the goals of this initiative, in FY 2012 the Obama Administration has requested $100M in support for multi-year programs that will launch various components of the Materials Genome Initiative. These programs are across: the Department of Energy (DOE), the National Institute of Standards and Technology (NIST), the National Science Foundation (NSF), and the Department of Defense (DOD)

While all aspects of this initiative will be coordinated among the participating agencies, this budget request includes the following new targeted activities:

1. The DOE Office of Science and NSF will work together to enable the development, maintenance, and deployment of reliable, interoperable, and reusable software for the next-generation design of matter. The DOE, through its *Computational Materials and Chemistry by Design* program, and NSF, through aspects of its *Cyberinfrastructure Framework for 21st Century Science and Engineering,* will coordinate activities on the development of high quality production software toolkits that both incorporate new algorithms and allow for interoperability with existing software tools.
2. In support of their advanced software programs, both the DOE and NSF will also coordinate activity in the development of next-generation characterization tools that provide the fundamental basis for development of and validation of the algorithms and software tools.
3. An *Advanced Materials by Design* program led by NIST will target the development of standards infrastructure, reference databases, and centers of excellence that will enable reliable computer modeling and simulation for materials discovery and optimization. This activity will be coordinated closely with the DOE and NSF efforts on software and experimental tool design.
4. The DOD will invest in basic and applied computational materials research directed toward enhancing performance and accelerating transition of advanced materials to meet a broad array of national security needs and maintain a technological advantage in defense systems along the full materials continuum from discovery through deployment, including maintenance and recovery of assets. These efforts will be integrated across the science and technology programs of the military services (i.e. Army Research Labs, Office of Naval Research, and Air Force Research Labs).
5. DOE's Energy Efficiency and Renewable Energy *Next-Generation Materials* program will leverage computational tools to accelerate manufacture and characterization of new materials for energy technologies. It will invest in such areas as: new materials used in manufacturing processes, new hybrid composite material systems with improved materials properties and lower manufacturing cost, modeling and simulation tools for predicting spatial and temporal variability of new materials, and tools for rapidly verifying fitness of new materials for intended use.
6. NSF and DOD will play a lead role in addressing the next-generation workforce goals by: facilitating new partnerships between the relevant science and engineering communities in academia, government and industry to promote a culture supporting and embracing the use of the capabilities developed within this initiative; and engaging with students and colleagues to develop the culture and relevant training of the next-generation workforce.

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Conclusion

In summary, advanced materials are essential to human well-being and are the cornerstone for emerging industries. Yet, the time frame for incorporating advanced materials into applications is remarkably long, often taking 10 to 20 years from initial research to first use. The Materials Genome Initiative is an effort that will address this problem through the dedicated involvement of stakeholders in government, education, professional societies, and industry, to deliver: (1) the creation of a new materials-innovation infrastructure, (2) the achievement of national goals with advanced materials, and (3) the preparation of a next-generation materials workforce to sustain this progress. Such a set of objectives will serve a more competitive domestic manufacturing presence — one in which the United States will develop, manufacture, and deploy advanced materials at least two times faster than is possible today, at a fraction of the cost.

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About This Document

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