EXECUTIVE OFFICE OF THE PRESIDENT OF THE UNITED STATES

MATERIALS GENOME INITIATIVE STRATEGIC PLAN

A Report by the

SUBCOMMITTEE ON THE MATERIALS GENOME INITIATIVE

COMMITTEE ON TECHNOLOGY

of the

NATIONAL SCIENCE AND TECHNOLOGY COUNCIL

November 2021

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The Subcommittee on the Materials Genome Initiative (SMGI) defines and coordinates Federal efforts in support of the goals of the Materials Genome Initiative (MGI) and identifies policies that will accelerate deployment of advanced materials. SMGI also tracks national priority needs that would benefit from MGI, identifies extramural activities that connect to MGI goals, and explores ways the Federal Government can advance the development of the Materials Innovation Infrastructure. More information is available at https://www.mgi.gov/.

About this Document

The Materials Genome Initiative was launched in 2011 to accelerate the discovery, design, development, and deployment of new materials, at a fraction of the cost, by harnessing the power of data and computational tools in concert with experiment. The 2021 Materials Genome Initiative Strategic Plan updates and replaces the previous strategic plan released December 2014, and reflects the significant advances that have been made over the past ten years. This document provides a vision to align the MGI community across the continuum from research and development through deployment, and identifies goals for the next five years with objectives and actions to be taken by the community to advance the MGI.

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Abbreviations and Acronyms

3D	three-dimensional
AI	artificial intelligence
AM	additive manufacturing
DMP	data management plan
DOC	Department of Commerce
DOD	Department of Defense
DOE	Department of Energy
DOI	Department of the Interior
DOS	Department of State
FAIR	findable, accessible, interoperable, and reusable (data)
HBCUs	historically black colleges and universities
HGP	Human Genome Project
HHS	Department of Health and Human Services
ICME	integrated computational materials engineering
MGI	Materials Genome Initiative
MII	Materials Innovation Infrastructure
MIP	Materials Innovation Platform
MSI	minority-serving institution
MURI	Multidisciplinary University Research Initiative
NASA	National Aeronautics and Space Administration
NIH	National Institutes of Health
NIST	National Institute of Standards and Technology
NMDN	National Materials Data Network
NSF	National Science Foundation
NSTC	National Science and Technology Council
OMB	Office of Management and Budget
OSTP	Office of Science and Technology Policy
R&D	research and development
STEM	science, technology, engineering, and mathematics
U.S.	United States
USDA	U.S. Department of Agriculture
USGS	U.S. Geological Survey
USPTO	U.S. Patent and Trademark Office

Executive Summary

The Materials Genome Initiative (MGI) was launched in 2011 to accelerate the discovery, design, development, and deployment of new materials, at a fraction of the cost, by harnessing the power of data and computational tools in concert with experiment. Significant advances have been made by scientists and engineers from academia, industry, and government in both expanding understanding and building the foundation of the required infrastructure of models, computational and experimental tools, and data. Using the existing foundation as a springboard, this strategic plan identifies three primary goals to guide the community over the next five years to expand the impact of the MGI.

While the MGI approach has already led to the accelerated deployment of advanced materials in select applications, realizing the full potential of the initiative will help the Nation and the world build back better from the effects of the global pandemic. Rapid design, development, and use of new materials will enable infrastructure such as roads and bridges that last longer, a more resilient and efficient energy system, reduced dependence on critical minerals, higher-quality health care delivery, and better, smarter, and more useful technologies that power our economy and maintain our national security.

The ability to rapidly share materials knowledge among scientists, engineers, and manufacturers yields accelerated discovery and fabrication of more capable materials, better tools to design devices and structures with materials, and more efficient manufacturing. This knowledge sharing is at the heart of the MGI, and it is realized through the Materials Innovation Infrastructure (MII): an evolving and dynamic accessible framework of seamlessly integrated advanced modeling, computational and experimental tools, and quantitative data. The MGI seeks to provide access to tools for knowledge exchange in a way that maximizes opportunities for contributors from all of America, especially in communities that have traditionally been left behind. By expanding capabilities and reducing barriers for engagement, the efforts described here will have a profound impact among educators, researchers, and manufacturers.

Expanding and fully utilizing the MII requires attention to its physical infrastructure, theoretical developments and computational tools, robust data curation that enables the application of artificial intelligence (AI) and other revolutionary capabilities, and the human genius that fills American laboratories, engineering studios, and industrial shop floors. The MGI Strategic Plan acknowledges the roles of all stakeholders along this continuum of distinct scientific disciplines and technological maturation. Through an examination of the current materials research and implementation landscape, this strategy document defines three primary goals for the next five years:

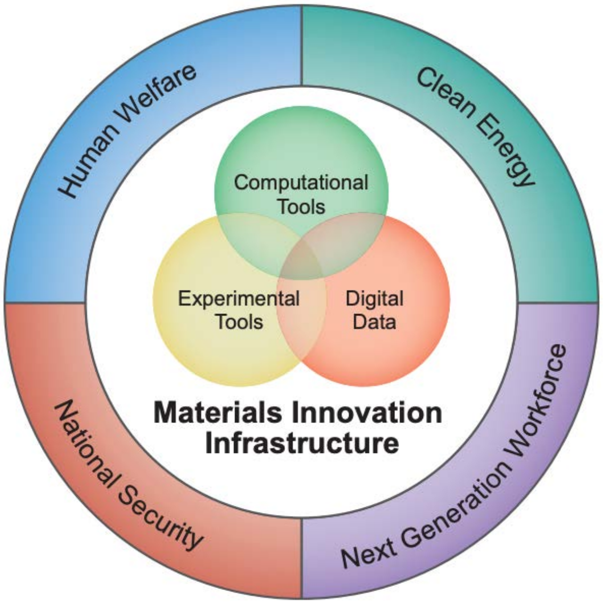
1. Unify the Materials Innovation Infrastructure
2. Harness the Power of Materials Data
3. Educate, Train, and Connect the Materials R&D Workforce

This strategic document elaborates on the rationale and motivations for the three primary goals introduced above. In doing so, objectives and supporting actions are identified and presented with the intent of guiding the work of the full MGI community to realize an ecosystem uniquely optimized for the accelerated discovery, development, and utilization of materials knowledge to address critical challenges such as climate change. Achieving these three goals is also essential to U.S. competitiveness in the 21st Century and will help to ensure that the United States maintains global leadership in innovation of emerging materials technologies in sectors including health, defense, and energy, and to broadly support technologies of the future.

Introduction

Throughout the ages, materials have defined civilizations. From chipped stones for effective tools to the semiconductors that power the most sophisticated computers today, the ability to manipulate materials has led to advances that benefit humankind. The Materials Genome Initiative (MGI) was launched to accelerate the discovery, design, development, and deployment of new materials by harnessing the power of data and computational tools in concert with experiment. Significant advances have been made under the auspices of the MGI, including the formation of a strong community of researchers, engineers, and manufacturers and the establishment of the Materials Innovation Infrastructure (MII) consisting of modeling, computational, and experimental tools and data. The MGI includes the entire materials continuum from discovery through use. In advanced manufacturing, the MGI supports new materials fabrication techniques for a range of applications, including additive manufacturing, and accelerates the availability of materials with the unique properties required for new product innovation in areas as diverse as quantum information sciences, space exploration, sustainable energy development, and biotechnology.

The MGI was launched ten years ago with a grand vision. It encompassed not only the work of materials scientists and engineers but aimed to use quantitative data and computational codes to discover and predict material behavior as a function of composition, processing, and service history—and most important, those predictive capabilities were meant to be captured in computational tools that interact seamlessly with the engineering tools that are used in system design, manufacturing, and maintenance decisions.



The founding conceptual structure of the Materials Innovation Infrastructure

Linking knowledge from first principles quantum mechanical calculations through the entire life cycle of a product is ambitious. It requires multiple codes at various length and temporal scales that are dynamic and iterative. It requires attention to a broad spectrum of phenomena, the relative importance of which vary by application and industrial sector. It requires quantitative characterization and the instruments that capture material feature and property data efficiently with the appropriate level of precision. Yet, it is not impossible. At the onset of the MGI there were isolated examples of where significant returns on investment had been demonstrated when such linkages were made. The MGI was formed as a community to expand the number of materials systems and applications benefitting from the integrated computational approach by providing more effective means of sharing data and communicating knowledge and understanding among the diverse researchers and practitioners who advance materials from discovery along the continuum of technological maturation and product life.

This strategic plan reflects the current materials research[1] and implementation landscape and identifies goals, objectives, and supporting actions required by the full MGI community[2] to realize the accelerated development and utilization of materials knowledge for a robust and secure future. The three primary goals to guide the community over the next five years are to: (1) unify the Materials Innovation Infrastructure; (2) harness the power of materials data; and (3) educate, train, and connect the materials research and development workforce.

To unify the MII is to make the individual tools more valuable, and access to them more readily available. As additional research disciplines and industrial sectors engage and explore the MII, existing capabilities will be challenged and improved. Recognizing this powerful and integral relationship between the use and strengthening of the innovation infrastructure, the MGI will incentivize interdisciplinary teaming to identify gaps for further work and create opportunities for expanding reach and enhancing efficiencies. Imminent leaps in computational power, instruments for more rapid and precise synthesis and characterization of material structure and properties, as well as modeling enhanced by artificial intelligence (AI) and machine learning must be embraced to realize the full potential of the MII. Of equal importance are the platforms that incentivize and enable integration of increasing volumes of data and understanding to be shared easily among all stakeholders along the materials development continuum. To meet current and emerging needs of the full spectrum of the MGI community, special emphasis is placed on establishing a National Materials Data Network (NMDN).

Materials data powers the innovation and exploitation of materials research and technology. Artificial intelligence techniques offer the potential to markedly increase the utility of that data by accelerating research and uncovering insights at remarkable speeds. Ensuring that the MGI community is poised to take full advantage of AI requires, among many issues, attention to curation of data that is interoperable and reusable and that formally acknowledges the generators of data. Additionally, AI-driven techniques must be developed specifically for the MGI community. High-impact examples span from autonomous control of research instrumentation to enhanced process and quality control systems for manufacturing.

As the MGI community concomitantly builds upon and harnesses technological advances emerging at increasingly rapid rates, a diverse, agile, and adaptive workforce that is prepared to fully utilize new tools and thrive becomes imperative. Informed by analyses of competencies required by academic,

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[1] Materials research is defined by the broad intersection of many disciplines, including chemistry and chemical sciences, materials science and engineering, physics, biology, mathematics, and other engineering disciplines and research domains, enabling myriad technological advances that benefit society and provide the fuel that feeds innovation. Systems and products for health care and wellbeing, energy and environmental stewardship, manufacturing and economic competitiveness, and national security are driven by advances inspired in the laboratory and brought to practice only with the contributions of many talented researchers and practitioners who bring their unique expertise and perspectives as ideas progress to tangible, implemented capabilities.

[2] In this plan, the "MGI community" is referenced frequently. This broad term is meant to encompass both the stakeholders invested in achieving the goals of the MGI and the numerous supporting communities providing the intellectual and technical means to attain those goals. Members of the MGI community include students, teachers, researchers, developers, and practitioners from academia, industry, and government.

national, and Federal laboratory researchers and industrial practitioners, the MGI community will emphasize development of curricula. This includes K-12 science, technology, engineering, and mathematics (STEM) education through university graduate student programs that promote fluency in data science and informatics, computing and modeling, experimentation and characterization, as well as critical aspects of materials science, manufacturing, and sustainable development. Further, recognizing the inherent and complex interdisciplinary nature of materials research and development, opportunities for internships and multidisciplinary team assignments will be encouraged in undergraduate and graduate curricula. Filling the knowledge gaps along the materials development continuum will require expansion of training programs and creation of new job opportunities.

Achieving these three goals will be critical to addressing global challenges and will help ensure that the United States maintains leadership in the innovation and utilization of emerging materials technologies that underpin manufacturing, healthcare, sustainable energy production, industrial innovation, and safeguarding U.S. national and economic security.

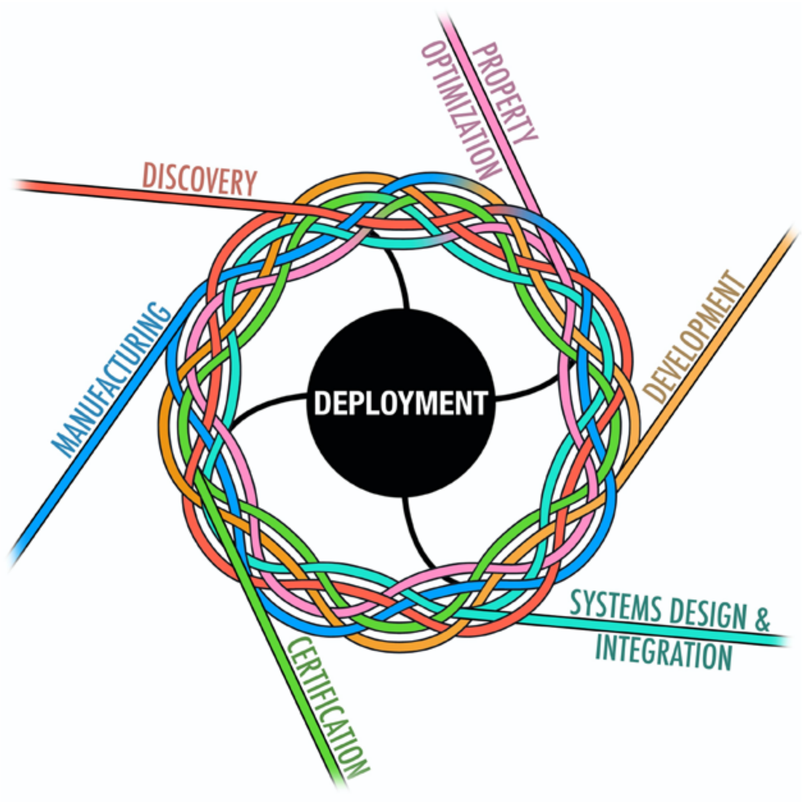
Goal 1. Unify the Materials Innovation Infrastructure

The Materials Innovation Infrastructure provides a national framework to generate, manage, integrate, and share knowledge to accelerate materials research and development (R&D), manufacturing, and deployment. This national framework encompasses the entire materials development continuum with integrated and iterative coupling from new discoveries and fundamental research advances to engineering design and manufacturing. It will enable the use of deep and vast materials knowledge to accelerate translation of innovations to product development, certification, and deployment. The materials R&D enterprise is inherently interdisciplinary. The MII must leverage the tools and knowledge developed in the numerous disciplines that place the understanding and control of matter at their core, including chemistry, physics, materials science, biology, the full range of engineering disciplines, as well as insights from computer science, software engineering, applied mathematics, and statistics. The MGI can further maximize its impact by capitalizing on the breadth of capabilities across the Nation, working to integrate the talents and experiences from all regions and underserved communities.

Over the past decade, the Federal agencies have fostered the development of the main elements of the MII through the implementation of the MGI. These elements include:

- Computational (theory, modeling, and simulation) tools.
- Experimental (synthesis, characterization, and processing) tools.
- Integrated research platforms.
- Data infrastructure.

Attaining the bold vision of the MGI now depends on unifying these elements into a broadly accessible and tight-knit network. Unification requires filling in the gaps and strengthening the connections across the broad U.S. portfolio of materials R&D, from discovery through deployment, across industry, national and Federal laboratories, and academia. The MII will facilitate the exploration and use of the full range of material properties, the synthesis and processing methods to produce a material, and the manufacturing techniques necessary to incorporate that material into a product. The data generated during materials R&D is vast and heterogeneous, encompassing diverse electronic, atomic, and molecular phenomena; processing effects on multiscale material properties and performance; application design; and manufacturing know-how. Management of this data will require the MGI community to coordinate and establish common protocols for seamless sharing of heterogeneous data sets.



The MGI paradigm promotes integration and iteration of knowledge across the entire materials development continuum. Unification of the MII will provide a framework for seamless, convective flow of information and a weaving of knowledge among all stakeholders contributing to the materials R&D enterprise, accelerating the deployment of new materials.

Recent studies and reports[3] have emphasized that new experimental tools coupled with computational tools and facilities are needed to automate materials synthesis and characterization across all materials classes.[4] Opportunities to access these coupled tools can be found at research centers and national user facilities, but access to these scarce resources is highly competitive and cannot meet the full needs of the MGI community. Furthermore, support for sustainable operation and maintenance of the tools is an ongoing challenge. Federal agencies have been exploring programs[5] that aim to automate synthesis and characterization protocols via the use of modular robotics, machine learning, and inverse design concepts. A mechanism to expand these efforts and accelerate the development of tools across the vast array of materials classes is the establishment of a national agenda of grand challenges with focused efforts to build the infrastructure for the materials needed to meet those challenges.

Another driver for the unification of the MII is to substantially lower the entry barriers and increase access for smaller companies and less resourced academic institutions, powering innovations across a diverse pool of research scientists and engineers, developers, product designers, and manufacturers.

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[3] *Frontiers of Materials Research: A Decadal Survey*, The National Academies Press, Washington, DC, 2019.

[4] Here materials classes refers to types of materials, e.g. polymers, metals, ceramics, composites, etc.

[5] http://mission-innovation.net/wp-content/uploads/2018/01/Mission-Innovation-IC6-Report-Materials-Acceleration-Platform-Jan-2018.pdf

This view of the MII informs the strategy of how to best unify and amplify its impact. Specifically, over the next five years the following strategic objectives are vital to advancing Goal 1:

1. Bridge, Build, and Bolster Elements of the MII.
2. Establish a National Materials Data Network.
3. Accelerate Adoption of the MII through National Grand Challenges.

Objective 1: Bridge, Build, and Bolster Elements of the MII

A major consequence of a unified MII will be the efficient and "convective" flow of knowledge along the entire materials development continuum. The creation of knowledge from the MGI paradigm requires not only the appropriate experimental and computational tools, but also a framework that can store and share the data and software produced by the research community. The MII will be dynamic and adaptive in order to respond to the need for new tools generated by the iterative process of knowledge sharing. In an effort to successfully bridge, build, and bolster the elements of the MII, Federal agencies will need to collaborate with the MGI community to understand the current status of computational, experimental, and data infrastructure tools. The growing computational power that will soon reach the exascale (10^{18} floating point operations per second—flops), experiments that are producing massive data sets, and automated synthesis techniques that can systematically produce vast numbers of new materials, highlight the urgency to build a unified MII. The vignettes included below highlight the efficacy of MGI-based approaches to dramatically accelerate the development and application of materials knowledge, the vast breadth of applications, and the diverse teams needed to realize a unified MII infrastructure.

Computational Tools

A combination of algorithmic and hardware advances has led to a phenomenal increase in computational power over the past four decades. This has made many real-world materials problems tractable. Federal agencies have responded to these developments with targeted projects for data repositories, data science and analytics approaches, as well as computational materials and chemical sciences centers and software institutes charged with developing and distributing broadly applicable, open-source, community software. Other program efforts include integrated computational science and applied mathematics activities for improved algorithm development, co-design of next-generation hardware and software for exascale computing, and integrated experimental programs for validation of predictive materials theory to drive new model development in a feedback loop.

Early projects focused on advancing high-throughput quantum mechanical calculations of molecules and materials, leading to curated databases supported by software tools for automated computational workflow, data mining, and knowledge extraction, and are now being enhanced by the recent inclusion of AI approaches. These computational tools and data cover most classes of materials and are now used worldwide by many research communities. Efforts are underway globally to integrate these resources.[6]

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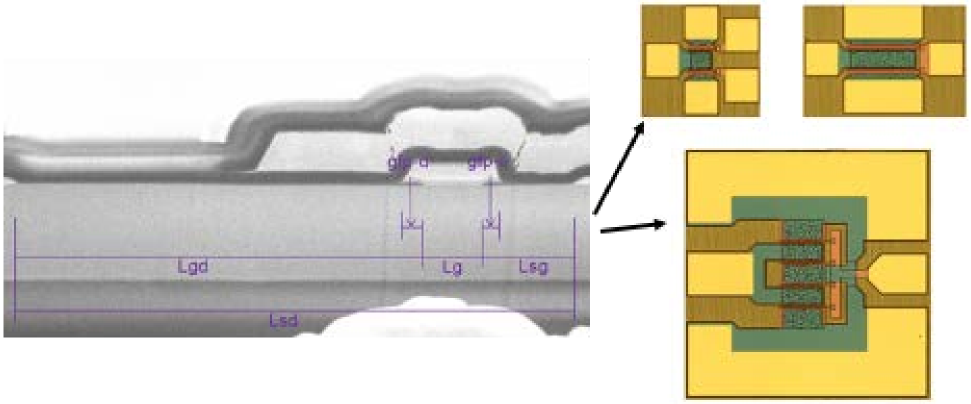
[6] https://www.optimade.org

MGI Vignette — *Engineering predictable behavior into GaN devices: An approach to accelerating design and optimization*

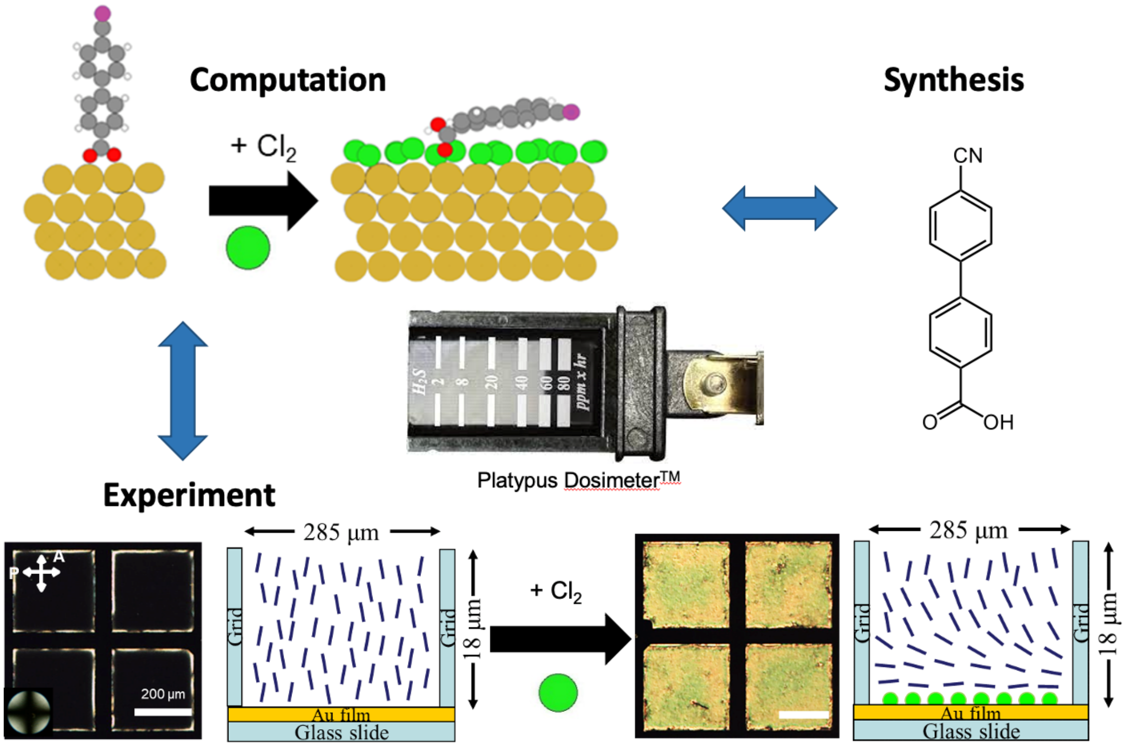
Like the shift from propeller to jet power, gallium nitride (GaN) transistors promise more speed, power, and agility to everything emitting radio or microwave power: radar, electronic warfare, and communications systems. This comes with initial cost and reliability concerns, especially for the most risk-averse applications, because the new technology has different characteristics than the old. DOD has developed a program in partnership with industry that endeavors to build a GaN transistor circuit model that covers a broad swath of process performance, design, and usage space to benefit the entire U.S. industrial base. In the spirit of the MGI, this program seeks to improve upon today's "point circuit models" that predict performance characteristics in a narrow electrical, thermal, and process range, and that rely on proprietary test datasets. Instead, this activity seeks to create a complete "computational toolset" that will include all relevant physical effects needed to fully model performance and reliability within the design phase and prior to expensive system integration. This program has already successfully demonstrated the initial design toolset, capturing those effects for the first time for this industry, by implementing GaN physics of failure as part of the circuit design process to optimize a GaN device. Both circuit and system designs are included early in the design phase, with the primary objective of reducing the number of iterative design/build/test cycles, along with attendant reductions in development cost and time delays. The integrated modeling tools that result from this program will enable the U.S. industrial base to more efficiently develop and deliver transformational capabilities to the U.S. Air Force.



Thousands of transistors within unique devices having varied micrometer-scale physical dimensions were manufactured. The electron micrograph cross section (left) has many possible transistor designs (three examples at right) that were tested over many thermal and electrical loading conditions. Graphics from Air Force Research Laboratory. See https://doi-org.wrs.idm.oclc.org/10.1016/j.jcrysgro.2019.04.008.

MGI Vignette — *DMREF: Accelerating the deployment of toxic gas sensors*

A collaborative team from Cornell University, Kent State University, and the University of Wisconsin-Madison, supported by the NSF Designing Materials to Revolutionize and Engineer our Future (DMREF) program, has employed the MGI philosophy to accelerate the design and deployment of metal alloy surfaces for chemoresponsive liquid crystals (LCs). Whereas the design of the first LC chemical sensor for hydrogen sulfide took almost ten years to complete, by iteratively developing over four generations of progressively more sophisticated computational chemistry models of competitive interactions of LCs and targeted chemical species with metal cation binding sites, the team has managed to shorten the timeline for design of chemoresponsive LCs to a few months per analyte. The designs of liquid crystals that respond to chlorine gas, which emerged from cycles of feedback between computations and experiments, enable the sensing of concentrations of chlorine gas as low as 200 ppb within 15 minutes, which satisfies Occupational Safety and Health Administration (OSHA) personal exposure limits. The team has extended this work to address the design of nerve agent (NA) sensors based on the competitive binding of NAs and liquid crystalline compounds on metal salts. NAs pose a great threat to society because they are easy to produce and are deadly in nature, which makes developing methods to detect, adsorb, and destroy them crucial. This team has collaborated with an industrial partner, ClearSense™, to develop wearable liquid crystalline sensors for monitoring human exposure to toxic gases. This research has also led to the discovery that machine learning techniques can uncover valuable feature information in the liquid crystal response that has not previously been recognized, and as a result, sensor accuracy increased from 60% to 99%. Results of the project are disseminated through the Chemoresponsive Liquid Crystal Research Database, where a built-in analyte search feature enables the efficient identification of the most promising liquid crystal designs for a desired analyte.



Computations predicted (top left) that chlorine gas will displace liquid crystals on metallic gold surfaces to give an optical response. A thin gold film and liquid crystals (top right) were synthesized. Experiments confirmed a change in the optical output of the system upon exposure to chlorine gas (bottom). The technology has been deployed in a commercial sensor (center). See http://ls-staging.doit.wisc.edu/liquid-crystals/.

To achieve the full potential of the MGI, a grassroots community movement is required to create and validate data and its transformation through the MII into the deeper knowledge that informs the creation of new, transformative materials. The community that develops models and software is typically much smaller than those who could make productive use of them. Complicated, research-grade computer codes need to be transformed into robust and sufficiently user-friendly software that meets the needs of novice user communities in industry, academia, and national and Federal laboratories. Ideally, such scalable software should run efficiently across the entire spectrum of computing platforms, from a laptop to the exascale supercomputer. In addition, pathways need to be identified and supported to bolster the long-term development and maintenance of codes and software packages. Cross-disciplinary research programs that include computer science, applied mathematics, information technology, and materials science can be used to bridge research disciplines and accelerate algorithm and software tools development. In parallel, more conventional software development and support models, mixed with co-design principles, will continue to play an important role in this evolving field. The commercial software industry can play a critical role through the incorporation of the newest, community-developed, algorithms and techniques into broadly accessible codes. Actions the MGI community should take to bridge, build, and bolster computational tools, a central element of the MII, include:

- Identify and bridge the current computational tool gaps, especially those that present barriers to accessibility to the diversity of stakeholders along the materials development continuum.
- Leverage and build on the national computational infrastructure by nurturing the development of community codes, and the incorporation of these techniques into commercial codes.
- Build connections to and strengthen collaboration with related communities to bolster cross-disciplinary computational research and tool sharing and development.

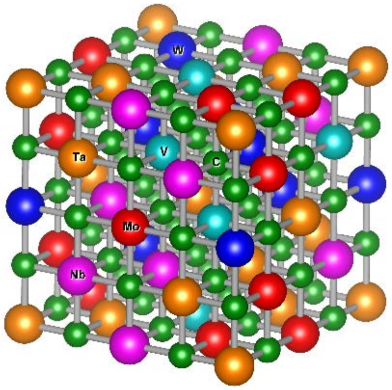
Experimental Tools

Materials are intrinsically hierarchical, from the atomic to the product scale. Such hierarchies pose formidable challenges to ensure adequate experimental and computational coverage of the vast spatial (from angstroms to meters) and temporal (picoseconds to years) domains. Experimental tools to measure changes in structural, chemical, and physical properties that have advanced the understanding of materials are found at x-ray, neutron, microscopy, and high-magnetic-field facilities as well as in laboratories for electron, ion, and laser spectroscopy. Many of the best characterization techniques still rely on sample preparation methods that are extraordinarily time-consuming and may modify or destroy the structures associated with the most interesting properties. More multimodal characterization tools, including non-destructive techniques, are needed to help mitigate this challenge and enable comparative data to be garnered from a single sample. The chemistry community has made significant strides in automation of synthetic chemistry, which is informing efforts in complex materials systems. Advanced tools for synthesis and processing are now available for materials research, some with atomic-level control of composition and structure and extensive diagnostics capabilities for iterative feedback optimization and control. However, the “best” of these tools are

MGI Vignette — *Seeking materials with high melting temperature and structural stability*

What is the highest melting temperature material one can conceive, and how would you make it? That deceptively simple question is actually unimaginably complicated. Materials that are able to maintain their load-bearing capability to the very highest temperatures in extreme environments will enable technological achievements such as advanced manufacturing tooling and leading edges for hypersonic aerospace vehicles. But understanding the factors that influence interatomic bonding and then harnessing the controlling physical mechanisms to deliver such materials has been elusive until now. A Multidisciplinary University Research Initiative (MURI) award supported by the Office of Naval Research is applying integrated computational materials engineering (ICME)-based and MGI-based approaches to design ultrahigh-temperature ceramics (UTHCs) with enhanced hardness to meet this challenge.

The project is focused on UHTCs, also called high-entropy ceramics, by combining carbon, nitrogen, and boron with refractory metals (Hf, Mo, Nb, Ta, Ti, V, W, and Zr) to produce complex atomic structures that are predicted to be harder and have higher melting temperatures than previously known ceramics. The team is using the automatic FLOW (AFLOW) repository with a partial occupation method to rapidly generate distinct quasirandom unit cell configurations and screen them for synthesizability and stability at elevated temperature. Then, employing accelerated synthesis and analysis techniques, the team of materials scientists and engineers has demonstrated several compositions with a Vickers hardness up to 50% higher than those predicted by a simple rule-of-mixtures calculation. This promising result illustrates that materials discovery of combinatorially complicated systems like this can only be accomplished in a sufficiently fast and affordable way with ICME and MGI concepts.



A high-entropy carbide HEC-16: MoNbTaVWC$_5$ that forms a single phase with spark plasma sintering. It was designed, synthesized, and tested using MGI-facilitated strategies. Graphics from Duke University. See https://www.nature.com/articles/s41524-020-0317-6.

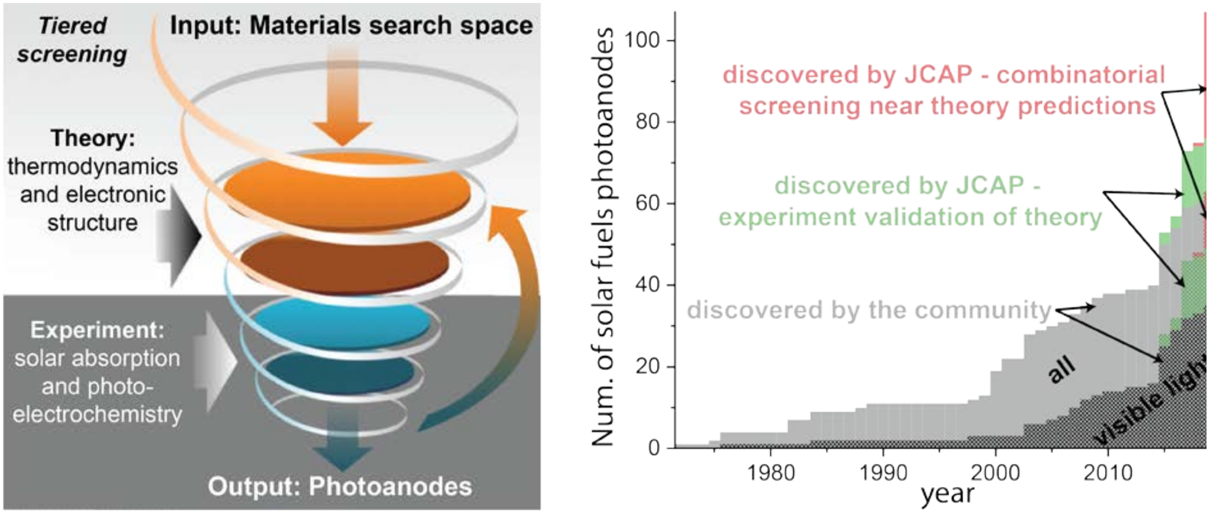
typically limited to specific materials classes and/or to small quantities of materials (e.g., thin films and nanoparticles). To generate the vast quantities of experimental data needed to validate and drive refined predictions from theory, modeling, and simulation, advances in experimental tools, especially high-throughput instruments for integrated synthesis, characterization, and processing, are needed. Availability and access to experimental tools critical to materials R&D is often through user facilities, research centers, or specialized platforms. This can be especially daunting for potential industrial users. Streamlined and inclusive access policies to the tools and to the associated expertise will be critical to advance the MGI.

To accelerate and expand the acquisition of experimental tools, the MGI community and Federal agencies should work together to:

- Develop a strategy to expand synthesis and processing tools to more materials classes and to develop multimodal characterization tools.
- Leverage advances and bolster development of modular, autonomous, integrated, high-throughput experimental tools—from lab to manufacturing.
- Identify and remove barriers that limit access by a diverse user community, including Historically Black Colleges and Universities (HBCUs) and other Minority Serving Institutions (MSIs), to state-of-the-art instrumentation.

MGI Vignette — *Integrated research drives the creation of materials knowledge for clean energy*

The Department of Energy supports the MII and creation of materials knowledge through integrated research at its Energy Innovation Hubs. Their mission is to discover, understand, control, and deploy clean energy solutions for energy storage in batteries and fuel from sunlight. The Joint Center for Artificial Photosynthesis (JCAP) finds new and effective ways to produce fuels using only sunlight, water, and carbon dioxide. Solar fuel technologies require durable and scalable materials that evolve oxygen from water to enable fuel synthesis. Researchers at JCAP integrated combinatorial synthesis with high-throughput electrochemistry to discover 49 ternary oxide photoanodes, 36 with visible-light response for oxygen evolution, which equals the number of photoanodes with visible-light response discovered in the 50-year history of solar fuels research. Computational guidance of high-throughput experiments has been particularly effective in dramatically increasing the list of metal-oxide photoanodes for water splitting and hydrogen production, motivating a new era of photoanode development where the characterization and optimization techniques developed on traditional materials are applied to next-generation photoanodes that exhibit visible-light photo response. The accelerated discovery of photoanodes illustrates success via harnessing the complexity of metal oxides.



JCAP discovers metal oxides having sufficiently low photon energy onset for efficient solar photoelectrochemistry. See https://solarfuelshub.org.

Integrated Materials Platforms

As the MGI community works to bridge the computational and experimental tool gaps and expand integrated capabilities to span more materials classes, a new type of platform must emerge. Many research centers and user facilities provide a substantial data infrastructure allowing fast analysis on-site and integration with experimental tools. However, national integrated materials platforms are required to fully break down barriers between materials discovery and deployment by providing workspaces (both real and virtual) for materials discoverers and innovators (scientists and engineers) to generate, communicate, and circulate knowledge with materials/product designers and manufacturers in a way that does not currently exist in the United States or worldwide. These integrated materials platforms would serve as innovation "nodes" of the MII, engaging and providing access among stakeholders along the entire materials development continuum. Indeed, these platforms will provide the crucial infrastructure needed to address the grand challenges discussed in Objective 3. Federal agencies and the MGI community should:

- Convene workshops to build community and identify incentives and barriers to collaboration.
- Identify pilot projects to seed the development of integrated materials platforms.
- Learn from industrial exemplars of integrated materials platforms.

Data Infrastructure

Materials data and its integration is essential to the success of the MGI. Data generated from experiments and simulations can be extraordinarily rich—often expressing many complicated and complex phenomena. The potential value for reuse across a number of applications is extremely high, and therefore critical to accelerating materials R&D. The unification of the MII hinges upon the successful creation and integration of the emerging data management capabilities that were non-existent a decade ago.

A recent study[7] outlined the requirements and current status of the U.S. materials data infrastructure and enumerated a set of priorities for achieving a sustainable and broadly useful set of resources to accelerate materials R&D and bolster the MII. The recommendations can be synthesized into four main themes:

1. Establishing and sustaining data repositories and analysis tools.
2. Integrating these distributed resources into a federated system.
3. Continuing to engage with researchers to inform them of existing capabilities, and, critically, to determine how the infrastructure meets, or fails to meet, existing needs.
4. Developing incentive mechanisms to accelerate adoption of the materials data infrastructure.

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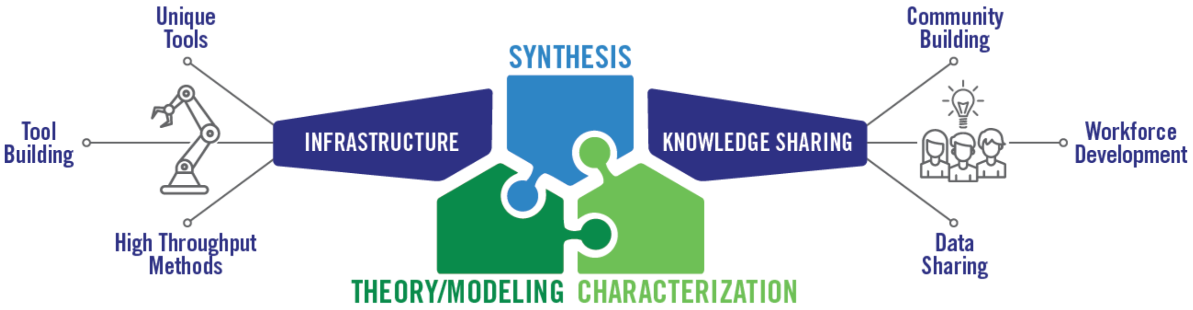
[7] www.tms.org/portal/PUBLICATIONS/Studies/portal/Publications/Studies/Studies.aspx

MGI Vignette — *Materials Innovation Platforms (MIPs) — MGI-enhanced by infrastructure and knowledge sharing*

The National Science Foundation launched the MIP program in 2016 to create a new kind of national user facility. Two sets of platforms, established in 2016 and 2020, fulfill critical national needs for crystal growth and for materials-biology convergence to develop new materials.

The core of MIPs is the MGI approach, with tightly integrated activities of materials synthesis, characterization, and theory/modeling. Research infrastructure is crucial to the operation of the MIPs, consisting of a suite of experimental and computational tools that democratizes access and attracts hundreds of users nationwide. The 2016 MIPs feature molecular beam epitaxy for depositing a majority of the elements in the periodic table including alkalis, the world's first floating-zone furnace under 300-atm pressure of reactive gases, a transmission electron microscope with world-record spatial resolution, and reactive force field codes for two-dimensional materials that have been downloaded by hundreds of researchers. *De novo* glycan synthesis, automatic gene assembly, and robotic synthesis of non-petrochemical-based polymers anchor the 2020 MIPs. Knowledge sharing is a signature feature of MIPs. By design, each MIP is a scientific ecosystem, where materials researchers share tools, codes, samples, data, and know-how, as well as training of the next generation of scientists. MIPs enable the entire community of researchers to immediately benefit from the latest developments and to also build upon and improve them through the open exchange of ideas. The MIP program represents a new modality for research and training, for the purpose of accelerating discovery and development of new materials and novel materials phenomena/properties, as well as fostering their eventual deployment.



MATERIALS INNOVATION PLATFORMS

PARADIM — AN NSF MATERIALS INNOVATION PLATFORM
2D Crystal Consortium — NSF Materials Innovation Platform
BioPACIFIC — Materials Innovation Platform
GlycoMIP — NSF Materials Innovation Platform

(Top) Key MIP ingredients. (Bottom) [PARADIM](#) and [2DCC MIP](#) on electronic and quantum materials were launched in the inaugural class, in 2016. [BioPACIFIC MIP](#) and [GlycoMIP](#) on biomaterials and polymers were established in 2020. See https://www.nsf.gov/funding/pgm_summ.jsp?pims_id=505133.

The MGI has been successful in spurring action in theme 1, with numerous databases of computed and experimental data providing insights into materials design and manufacture.[8] Yet, there is still a great deal of work to be done to achieve the desired levels of integration and utility for the materials R&D enterprise (that is, themes 2 and 3). Furthermore, the incentives in theme 4 for adoption remain outside the research mainstream. To successfully build out and integrate the materials data infrastructure requires the identification of existing gaps in that infrastructure, a concerted effort to bridge those gaps,

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[8] https://materials.registry.nist.gov/

and the identification and use of best practices for utilizing the data infrastructure. To achieve much of this desired integration will take significant engagement across the MGI community, which is explored fully in Objective 2.

Any discussion of dissemination of data and associated tools naturally results in a discussion around intellectual property and export-controlled information that, for a variety of reasons, cannot be shared. Successful implementations of MGI concepts must exist in harmony with these constraints, either by instantiating MGI infrastructures within secure environments, or by creating vetting procedures, as has often been the case, that flag sensitive information. The MGI community will lean heavily on the security community to provide these solutions, because in general they lie outside the domain expertise of MGI practitioners.

In addition to efforts to identify and bridge data infrastructure gaps, there are specific actions that the Federal agencies can take to incentivize best practices in data management. Over the past decade, most Federal funding of materials research has mandated a comprehensive data management plan (DMP). Ideally, a DMP provides the details of how the data will be discoverable and accessible by other researchers and provided in a way that ensures maximum usability. These ideas fall under the so-called "FAIR" data principles, which posit that research data should be findable, accessible, interoperable, and reusable.[9] A number of Federal agencies, such as NIH, have recently embraced FAIR data requirements for funded research.[10] Such an undertaking will require significant efforts on the part of funding recipients, must be done in a staged manner, with an ongoing assessment of impacts on research, and in concert with a rollout of the data infrastructure that makes it possible. Actions by Federal agencies to foster unification of the MII include:

- Create tools, standards, and implement policies to encourage FAIR data principles.
- Support the bridging, building, and bolstering of data infrastructures.

Objective 2: Foster a National Materials Data Network

The materials data infrastructure is critical in the overall unification of the MII. It is in this context that the need for a coordinated, community-led alliance, here called a National Materials Data Network (NMDN), becomes clear. The NMDN can drive the creation and integration of the materials data infrastructure. The generators and users of data span the materials development continuum, from pure research to the manufacturing shop floor, to recycling, and at each point on the continuum is a knowledge resource for all. There are robust communities where best practices and classes of materials data can already be obtained, and as the materials data infrastructure builds out, it must integrate these resources and learn from their successes. The NMDN will drive the further development and integration of the data infrastructure and work to solve the incentive problems (detailed below) that currently impede its adoption.

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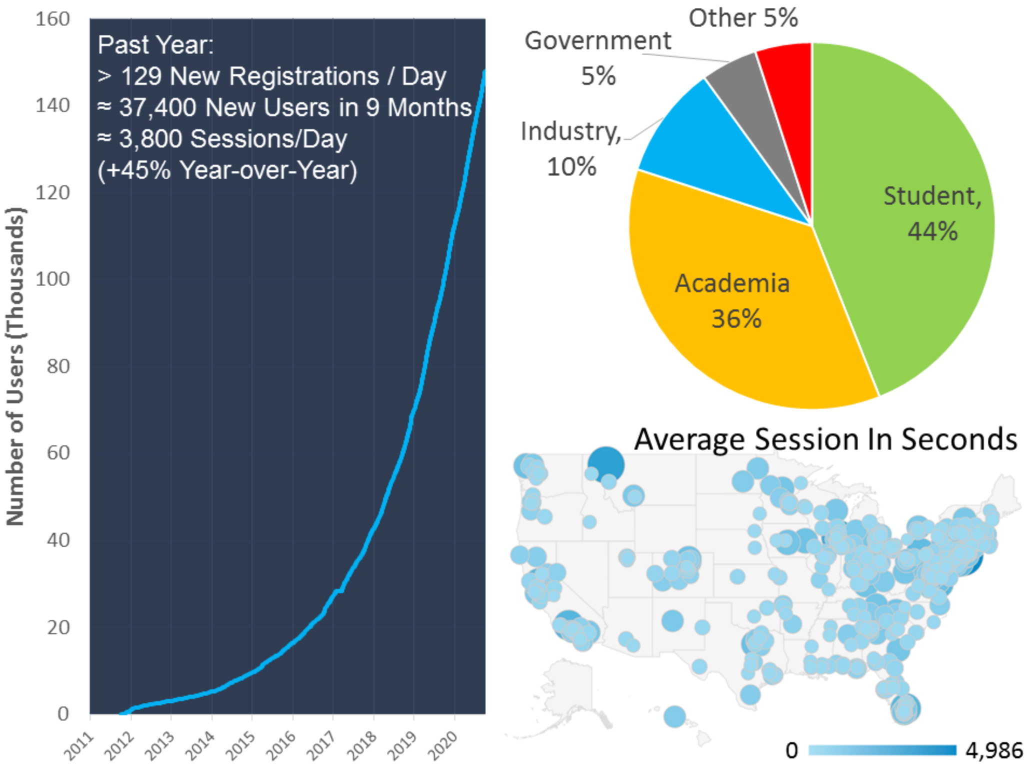
[9] Wilkinson, M., Dumontier, M., Aalbersberg, I. *et al.*, *Sci Data* **3,** 160018 (2016).

[10] https://grants.nih.gov/grants/guide/notice-files/NOT-OD-21-013.html

MGI Vignette — *Adoption of data tools*

Early builders of the MGI materials information infrastructure assembled data on hundreds of thousands to millions of compounds and made them available online in public repositories. These data can be used by scientists and engineers to search for previously unknown materials or to find materials with specific properties that may not have been measured. The Materials Project at Lawrence Berkeley National Laboratory has more than 140,000 registered users worldwide and users in every U.S. state. Currently the Materials Project contains more than 131,000 compounds, 49,700 molecules, and 530,000 nanoporous materials. This extensive database, with an arsenal of sophisticated workflow and analysis software, was developed and deployed to predict several new battery and photoanode materials that were made and tested in the lab. Recently, new transparent conducting oxides and thermoelectric materials were identified using a combination of computational and experimental screening along with high-throughput approaches.



Growth, demographics, and usage of the Materials Project by registered users.
See https://materialsproject.org/.

Addressing the Stakeholder Incentive Challenge

The materials R&D community is extremely heterogeneous. This presents considerable challenges for the data infrastructure and is reflected in the unevenness of the infrastructure's maturity across the diverse breadth of materials R&D. Part of the challenge is how stakeholder needs are articulated. A sizeable fraction of the materials R&D community does not yet see the entire value proposition in having a materials R&D data infrastructure, and the community does not speak with a single voice on the need for it. Part of the role of the NMDN is to provide a coherent voice to both articulate this need and to illustrate the value and potential impact of the data infrastructure on materials R&D.

There are grass-roots efforts in the materials R&D community attempting to address these issues. Recent conferences[11,12] were convened to explore how to improve the materials data infrastructure and enable accelerated materials discovery to deployment. The materials community has identified the need to foster entities in the spirit of an NMDN to leverage strengths and push forward better capabilities and stronger integration of materials data resources.[13] The NMDN can serve as a clearinghouse for best practices in materials data management, capabilities, and stakeholder needs, and serve to foster excellence in data stewardship throughout the community. Actions to support a NMDN include:

- Identify, collaborate with, and support community efforts towards creating an NMDN.
- Develop a framework for coupling and integrating public and private data repositories.
- Pilot efforts in automated data workflows from experimental equipment to data repositories.

Identifying and Bridging Gaps

Ensuring that the NMDN is informed by the broad diversity of stakeholder needs and perspectives is both essential to its success and a significant challenge. As the NMDN details the stakeholder requirements for the materials data infrastructure, the process of deploying that infrastructure moves to the fore. The NMDN then must transition the infrastructure from its present state, characterized by a wide variety of independent efforts, to a tightly integrated whole that can deliver on the promise of MGI with faster discovery to deployment of advanced materials and a subsequent driving force to enable new technologies.

The gap analyses discussed earlier are crucial, but the existing infrastructure providers must also work together to realize the desired integration. The NMDN should create a governance model that includes materials data infrastructure providers, data generators, data and computer scientists, and representative stakeholders to guide integration by identifying and prioritizing projects based on needs and tractability. This leadership team could in turn help the community speak with a coherent voice.

While a coherent voice will certainly help, achieving such goals will take a lasting commitment from industry, academia, and government, working in concert, albeit with varying goals and missions. A distributed and federated materials R&D data infrastructure landscape will propel materials R&D to previously unreachable performance and productivity levels. This reality will then augment buy-in as the value of a coordinated materials data infrastructure becomes apparent, and, where lacking, spark improvement. A focus on grand challenges can help demonstrate the significant return on investment associated with the development of a materials data infrastructure.[14] To further solidify its leadership role, the NMDN will foster "grand challenge R&D" as detailed in Objective 3.

The ultimate success of the NMDN will be measured by the deployment of a robust materials data infrastructure with users around the entire materials development continuum. In driving such change, the data generators, both large and small, will play a critical role in both the supply and demand considerations that the NMDN must address. Taking the lead from other disciplines, where large instruments like telescopes, the Human Genome Project, and particle accelerators have driven the creation of successful data infrastructures, the NMDN should coordinate with integrated materials R&D platforms as detailed in Objective 1. These platforms are generating enormous amounts of data,

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[11] Convened in Rosemont, IL on November 21–22, 2019, and virtually Feb 23-25, 2021, with NSF support.

[12] M. Akyol et al., *Matter,* 1, 1433–1438, December 4, 2019.

[13] https://www.marda-alliance.org/

[14] T. Scott et al., "Economic Analysis of National Needs for Technology Infrastructure to Support the Materials Genome Initiative," https://www.nist.gov/system/files/documents/2018/06/26/mgi_econ_analysis_brief.pdf.

requiring storage and ease of access to information to support their respective research communities. The demands of the user communities who need the data will help the NMDN refine its strategy and drive the evolution of the MII. Actions supporting the success of an NMDN include:

- Identify and bridge gaps, and unify existing data infrastructures.
- Develop data exchange standards and protocols.
- Identify complementary international efforts for collaboration where practical.
- Develop and implement sustainment strategies, including data infrastructure roadmaps.

Objective 3: Accelerate Adoption of MII through National Grand Challenges

Widespread adoption of the MII will accelerate materials development to address national needs in energy, healthcare, defense, and consumer technologies. Many of these issues are deeply connected with global concerns such as climate change, sustainable manufacturing, critical materials supply chains, environmental mitigation and remediation, and countless other areas where new materials act as core enablers of transformative technologies.

Encouraging the MGI community to rally around addressing grand challenges through targeted activities is a potent means to accelerate adoption of the MII. Adoption can be accelerated through the promotion of MGI successes, raising awareness of the potential inherent in the MII. Concurrently, the MGI community must be brought together to define and develop solutions to national grand challenges through MGI-driven R&D. Additionally, there is a singular opportunity to define several Human Genome Project-scale efforts in the materials space that could lead to extraordinary breakthroughs in human welfare and economic and national security.

Raising Awareness and Building Community

Considerable progress has been made under the auspices of the MGI. Highlighting these successes demonstrates the opportunities afforded by the MGI approach and raises awareness within the materials R&D enterprise regarding the value in the existing capabilities of the MII as well as its potential scope. These practical successes are articulated via publications, patents, reported manufacturing efficiency gains, etc. Existing elements of the MII, such as software tools, experimental capabilities, and computational resources, must be showcased to drive stakeholder participation and evolution. Additionally, events where MII developers can interact and collaborate can drive deeper integration, which in turn further increases the value of the MII.

Part of the engagement process is clear articulation of the MGI value proposition. The MII may be viewed as a means to move the field beyond the notion that archival manuscripts are the ultimate research product. That is, a modern publication is greatly enhanced by the inclusion of data, models, and other encapsulations of materials knowledge into a readily usable form.[15] These types of success stories for the MGI have been unevenly distributed across materials systems and subdisciplines.

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[15] e.g., Qresp: http://www.qresp.org/

MGI Vignette — *An MGI approach to new dielectric polymers for wound film capacitors*

Energy-dense, easily manufactured, affordable capacitors are essential components for climate-sensitive power distribution. They must also be reliable and exhibit graceful failure, which means that if they are damaged the response is a measured reduction in performance rather than a sudden extinction. Metallized polymer-wound film capacitors are a natural choice. The energy stored in a film capacitor is proportional to the product of the dielectric constant and the square of the dielectric breakdown strength. The state-of-the-art polymer is biaxially oriented polypropylene, BOPP. It has a very high breakdown strength due to oriented crystallites, but also has a low dielectric constant due to the non-polar nature of the alkyl chains. The Office of Naval Research invested in the pursuit of other polymers that could store more energy. However, the chemical space of organic polymers is huge, raising the question, “Where does one start?”

In a recent MURI project led by the University of Connecticut, an MGI approach was employed, emphasizing computation with strong feedback from experimentation (polymer synthesis and chemical, morphological, and electronic characterization). Researchers used high-throughput density functional theory (DFT) to probe chemical space and identify materials with high dielectric constant and high dielectric breakdown. With computations on hundreds of materials, they noted an expected trend as nearly all materials fell on a line that showed as the dielectric constant increased, the breakdown strength decreased. More interestingly, there were outliers.

Key to the success of the research effort was the balanced, iterative input between computation and experimentation. Synthesis pathways for some compounds did not exist. Feedback from synthesis experts identified closely related materials that could be made, and new computations centered on these were carried out to identify the most promising materials. These materials were synthesized and characterized, which in turn led to more cycles of computation, synthesis, and characterization, and eventually to promising families of new dielectric materials.

For a film to be useful for capacitors, it needs to be processable to very thin thicknesses (4–20 micrometers) without pinholes, flaws, and with less than 5% thickness variation. Reel-to-reel processing used to manufacture large volumes of films provides many parameters that can be monitored in-line and manipulated. With quantitative understanding of the parameters that can be controlled during fabrication, the computation/synthesis/characterization process was applied to the most promising new materials to find optimal properties that, in turn, provided predictable processing windows. Recently, with the benefit of the data generated to date, machine learning approaches to materials design are being incorporated into the discovery-to-manufacturing continuum for advanced dielectric films and advanced capacitors.

Creating the next generation of wound film capacitors. See https://doi.org/10.1002/adma.201600377.

Additionally, the materials R&D enterprise is highly diverse, drawing from many disciplines, with all sorts of material types and processes spanning basic research to industrial application. It will be crucial to foster deeper connections between academia and industry, allowing for cross-fertilization of the best ideas of materials researchers with the best of designers and manufacturers. This could be pursued by creating analogous entities to the extremely successful National Academies of Sciences, Engineering, and Medicine Chemical Sciences Round Table,[16] or similar more specific entities. Agencies could then use the findings of such roundtables to inform the creation of new programs to more deeply connect academic, governmental, and industrial research. Actions to increase MGI stakeholder integration with the MII include:

- Engage with manufacturers to identify critical capabilities the MII can address.
- Develop opportunities for sustained engagement with industry, academia, and government.
- Promote activities and methods to promulgate successes and tackle our greatest challenges.

Meeting National Needs and Addressing Global Concerns

Full unification of the MII is a truly ambitious goal that will only be achieved by broad engagement across the full spectrum of the materials development continuum. The MGI community has an enormous opportunity to both meet national needs and address global concerns. These third-millennium challenges including climate change, environmental degradation, energy storage, renewable power generation, critical materials substitution, advanced healthcare technologies that rely on new biocompatible materials, new manufacturing capabilities that address the lack of resilience in existing systems, and improved materials to rebuild an aging physical infrastructure. The reverse argument is also true. Overcoming the challenges that the Nation faces will, from the perspective of the MGI, *require* a unified MII. Thus, the solution to these third-millennium challenges proceeds hand-in-hand with the unification of the MII.

While the development of new materials manifestly plays an important role in tackling our greatest challenges, the specifics of where the critical breakthroughs remain will vary by application. The MGI community must be brought together to define, roadmap, and solve these challenges. Actions that can be taken to address national needs and address global concerns include:

- Convene a series of third-millennium challenge workshops.
- Develop a multiagency effort to foster MGI community unification of the MII around third-millennium challenge problems.

Learning from the Human Genome Project

When the MGI was rolled out in 2011, the Human Genome Project (HGP) was an extraordinarily useful analogy. It neatly conveyed the concept that the development of deep knowledge of materials through the construction of the MII would lead to great advances. However, there is a case to be made that there are a number of HGP-inspired efforts that are within the remit of the MGI that could take the analogy significantly further and could greatly spur progress in general.[17] Such an undertaking would have enormous long-term benefits, further unify the MII, and also help push efforts focused around grand challenges going forward. As such efforts evolve, they will drive the cost of further progress down, in a virtuous loop of discovery and technological advancement. Indeed, the first human genome sequence cost more than a hundred million dollars, and now one can obtain a sequence for about $1,000.[18]

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[16] https://www.nationalacademies.org/our-work/chemical-sciences-roundtable

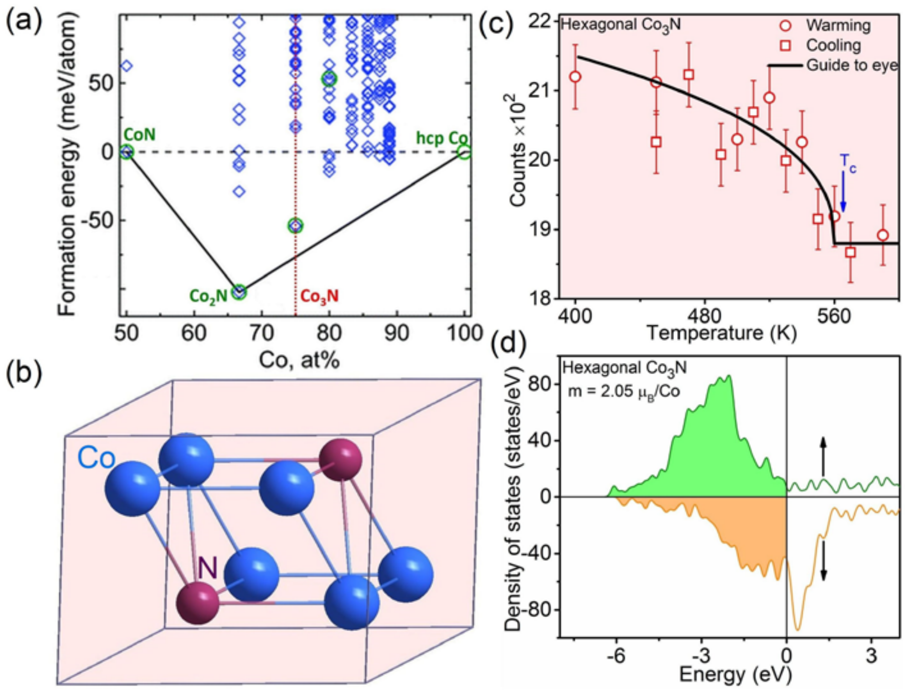
[17] http://nap.edu/11108

[18] https://www.genome.gov/about-genomics/fact-sheets/DNA-Sequencing-Costs-Data

MGI Vignette — *Securing America's future through rare-earth-free magnets*

Magnets are key components in modern technologies including electrical vehicles, wind turbines, medical equipment, cell phones, and computers. Most high-performance permanent magnets contain rare-earth elements such as neodymium (Nd) and dysprosium (Dy). These "strategic" elements are of particular importance to improve performance in permanent-magnet applications. The demand for rare-earth-based high-performance permanent magnets continues to grow, putting economic and national security pressure on the supply of rare-earth elements. China produces 97% of all rare-earth elements, and their mining can have detrimental impacts including the release of dangerous radioactive elements such as uranium into the environment.

A collaborative DMREF team from the University of Texas at Austin, University of Nebraska-Lincoln, and Iowa State University has employed the MGI philosophy to accelerate the design of rare-earth-free magnetic materials. Specifically, they have developed an open-access database of magnetic materials to facilitate a data-intensive machine-learning design of new rare-earth-free magnets. The database currently has over 3,800 entries. The team has demonstrated that its data-intensive methods improve efficiency of the experimental fabrication of new rare-earth-free and Pt-free magnetic materials and has predicted and synthesized a set of several cobalt nitride compounds that exhibit high magnetocrystalline anisotropy and Curie temperature (necessary properties for commercial applications). In order to translate promising magnetic materials toward application, the team has partnered with the Air Force Research Laboratory and industry.



(a) Calculated formation energies for new Co-N compounds. (b) Experimentally synthesized hexagonal Co_3N structure using cluster deposition. (c) Neutron diffraction data showing magnetic transition $T_c \approx 550$ K. (d) Total density of states revealing strong ferromagnetism. See https://www.novomag.physics.iastate.edu/structure-database.

The general idea behind such efforts is to identify a core set of measurements or computations, that, when amassed, forms a foundational resource that can be mined for deep insight and predictive power. The advent of advanced AI techniques has further enhanced the predictive power of these databases. Some of the early successes in these HGP-inspired MGI projects include the wide variety of density functional theory databasing efforts. While these efforts have yielded substantial insights and predictive capacity, there is even more to be gained through the amassing of experimental data. Experimental HGP-inspired MGI efforts are much rarer due to several factors, the most salient being cost, although there are some exceptions.[19] Yet, with the advent of autonomous laboratories, it is quite conceivable that such efforts are now within reach, and the potential payoffs could be orders of magnitude greater than the investments. Given the enormous diversity in materials scales and processes, the challenge in these cases will be to identify the classes of experiments that should be conducted. Actions that can be taken to realize new HGP-inspired MGI efforts include:

- Conduct a series of workshops and studies to identify the highest risk-reward opportunities.
- Support the creation of HGP-style data and knowledge resources for materials R&D.

Goal 2. Harness the Power of Materials Data

The strategic value of a deployed materials innovation infrastructure was detailed in Goal 1. Goal 2 builds upon these ideas, leveraging and augmenting the materials innovation infrastructure to enable the application of artificial intelligence[20] approaches to profoundly accelerate materials R&D. The following strategic objective will be pursued during the next five-year timeframe:

Objective 1: Accelerate Materials R&D Deployment through the Application of AI

It is clear that AI techniques have the potential to radically transform the materials R&D landscape, and the availability of high-quality materials data is essential to realizing this opportunity. The last few years have seen exponential growth in the publication of AI-enabled materials discovery, and yet the field is only in its infancy. While the MGI anticipated the data-driven trend, the recent surge in efforts has been breathtaking, and the community must react to fully leverage these developments.

AI provides a number of exciting opportunities for materials research. In general, a machine learning model of a material can be developed to provide predictive capabilities where traditional, physics-based models either do not yet exist, or remain so challenging (and slow) as to be too expensive in time or other resources to be useful. In fact, AI models can aid in the development of new physical models by elucidating previously hidden, complex relationships. Similarly, sophisticated use of AI tools will open opportunities for understanding increasingly complex systems. Of course, AI is a tool like any other, with advantages and disadvantages. As such it is not a panacea for materials R&D, and assessing the risks and benefits associated with each application of AI will form an important research topic in itself.

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[19] http://nanocrystallography.org/

[20] Here, the term AI is used interchangeably with machine learning (ML).

MGI Vignette — *Ensuring reproducibility in the application of AI to materials R&D*

The Center for Hierarchical Materials Design (CHiMaD) (https://chimad.northwestern.edu/), a NIST Center of Excellence, established the Materials Data Facility (MDF) (https://www.materialsdatafacility.org/) to build and maintain the data infrastructure for CHiMaD. In 2018, the MDF received support from the Department of Energy to create the Data and Learning Hub for Science (DLHub) (https://www.anscenter.com/). DLHub leverages existing CHiMaD data publication and sharing tools and builds a new set of capabilities to collect, publish, and categorize artificial intelligence models and other functions to be applied to data. DLHub allows others to run those models on leadership computing resources or in the cloud with a few lines of code, search among published models, and overall increase the reproducibility of machine learning applications to materials R&D (and beyond to the entire portfolio of scientific research). Example applications in x-ray science, batteries, and microscopy have been demonstrated.

The MDF/DLHub effort has now been further augmented through an NSF-supported collaborative Cyberinfrastructure for Sustained Scientific Innovation (CSSI) award to the University of Wisconsin-Madison and the University of Chicago that will smooth the interfaces between data providers (i.e., MDF) and AI-model providers (i.e., DLHub) (https://matmodel.engr.wisc.edu/products/). This effort seeks to collect and describe all of the best machine learning input datasets for materials and publish them in a well-structured format in the MDF. Concurrently, the DLHub will capture and describe the best AI models and build an interface to allow researchers to quickly pull data from MDF, including any number of well-aligned datasets, and execute the appropriate AI methods on DLHub for improved, reproducible, materials property prediction.

As discussed in Goal 1, one of the most exciting developments in AI approaches to materials R&D is the advent of "autonomous" materials research.[21,22] These approaches allow AI-driven robotic systems to develop hypotheses, synthesize and develop new materials based on such hypotheses, characterize the materials to determine their properties, ascertain if they are an improvement over previous iterations, and then specify the next round of synthesis or modification. In this way a "closed-loop" AI-driven system can rapidly iterate over processes and compositions in the search for the next great material. For relatively well-posed systems, including small molecule chemicals, preparation of monodispersed nanoparticles via flow syntheses, and use of an autonomous researcher for mechanical design, there has been significant progress (see vignette below). The opportunities for AI at scientific user facilities and for materials platforms to drive experiments in real time is within reach.[23]

"AI-Ready" Materials R&D Data

The raw inputs for AI approaches are, of course, data. Those data must either be generated by the materials researcher (via experiment or models) or harvested from already published data residing in the materials data infrastructure. As discussed in Objective 1 of Goal 1, achieving FAIR materials data can further the goals of the MGI. It also serves as a useful rubric for making materials data "AI-ready."[24]

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[21] Workshop on Autonomous Systems for Materials Development: https://www.nano.upenn.edu/autonomous-systems-for-materialss-development-workshop/.

[22] https://cen.acs.org/business/informatics/lab-future-ai-automated-synthesis/99/i11

[23] Basic Energy Sciences Roundtable on Producing and Managing Large Scientific Data with Artificial Intelligence and Machine Learning: science.osti.gov/-/media/bes/pdf/reports/2020/AI-ML_Report.pdf.

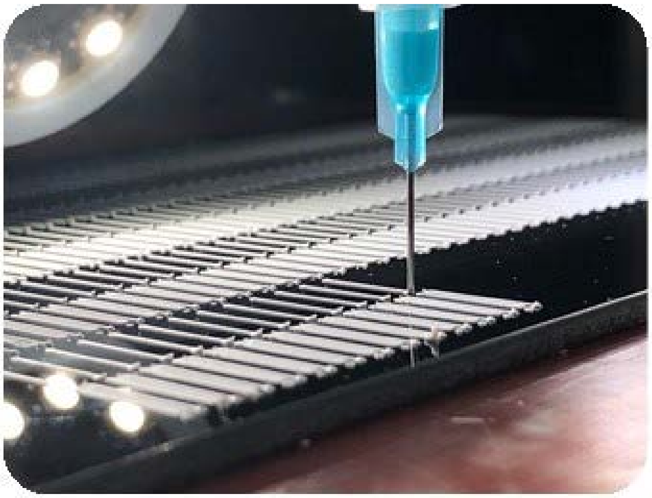
[24] Technical Report: *Data and Models: A Framework for Advancing AI in Science*: https://www.osti.gov/biblio/1579323-data-models-framework-advancing-ai-science.

MGI Vignette — *Using ARES OS™ software to build your own autonomous research robot*

Autonomous research systems have the potential to revolutionize the way research is done by using AI to drive robotic experiments over hundreds or thousands of iterations. Already, autonomous research robots such as ARES™ have learned to grow carbon nanotubes at controlled rates and optimized the structure of a 3D-printed twisted barrel to maximize energy absorption. However, to date, building a research robot has required significant investments in software development.

ARES OS™ has been freely available since the fall of 2020 as open source software from the Air Force Research Laboratory that researchers can use as a foundation to build their own research robots. With roots in autonomous robotics, ARES OS™ is architected to lower the barrier to entry to autonomous research systems by structuring hardware/software interface modules, analytical modules that provide feedback information, and planning modules that can use AI and machine learning to direct iterative experiments. ARES OS™ can save months or years of time compared to custom code.

Already several groups are evaluating ARES OS™, including in industry, academia, and government laboratories. ARES OS™ has been successfully deployed on three autonomous research robots to date, including for carbon nanotube synthesis, flow chemistry, and additive manufacturing.



ARES OS™ software drove an autonomous research system 3D (additive manufacturing) printer, AM ARES™, which taught itself to print simple structures controlling four independent parameters: Speed, prime delay, and X and Y offsets. Graphic from the Air Force Research Laboratory.
See https://afresearchlab.com/technology/successstories/polymer-and-responsive-materials-team/

While FAIR data cannot, in and of itself, make data AI-ready, it lays the crucial groundwork. The materials data infrastructure will ensure that data are both findable and accessible. One of the great potentials of AI for materials R&D is realized when the algorithms can be applied across disparate data sets. That, in turn, requires that the data has been curated in such a way that the information is interoperable (curated and presented in a manner that the data is machine-actionable with minimal human intervention) and reusable (data provenance is documented and appropriate uses for the data are understood). In this way, a crucial aspect of the strategy for the data infrastructure is directly linked to the application of AI to accelerating materials R&D. Actions to improve the utility of MGI data include:

- Build upon FAIR data policies to ensure more AI-ready datasets.
- Incentivize the implementation of FAIR data practices.
- Provide tools to assess the quality of data.
- Develop and incentivize the adoption of community-developed metadata standards.

AI-Driven Materials R&D for U.S. Manufacturing

A number of barriers exist before adoption of AI-driven materials R&D becomes pervasive and is transitioned to U.S. manufacturing. Yet, some companies have already established successful business models around this application, demonstrating that the primary impediments are not around the inherent value proposition. In order to eliminate the remaining barriers, the MGI must foster:

- Trust and associated understanding of the uncertainties in the results of AI.
- Widespread knowledge of the capabilities and limitations of these techniques.
- Ease of access to these techniques across U.S. manufacturing.
- Methods and tools to protect intellectual property as well as national defense resources.

In addition to accelerating materials exploration and development, AI can provide enhanced understanding and control of the materials processes used in manufacturing. Embedding AI approaches in the sensing and control systems of manufacturing processes enables instantaneous corrections to materials processing conditions to assure that performance and tolerance specifications are met with less variability. This translates to higher product yields and an ability to design components using tighter materials allowables. Furthermore, when health monitoring systems are installed during deployment of a product, measurement of material performance during operation becomes possible. These systems gather performance data during real-world product use, eliminating the assumptions and approximations necessarily made during laboratory testing. When implemented during product manufacturing and deployment, a natural feedback loop can provide refined AI models back to the materials R&D community. The availability of these AI models would allow researchers to better understand materials processes when implemented on the manufacturing floor, and also provide insights to more precise physics-based models of materials behavior during operation. Introduction of these improved materials models into new product development results in faster design and manufacture of improved products with higher yield and at lower cost. The National Science and Technology Council (NSTC) Subcommittee on the Materials Genome Initiative is coordinating with the NSTC Subcommittee on Advanced Manufacturing to harmonize their approaches and optimize engagement with industry. Ultimately, industry will play a vital role in shaping the agenda of the National Materials Data Network, and thereby help to get crucial data into the hands of industrial researchers, where it can be combined with proprietary data to accelerate R&D goals. Actions to accelerate AI-driven materials R&D by U.S. manufacturing include:

- Demonstrate application of materials-informed AI approaches to *in operando* manufacturing processes.
- Translate autonomous R&D techniques from the laboratory to the shop floor.
- Promote AI-driven techniques through workshops, symposia, and the articulation of third-millennium problems.

Goal 3. Educate, Train, and Connect the Materials R&D Workforce

The MGI requires a connected ecosystem that spans from fundamentals to application, in which fundamental activities are motivated and enriched by the complex challenges of designing *with* materials and new products, and applications are inspired by fundamental advances in the design *of* materials. Given this need, a range of talent sets is required, and new pedagogies are needed to educate and train from K-12 to graduate levels, and to train/retrain at the post-doctoral, faculty, and vocational levels. Success will require a diverse and inclusive workforce that can communicate across all components of the materials development continuum, with approaches to solutions as diverse as the workforce.

A key objective since the inception of the MGI has been "…creating a world-class materials workforce—that is trained for careers in academia or industry, including high-tech manufacturing jobs."[25] In light of the impact that AI is already having on scientific research and development, let alone society, training in data science is essential, as was noted in the recent NSTC Strategy for STEM Education.[26] Federal agencies have successfully encouraged and supported education and research programs that integrate and iterate between computation, experiment, and data-driven research, providing essential experiences for the next-generation MGI workforce. Further, significant changes have been undertaken by many colleges and universities across the Nation to better align materials science and engineering curricula with MGI goals, and students are being presented with new research opportunities that reinforce the fundamental materials curriculum through industrial experience and entrepreneurship. Such efforts in other MGI-relevant disciplines, including chemistry, physics, mathematics, and engineering, are being explored or are underway.

The MGI has the potential to further lead the charge to transform education and training by tackling persistent challenges in academia, including recruitment and retention, mastery of fundamental technical skills, and broader skills involving communication, ethics, shared leadership, and an awareness of cultural, social, environmental, and economic implications of materials. MGI is also, by its inherent interdisciplinarity, inclusive across the science, engineering, and math enterprise and offers a compelling platform to educate and train in a diverse, team-based environment.

Three strategic objectives will be pursued during the next five years to realize these benefits:

1. Address Current Challenges in Materials R&D Education.
2. Train the Next-Generation Materials R&D Workforce.
3. Connect Talent to Opportunity.

Objective 1: Address Current Challenges in Materials R&D Education

A recent report on the needs of the MGI workforce[27] identified three key competencies needed by materials researchers: data management, computation, and experimentation. Students need not be experts in all three areas but should be conversant in multiple topics across this spectrum. A recent review of the MGI similarly notes that students should be trained in both theory and experiment because there exist different jargons, working cultures, and expectations between experimentalists and computationally focused groups, as well as the array of science and engineering disciplines that are needed to realize the vision of MGI. Furthermore, it is now evident that STEM majors should be articulate in data science and in core teamwork and the broader skills emphasized above. While some departments and universities have pioneered efforts to encompass new MGI-inspired programs both at the undergraduate and graduate level,[28] and new programs are being rolled out,[29] acceleration and adoption of such approaches to education and training are needed at all education levels in support of the materials R&D enterprise.

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[25] National Science and Technology Council, Committee on Technology, Subcommittee on the MGI Initiative, *Materials Genome Initiative - Strategic Plan* (2014).

[26] National Science and Technology Council, Office of Science and Technology Policy, *Charting a Course for Success: America's Strategy for STEM Education* (2018).

[27] The Minerals, Metals & Materials Society, Creating the Next-Generation Materials Genome Workforce (2019).

[28] e.g., https://d3em.tamu.edu/ and http://engineering.buffalo.edu/materials-design-innovation.html

[29] e.g., https://digi-mat.ncsa.illinois.edu/ and https://aim-nrt.pratt.duke.edu/

Foundational K-12 STEM Education

MGI-inspired thinking can offer a transformational approach to teach and reinforce fundamental knowledge in STEM for primary (K-8) and secondary (9-12) education.[30] Students in these age groups are often adept at using electronic and data-related resources. Fostering strong support for science, technology, engineering, and math, including computer science (STEM/CS)[31] and focusing these talents on materials-relevant problems will provide a stronger foundation for student success and interest in materials research and relevant careers at an early age. Materials and associated disciplinary professional societies offer K-12 programs and elective high-school courses that teach the importance of materials to our everyday lives. These programs can be augmented, refined, and leveraged to include and accelerate data science literacy.[32] Actions the MGI community should take to enhance K-12 STEM/CS education include:

- Foster training in data science for K-12 science educators.
- Develop MGI educational materials for science museums, scouting, science fairs, and other extracurricular experiences.
- Unify, refine, and amplify materials and MGI-relevant disciplinary programs for K-12 students and educators.

Undergraduate Education

Academia has incorporated data-driven and computational techniques into undergraduate materials R&D curricula over the last decade. Various approaches include the development of professional certificate programs in integrated computational materials engineering,[33] the addition of advanced materials design and data science courses to traditional degrees, and the development of online and in-person courses in MGI-inspired approaches. Materials science and engineering (MSE) departments and other relevant disciplines including the chemical sciences have responded positively to data-driven and computational research training programs.[34] Several project-based, active-learning opportunities for undergraduate students have also been developed under the MGI.[35] Despite these advances, there is still a dearth of data-related relevant course offerings and experiential opportunities to satisfy the current growth of automation and artificial intelligence/machine learning in the existing materials workforce. To effectively educate undergraduate students in applying the MGI approach, college educators in relevant disciplines will need the tools and training to teach these principles. Development and distribution of online information, lectures, and courses will promote a broader impact of these resources.[36]

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[30] e.g., ASM Materials Camps, https://www.asmfoundation.org/teachers/materials-camps/year-one/.

[31] https://www.ed.gov/stem

[32] https://www.asmfoundation.org/teachers/k-12-grants/

[33] The National Academies of Science Engineering and Medicine, Integrated Computational Materials Engineering: A Transformational Discipline for Improved Competitiveness and National Security (2008).

[34] e.g., The NSF Division of Graduate Research (DGE) National Research Traineeship (NRT) Program provides one example.

[35] e.g., see https://skunkworks.engr.wisc.edu/, and vignette herein.

[36] e.g., Summer School for Integrated Computational Materials Engineering. See https://icmed.engin.umich.edu/.

MGI-inspired education that translates fundamentals into use cases will aid in recruitment and retention of a new cadre of young people searching for both societal relevance in their studies and a clearer view of future job prospects. These benefits also translate well to community colleges where unique opportunities exist to broaden workforce participation in the MGI enterprise. Actions by the MGI community to enhance undergraduate education to realize these benefits will include:

- Promote MGI-savvy curricula development.
- Create an MGI Educators Network.
- Enable MGI-focused undergraduate research and capstone experiences.
- Deepen ties and outreach to community colleges.

Graduate Education

Full realization of the MGI will require innovative MS and PhD graduates who lead the Nation in devising both computational and experimental methods to generate, validate, curate, and unify data and data structures needed for the MGI; and who navigate complex design spaces involving materials processing, structure, properties, and manufacturing as well as life-cycle, economic, sustainable development, and critical materials factors. To meet this challenge, interdisciplinary graduate programs will need to combine fundamental materials science expertise that spans from atomic to industrially relevant scales, computational and experimental approaches to deliver high-throughput data, informatics to enable inquiry-based thinking, and engineering design theory to guide complex, team-based decision making.

MGI-inspired graduate education should also provide the professional and technical skills to effectively communicate, collaborate, and lead interdisciplinary teams[37] while understanding the relevance, purpose, interdependence, and underpinnings of fundamental science and engineering training. Traditional graduate programs need to broaden participation by employing contemporary, effective learning mechanisms for a diverse and inclusive student population[38] and virtual training opportunities for those unable to participate in traditional class offerings. Graduate programs should also consider the development of interdisciplinary minors and graduate certificates with industry-relevant skills[39]. To put MGI education into practice, graduate programs should partner with industry, government and non-profit agencies to offer university, regional, and national MGI-based challenges that showcase entrepreneurial thinking and develop MGI-based communities and networking.[40] To summarize, actions to advance graduate education in MGI principles include:

- Develop and disseminate effective interdisciplinary programs and practices in data-enabled materials research, education, and training.
- Promote interdisciplinary graduate certificates with skills sets relevant to industry.
- Foster MGI-relevant internship and other experiential learning opportunities.

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[37] e.g., Data-Enabled Discovery and Design of Energy Materials effort at Texas A&M, https://d3em.tamu.edu/; vignette below.

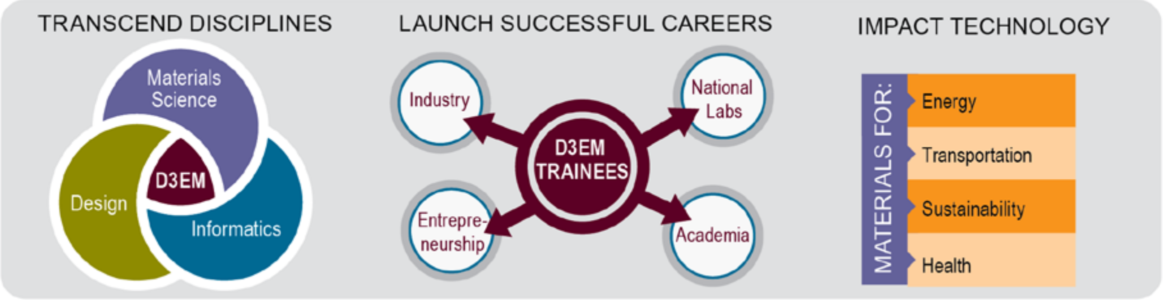
[38] The National Academies of Science Engineering and Medicine, *Graduate STEM Education for the 21st Century* (2018): https://www.nap.edu/catalog/25038/graduate-stem-education-for-the-21st-century.

[39] e.g., see CoMET: Computational Materials Education and Training, https://dftcomet.psu.edu/computational-minor/ and also SEAS: Data-Enabled Science and Engineering of Atomic Structure, https://www.mse.ncsu.edu/seas/about/.

[40] e.g., the "From Learning, Analytics, and Materials to Entrepreneurship and Leadership" (FLAMEL) Traineeship program at Georgia Tech helps students develop the skills and tools needed to pursue careers at the intersection of materials science, mathematics and computing: http://flamel.gatech.edu/goals.

MGI Vignette — *An MGI-powered curriculum*

Universities have begun to embed MGI principles into the undergraduate and graduate curricula, although much remains to be done. Modifying the undergraduate curriculum is challenging, given the highly structured nature of most curricula in materials science and engineering and related fields. At the graduate level, however, there tends to be considerably more flexibility in the curriculum, and several programs have developed comprehensive self-contained programs (as minors, certificates, or even specialized Masters-level degrees) focused on training graduate students on concepts related to the MGI. One such effort initiated by Texas A&M University is the Data-enabled Discovery and Design of Energy Materials (D^3EM) program (https://d3em.tamu.edu/). Initially funded by the NSF Research Traineeship (NRT) program, D^3EM now has institutional support as an Interdisciplinary Graduate Certificate on Materials Science, Informatics, and Design, and spans six departments in the Colleges of Science and Engineering at that university.



Programmatic structure of the D^3EM program. Graphic from Texas A&M University. See https://d3em.tamu.edu.

D^3EM combines the forward and inverse exploration and exploitation of materials design spaces by including a cross-disciplinary curriculum including courses on materials science, informatics, and engineering design. Scheduled after the participants' grounding in their own disciplines, D^3EM provides MGI-focused training in machine-learning-enabled exploration of materials spaces, and their design or optimization through goal-oriented engineering design principles. The technical element of the curriculum culminates with an interdisciplinary "Materials Design Studio," a project-based course aiming to address actual materials discovery/development problems. D^3EM also provides training in the skills essential to fruitful interdisciplinary research, including communication and collaboration, technical writing, team science, and leadership. Participating faculty are organized through a community of scholars whose focus is the continuous improvement of the students' educational experiences.

Thus far, D^3EM has trained over 40 PhD and MS students from eight different academic departments, and it is shaping a new Transformative Doctoral Education Model at the university that emphasizes critical reflection, problem solving, discourse, and mentorship. Roughly half of all projects in the Materials Design Studio have been further developed into peer-reviewed publications ranging from the accelerated design of specific materials to pedagogical aspects of teaching MGI principles. The program seeks to prepare its trainees for success in any career of their choosing and has thus partnered with national laboratories and industry to create a variety of internships, including a data-enabled materials discovery program with the Air Force Research Laboratory (AFRL) focused on broadening participation by underrepresented groups. The program leverages the D^3EM educational model to conduct data-enabled research where students work in concert with AFRL mentors on projects ranging from defect prediction during additive manufacturing to discovery and design of 2D functional materials for novel properties. Of the 13 graduate students sponsored by AFRL to date, 10 have spent an extended research period in the laboratory at Wright-Patterson Air Force Base, and one is beginning a post-doctoral fellowship.

Objective 2: Train the Next-Generation Workforce

Post-graduate training is needed to remain abreast of and maximize the use of rapidly evolving tools in the materials R&D enterprise. These tools include experimental and computational techniques as well as those for the acquisition, curation, sharing, and statistical analysis of data. The maturation of AI and ML algorithms and increased automation in research laboratories and on manufacturing floors requires life-long learning opportunities to reskill workers. Continuing education, vocational, summer school, and other training programs should facilitate information exchange, collaboration, and creative problem solving. Online delivery should be supported to maximize inclusion of a broad and diverse audience.[41,42]

Mid- and late-career professionals in academia, national laboratories, and industry may be less familiar with emerging concepts in computation and data science than junior colleagues, and thus represent a significant training opportunity for MGI. "MGI sabbaticals" would relieve professionals and technicians from their normal duties in order to acquire and translate new skills and evolving tools into the workplace. Partnerships between industry, academia, national labs, and professional societies would enhance the ability to translate emerging best practices across the materials development continuum and between different use cases.

Training in research translation, entrepreneurship, and technology transfer can help mitigate the inevitable challenges that arise as fundamental discovery advances approach the proverbial "valley of death." Graduate students and post-doctoral scholars with established fundamental skills should have opportunities to apply their expertise in a use-inspired, MGI mindset. Partnerships between academia, national laboratories,[43] industry, and other entities such as the Manufacturing USA Institutes[44] can promote MGI internships that foster two-way convection—where new MGI tools and individuals propagate from academia to industry, national labs, and institutes, and where post-doctoral scholars who are bound for academia acquire use-inspired, industrially-relevant experiences before starting their academic careers. Interagency programs such as I-Corps™ and post-graduate translational fellowships should also be promoted to equip graduates with exploration of market need for MGI-based technologies.

To summarize, actions to train the next-generation workforce include:

- Promote and support continuing education, vocational, and summer school programs to maximize the impact of rapidly-evolving MGI-tools.
- Develop opportunities to retrain mid-career professionals through MGI sabbaticals.
- Foster programs to cross-train scientists and engineers in research translation, entrepreneurship, technology transfer, and commercialization.

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[41] For example, nanoHub has developed an extensive selection of online curricula, curated educational materials, courses, and lectures.

[42] K. Madhavan, L. Zentner, V. Farnsworth, S. Shivarajapura, M. Zentner, N. Denny, and G. Klimeck, *Nanotechnology Reviews* **2,** 107-117 (2013).

[43] DOE Office of Science Graduate Student Research (SCGSR) Program. science.osti.gov/wdts/scgsr.

[44] https://www.manufacturing.gov/

Objective 3: Connect Talent to Opportunity

To build the technology-savvy and connected workforce required to span the entire materials development continuum, a broad and diverse materials education and training effort must be undertaken that extends uniformly across gender, race, ethnic, geographic, and economic boundaries. This must include human resource development to promote diversity and inclusion in academic, national laboratory, and industrial settings. Achieving this and the bold objectives outlined in Goal 3 will require new coordinated partnerships across these sectors to connect talent to opportunity.

Ensuring a Diverse and Inclusive Materials Workforce

As emphasized above, the MGI offers the potential to enhance recruitment and retention of women and others traditionally left behind in undergraduate and graduate STEM/CS programs. By effectively connecting materials development to societal impacts, MGI-inspired education can be designed to resonate with different cultures of people and regions in the United States.

Activities to promote public awareness of opportunities in communities that are underrepresented in the contemporary workforce are too passive—more innovative approaches are needed. Federal agencies have and continue to support “bridge”-learning[45] and partnership programs at HBCUs and other MSIs. With guidance from thought leaders at these institutions, successful programs should be expanded and included in all efforts to improve MGI-savvy curricula, training, and experiential opportunities for undergraduate, graduate students, and associated faculty and staff. Computation and data analysis represent necessary skill sets that can be well suited for areas where traditional laboratories or instruction are prohibitively expensive or impractical. Community colleges represent a significant existing infrastructure with the potential to attract a socio-economic and geographically diverse segment of the population through effective outreach to faculty and students. Success of the materials R&D enterprise requires a stronger and concerted effort to overcome the challenges of diversity and inclusion across all sectors. To meet this challenge, actions by the MGI community include:

- Identify effective programs and fill in gaps.
- Increase attraction and cultivation of a diverse and inclusive workforce.

Partnerships in MGI Workforce Development

Fostering the connected ecosystem that spans from fundamentals to application will require more effective coordination between MGI stakeholders (i.e., government, academia, and industry). Education and research provided by academia needs to be better connected to the efforts residing in Federal and national laboratories and industry. It is thus important to promote opportunities for university principal investigators (PIs), post-doctoral scholars, and students to engage with research programs sponsored by mission agencies and the industrial sector. Such engagements lead to the formation of new collaborations that accelerate the development of materials into new technologies.

Scientists and engineers engaged in MGI-inspired research should be guided in part by a vision of materials application. In some cases, this could be accomplished by including industrial PIs in the research projects.[46] Alternately, industrial advisory boards that include multiple companies to guide fundamental research efforts toward application could be formed. The MGI community should play a

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[45] https://www.fisk-vanderbilt-bridge.org/

[46] NSF's Grant Opportunities for Academic Liaison with Industry (GOALI) program provides an opportunity for close partnership between an academic team and an industrial researcher.

foundational role for future advanced manufacturing[47] through partnerships with institutes such as those associated with Manufacturing USA, for example.[48] Such academia/industrial partnerships will provide valuable experiences for students to receive meaningful training and expand career opportunities. Over the next five years, actions the SMGI and MGI community will initiate include:

- Enhance and expand partnerships between academia, national laboratories, and industry.
- Foster cross-fertilization of expertise and knowledge along the materials development continuum from discovery, to design, to manufacturing, to deployment.

MGI Vignette — *Workforce development through Federal partnerships*

MGI principal investigator meetings convene PIs funded across the Federal Government's MGI portfolio, providing an effective means for scientists and engineers to present and exchange information about their research activities, foster new ideas, establish collaborations, and discuss future research directions. The 2018 meeting included a competition to encourage partnerships among MGI-related activities sponsored by various Federal agencies. Supplemental funding provided to NSF's DMREF teams enabled graduate students and academic post-docs to intern at Federal and national laboratories. Through use of MGI principles, these students have attacked contemporary materials challenges including the design of photocatalysts for water splitting with DOE's HydroGEN Energy Materials Network, the use of artificial intelligence to search for rare-earth-free magnetic materials with the Air Force Research Laboratory, the synergistic use of microscopy and computational modeling for the development of superalloys with NASA, and the data-driven discovery of organic semiconductors for electronic and light-based technologies with NIST. Furthermore, a partnership among a multiuniversity DMREF team, NIST, and HydroGEN has been established to attack the important challenge of developing effective anion exchange membranes for high-performance fuel cells and electrolyzers, in support of H2@Scale efforts in deep decarbonization across sectors. Such coordination of MGI-sponsored research across multiple Federal funding agencies provides an effective mechanism for workforce development while synergistically focusing research efforts on critical societal materials needs.

See, for example: https://www.mgi.gov/sites/default/files/documents/2018abstractbook.pdf.

How to Use this Strategy

This strategic plan has outlined three strategic goals for the Materials Genome Initiative that, if achieved, will further accelerate the discovery, design, development, and deployment of new materials into manufactured products. The calls to action outlined herein are directed not only to the Federal agencies working together to achieve these goals, but also to the full spectrum of the MGI community. All are encouraged to identify ways to make these goals a reality, yielding extraordinary benefits to the U.S. economy, defense, energy production, and health.

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[47] National Science and Technology Council, Committee on Technology, Subcommittee on Advanced Manufacturing, *Strategy for American Leadership in Advanced Manufacturing* (2018).

[48] *Manufacturing USA*. https://www.manufacturingusa.com/institutes.