CREATING THE NEXT-GENERATION

MATERIALS GENOME INITIATIVE WORKFORCE

TMS A Study Organized by The Minerals, Metals & Materials Society

Creating the Next-Generation Materials Genome Initiative Workforce

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A STUDY ORGANIZED BY

The Minerals, Metals & Materials Society (TMS)

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Cover: Representation of the four national objectives identified as part of the original announcement of the Materials Genome Initiative: clean energy, human welfare, national security, and developing the next-generation workforce. Bottom image of X-51A Waverider on date of hypersonic flight is courtesy of U.S. Air Force (photo by Bobbi Zapka). Cover design by Dave Rasel, TMS.

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Promoting the global science and engineering professions concerned with minerals, metals, and materials

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Kevin Anderson is a member of The National Academy of Engineering for his work on sustainable aluminum alloy design. He is a member of TMS and a Fellow of ASM. He received his B.S., M.S., and Ph.D. degrees in metallurgical engineering from the University of Illinois at Urbana-Champaign. Anderson was a leader of aircraft materials and physical metallurgy at Reynolds Aluminum Research and is presently a Senior Technical Fellow for Brunswick Corporation in the Mercury Marine Division in Fond Du Lac, Wisconsin. In this role he is responsible for both materials research and applications across the corporation. Anderson is an inventor of high damage tolerant diecasting alloys that are made from 100% recycled aluminum and are registered with the Aluminum Association. In addition to receiving several important industrial awards for his work, Kevin holds over 30 United States patents with the vast majority successfully in production. He has taught aluminum metallurgy on an international level since 1999, been the past chair of the Advanced Casting Research Consortium at Worcester Polytechnic Institute and the Materials Innovation Committee of TMS, and is a member of the Grainger Institute for Engineering Advisory Board at the University of Wisconsin.

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Mark Asta received his Ph.D. from the University of California (UC), Berkeley, in 1993. He subsequently joined Sandia National Laboratories as a postdoc, and then as technical staff. In 2000 he joined the Department of Materials Science and Engineering (MSE) at Northwestern University. In 2005 he moved to UC Davis, in the Department of Chemical Engineering and Materials Science, and became vice chair in 2008. In 2010 he joined the MSE Department at UC Berkeley, with a faculty scientist appointment at Lawrence Berkeley National Laboratory (LBNL). He served as department chair of MSE from July 2012–January 2018. Since January 1, 2018 he has served as Materials Sciences Division Director at LBNL. Asta's research focuses on the development and application of atomistic computational methods for calculating bulk and interfacial thermodynamic and kinetic properties, and for computationally guided discovery and design of materials. He was awarded ASM International's Materials Research Silver Medal Award in 2002, Fellow of the American Physical Society in 2010, the TMS Functional Materials Division Distinguished Scientist/Engineer Award in 2013, the TMS Hume-Rothery Award in 2019, and Fellow of TMS in 2020. In 2015 he was named the Arthur C. and Phyllis G. Oppenheimer Professor at UC Berkeley.

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Allison Beese received her B.S. degree in mechanical engineering from Penn State University. After her undergraduate study, she worked at Lockheed Martin's Knolls Atomic Power Laboratory in New York as an engineer. She then entered graduate school at MIT, where she earned her M.S. and Ph.D. degrees in mechanical engineering. She spent two years as a postdoctoral fellow at Northwestern University. She joined Penn State as an Assistant Professor in materials science and engineering in 2013. Her research focuses on developing experimental and computational tools to identify and model links among microstructure, multiaxial plasticity, and multiaxial fracture of metals. She has received an NSF CAREER award, the 2018 TMS AIME Robert Lansing Hardy Award, the 2017 International Outstanding Young Researcher in Freeform and Additive Manufacturing award, a 3M non-tenured faculty award, an Oak Ridge Associated Universities (ORAU) Ralph E. Powe Junior Faculty Award, and a TMS Young Leader Professional Development Award.

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Stefano Curtarolo's research interests lie at the intersection of materials science, artificial intelligence and autonomous discovery of new materials. After studying electrical engineering and physics in Padova, Italy, he received his M.S. in physics from Penn State University in 1999, and a Ph.D. in materials science from MIT in 2003. Since then, he has been on the faculty of the Materials Science Department at Duke University. During his time at Duke, he has received numerous awards and recognitions including the DOD-ONR-Young-Investigator (2007), the NSF-Career (2007), the Presidential PECASE Award (2008), the International Union of Pure & Applied Physics-Young Scientist Prize in Computational Physics (2011), the Stansell Research Award (2013), Fellowship by APS (2013) and the 2013 MURI Award for strategies in rare-materials replacement. In 2015 Curtarolo received the "Friedrich Wilhelm Bessel Research Award" from the Alexander von Humboldt Foundation. Stefano has more than 150 referenced publications, over 200 invited departmental seminars and talks in national and international conferences, and about 10,000 scientific citations. At Duke University, Curtarolo's group started and maintains the quantum-cloud aflow.org consortium containing materials information and tools for more than four million compounds. His teams focus on developing autonomous daemons for materials discovery as well as tackle problems of synthesizability and manufacturability of amorphous/disordered systems.

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Will Joost is a Principal Materials Engineer at Pratt & Whitney in East Hartford, Connecticut, where he focuses on applying computational materials science and integrated computational materials engineering (ICME) toward advances in jet engines. His primary area of research is multi-scale modeling of mechanical behavior and tribology in crystalline materials. Prior to joining Pratt & Whitney, Joost spent 7 years as the Program Manager for Lightweight Metals in the Vehicle Technologies Office at the U.S. Department of Energy where he oversaw a portfolio of R&D projects. He also spent time as a postdoctoral researcher in the Theoretical Division at Los Alamos National Laboratory writing high performance computing code for dislocation dynamics simulations. Joost holds a B.S. from Rensselaer Polytechnic Institute, an M.S. from Arizona State University, and a Ph.D. from the University of Maryland, all in materials science and engineering.

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Michele Manuel is the Department Chair of the Department of Materials Science and Engineering at the University of Florida. She received her Ph.D. in materials science and engineering at Northwestern University in 2007 and her B.S. in materials science and engineering at the University of Florida. She is and ASM Fellow and the recipient of the Presidential Early Career Award for Scientists and Engineers (PECASE), NSF CAREER, NASA Early Career Faculty, ASM Bradley Stoughton Award for Young Teachers, AVS Recognition for Excellence in Leadership, TMS Early Career Faculty, TMS Young Leaders Professional Development, and TMS/Japan Institute of Metals and Materials (JIM) International Scholar Awards. Her research lies in the basic understanding of the relationship between processing, structure, properties, and performance. She uses a systems-based materials design approach that couples experimental research with theory and mechanistic modeling for the accelerated development of materials. Her current research is focused on the use of systems-level design methods to advance the development of new materials through microstructure optimization. Of specific interest are lightweight alloys, self-healing metals, computational thermodynamics and kinetics, shape memory alloys, and materials in extreme environments—specifically under high magnetic fields or under irradiation.

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Regents' Professor and Carter N. Paden, Jr. Distinguished Chair in Metals Processing, Dave McDowell joined Georgia Institute of Technology (Georgia Tech) in 1983 and holds appointments in both the GWW School of Mechanical Engineering and the School of Materials Science and Engineering. He served as Director of the Mechanical Properties Research Laboratory from 1992–2012. Since 2012 he has directed the Institute for Materials (http://www.materials.gatech.edu), a Georgia Tech Interdisciplinary Research Institute charged with cultivating cross-cutting collaborations (user facilities, research proposals, workshops) and approaches to accelerate materials discovery and development. McDowell's research focuses on the development of physically-based, microstructure-sensitive constitutive models for nonlinear and time-dependent behavior of materials, with emphasis on wrought and cast metals. Topics of interest include microstructure-sensitive computational approaches to fatigue of alloys, atomistic and coarse-grained atomistic simulations of dislocations, multiscale modeling, and systems-based materials design under uncertainty. He has participated in prior TMS study groups and workshops and is a member of the TMS Materials Innovation Committee. McDowell currently serves on the editorial boards of *npj:Computational Materials*, *Journal of Multiscale Modeling*, and as co-Editor of the *International Journal of Fatigue*.

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Xin Sun is the Director for the Energy and Transportation Science Division at Oak Ridge National Laboratory (ORNL). Her research expertise lies in the areas of computational materials and applied mechanics, and her strength is in applying the mechanics and materials fundamentals in solving challenging energy materials problems ranging from multi-physics carbon capture device-scale simulations to lightweight materials manufacturing processes including casting, forming, joining and non-destructive evaluations. Sun received her Ph.D. from the University of Michigan, Ann Arbor. Prior to joining ORNL, Sun was a Laboratory Fellow at Pacific Northwest National Laboratory (PNNL) in Richland, Washington. A Fellow of ASME, Sun is a well-recognized expert in integrated computational materials engineering (ICME) for lightweight energy materials, and has authored/co-authored more than 190 peer-reviewed journal articles and 10 books/book chapters. Sun has earned many recognitions for her technical accomplishments, with the most notables including the R&D 100 Award (2016), the University of Michigan Alumni Society Merit Award (2009), Pacific Northwest National Laboratory Director's Award for Exceptional Engineering Achievement (2008), UT-Battelle Awards Night Research Leadership at the Division Level (2018).

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Cathy Tway is the Technology and Applications Director for Catalyst Technologies in Johnson Matthey. In her role, Tway is responsible for a global team of scientists and engineers specializing in catalysis, process technologies, and engineering design. She ensures customer-driven R&D and engineering is delivered efficiently and provides technical input, oversight, and direction. Prior to joining Johnson Matthey, Tway held positions at Dow, Celanese, Solutia, and Akzo Nobel, holding both R&D leadership and individual contributor roles. Her more than 25 years of industrial experience covers the entire catalyst project life cycle including front-end opportunity identification and creation of new technologies, process scale-up, commercialization, and plant support. Over her career, Tway has commercialized two new inorganic materials and four catalyst technologies, with two of these processes still in use today. She has served on numerous review panels, boards, and committees including her work on the Scientific Advisory Board for the Nanoporous Materials Genome Center. Tway earned her B.S. degree in chemistry from Wichita State University and her Ph.D. in physical inorganic chemistry from the University of Nebraska-Lincoln.

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Expert Contributor Satellite Meeting—Indianapolis, IN, July 25, 2019

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- **Charles Fisher**, Naval Surface Warfare Center-Carderock
- **T.D. Huang**, Huntington Ingalls Industries
- **Jonathan Madison**, Sandia National Laboratories
- **David McDowell**, Georgia Institute of Technology
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Preface

Who should read this report?

This report contains useful background and information for anyone who has an interest in the Materials Genome Initiative (MGI), especially those who are involved in the education, training, and development of the workforce. People with such interests are likely to include many in the materials science and engineering (MSE) community, as well as individuals from other related disciplines across academic, industrial, and government sectors. This includes not just educators and trainers but researchers and practitioners in industry who are seeking broad support for MGI-focused activities. Additionally, federal agencies, private enterprises, and other institutions that support and finance materials advancements will also find this report useful. Many readers will especially benefit from identifying how they can contribute to the various action plans identified within the report. Beyond those experts who can directly contribute to and benefit from the MGI, other groups who would be interested in reading this report include more peripherally related professionals or students who want to learn more about key issues associated with the MGI and how they may get more involved with this important national initiative.

More specifically, the report will be of value to the following individuals and groups:

- Materials Genome Initiative stakeholders including materials science and engineering professionals as well as others in related disciplines (e.g., physics, chemistry, engineering, mathematics, computer science)
- educators and teaching professionals
- managers in industry who have responsibility for materials design, development, or deployment
- funding officers and program managers
- policymakers
- students

How to navigate this report

Readers are encouraged to navigate this report by first examining the Executive Summary to get a general sense of the scope and outline of the document and how they might be of most relevance to your expertise, interests, and organization. It is our hope that this report will encourage you to take action related to your skills and interests to support developing the next-generation MGI workforce. The Background and Prior Efforts section provides insight into the existing landscape, and the Current State of MGI Curricula and Training section may prompt you and your colleagues to think about your past training and current approaches to the education of the materials workforce. As you explore the Action Plans, you can begin to focus on the tactical details that resonate most with your priorities, and you can think in more specific terms about the actions that you and your colleagues might undertake. Then, perhaps you can begin to take some concrete steps toward initiating activities with this report as a guide for next steps.

What actions could be taken after reading this report?

A primary goal of this project is to motivate direct action by a wide variety of stakeholders who read this report. These actions include individual, group, and organizational-level contributions to the development of the next-generation MGI workforce. After reading this report, some next steps to take might include: (1) identifying specific recommendations or tasks that you and your colleagues may address, and from which you and your colleagues would gain the most benefit, (2) sharing information about the MGI with your managers and leadership to help grow awareness, and (3) taking concrete steps to initiate one of the seven action plans by investment of resources. These steps would be different depending on your role and domain(s) of interest.

It is also important to acknowledge that this report contains several high-priority action plans but it is not intended to include all of the potential steps that might contribute to the creation of the next-generation MGI workforce. Readers are encouraged to consider what other actions they can pursue to impact the development of the future workforce. Accelerating the pace of change in materials discovery and development through the MGI will require a large undertaking that is inherently interdisciplinary—all who read this report are invited and encouraged to take part.

Executive Summary

Background

The Materials Genome Initiative was announced in 2011 with an ambitious vision to discover, develop, and deploy advanced materials at an accelerated pace and a fraction of the cost. The initiative recognizes the essential role of materials in national security, clean energy, and human well-being and aims to take steps to develop an underlying materials innovation infrastructure that would enable faster scientific and engineering progress while ensuring U.S. competitiveness in materials. At the heart of the initiative is the linking of experiment, computation, and data science.

Though much progress has been made in the eight years since the MGI was announced, most of the advancements have been in the technical elements of the initiative. While there are a growing number of examples of advanced high-throughput experimentation techniques, enhanced computational tools, data-driven approaches, and modern machine learning methods, there remains a paucity of capable workforce participants trained in MGI approaches that bridge modern materials science tools and approaches with a deep understanding of the underlying fundamental science and engineering principles. The need for developing this next-generation MGI workforce was acknowledged as a key goal in the announcement of the initiative and further underscored in the release of the 2014 MGI strategic plan.

Building on the foundations of past workshops, activities, and reports that examined aspects of education and workforce issues related to the MGI, this report begins with some context on the MGI, including the current state of education and training opportunities available in formal and informal capacities for undergraduate and graduate student populations all the way through senior leadership positions. Based on input from academia, government, and industrial participants, it also articulates the desired skills for the future workforce to ensure readiness for employing MGI approaches. In addition to outlining many of the barriers that prevent change in education and training, the report also describes seven detailed action plans designed to accelerate the pace of change and ensure near-term preparedness of students and existing professionals to take on the challenges that can be uniquely addressed by the MGI and speed the discovery, development, and deployment of advanced materials.

Study Process

A team of 16 internationally recognized experts from various materials backgrounds across government, academia, and industry was assembled to lead this effort. The group's insights were collected virtually via online meetings and homework assignments as well as during two separate two-day, in-person workshops (held in February and July 2019) to address the project's goals. The outputs from these workshops along with the outcomes of related discussions and activities including a satellite meeting and a survey have been captured and synthesized in this document. In addition to being iteratively edited by the study team and TMS science and engineering staff, a draft of this report was also reviewed by an independent group of experts.

Current State of Education and Training

Since the MGI was announced in 2011, there have been several substantive changes undertaken within colleges and universities across the country to align their undergraduate and graduate curricula with MGI-relevant goals, such as expanded incorporation of computational and data science tools and educational offerings, a shift to more relevant programming languages, and strategic hiring of faculty with interdisciplinary backgrounds.

To identify the current state of curriculum, a survey was distributed to members of the University Materials Council (UMC),[a] and 24 responses were received. For undergraduate programs, 79% of respondents agreed that MGI principles are "Somewhat Important" or "Very Important" for students to learn prior to graduation. That number increases to 96% for graduate programs, suggesting that some view the MGI as an advanced set of concepts that are more essential to graduate training. Nonetheless, responses to additional questions regarding the number of MGI-related courses offered suggests there is still room for more programs to introduce MGI components at the undergraduate and graduate levels.

Additionally, a separate investigation of existing coursework related to integrated computational materials engineering and the Materials Genome Initiative in U.S. universities was conducted. A total of 50 out of the approximately 114 U.S. undergraduate and graduate programs were evaluated

a The University Materials Council (UMC) is composed of department heads, chairpersons, directors, and group leaders from academic programs in the materials field in U.S., Canadian, and Australian universities.

to assess the prevalence of coursework that meets the MGI's strategic plan goal to "equip the next-generation materials workforce." Of the 50 universities sampled, 40 offer computational materials science and engineering (CMSE) related coursework, specifically courses that contain keywords such as "computational materials," "modeling," or "simulations" in the title and/or course description. However, the success seen with incorporating CMSE concepts into MSE curricula has not yet extended to the third pillar of the MGI: data science.

Only nine out of the 50 institutions included in the research sample currently offer courses in their undergraduate or graduate materials science departments that reference "data science," "data handling," or the utilization of "databases." This dearth of data–or data-science-related–MSE course offerings highlights the work still needed to develop a modern curriculum within MSE. This will require connectivity to other fields contributing to the MGI, exposing students to the tools and concepts that will be ubiquitous in the workplace of tomorrow.

Outside of the traditional classroom offerings, many stakeholders host summer schools, online courses, or training opportunities on topics related to computational materials science and engineering. Several examples are detailed including the multi-day Machine Learning for Materials Research workshops offered through the National Institute of Standards and Technology. The mix of various styles of standalone programming to address specific needs of the evolving MSE community is a vital component to the development of the next-generation MGI worker.

Another critical learning opportunity outside the traditional classroom is hands-on experience in research laboratories and industrial environments. Examples of programs that support such activities include the longstanding Designing Materials to Revolutionize and Engineer our Future (DMREF) program as well as MGI-related programs supported by the NSF Research Traineeship program and the Department of Defense effort in preparing the lightweight materials manufacturing workforce through the offering of internships in the Lightweight Innovations for Tomorrow (LIFT) program.

Defining the Future MGI Workforce

With input from industry, government, and academia, the project team identified and prioritized the knowledge and skills that are essential to preparing the next-generation MGI workforce. In Table 1, they are organized into the three foundational pillars that map to the MGI: data, computation, and experiment. For each of the foundational pillars, a group of subtopics is listed that depicts the key competency areas associated with it. A set of core knowledge and skills as well as advanced/ specialty knowledge and skills are also provided for each subtopic, along with examples in a set of more detailed tables.

The knowledge and skills described in the tables are in addition to the core requirements needed for materials science and engineering. While it is not necessary for someone to become an expert in all of the knowledge and skill areas described, it is important for students–undergraduate and graduate–to be aware of these concepts and the engineering and scientific sub-fields in which they can be accessed, and to be conversant in multiple topics across the spectrum of data science, computation, and experiment.

Soft skills, such as working within interdisciplinary teams, were also acknowledged by the study team as being of critical importance to advancing the MGI. However, the emphasis in this work was placed on the technical concepts that are required to contribute to the progress of the MGI.

Reproduction of Table 1. Summary of Foundational Pillars and Key Competency Areas for the MGI Workforce.

Foundational Pillars	Key Competency Areas
Data	• Data handling • Modeling and simulation visualization • Software and codes to manage MG workflows
Computation	• Quantum and atomistic modeling methods • Microstructure evolution and material response • Multiscale and continuum modeling methods • Integrated workflows for computational tools
Experiments	• Multi-objective design and decision-making under uncertainty • Measurement methods and tools • Sensor fusion, high-throughput methods, and automation

Action Plans

The study team identified a total of seven recommended action plans to serve as guidance regarding next steps the stakeholder community should take over the coming 5–10 years that will help lead to significant progress in creating the next-generation MGI workforce. Action Plans are organized into two categories of recommendations: supply side and demand side. In the case of supply-side recommendations, there is an immediate impact on near-term workforce readiness and the supply of trained scientists and engineers who are prepared to address MGI challenges. In the case of demand-side action plans, the impact of the workforce is primarily in identifying organizational needs and building the demand for a sufficiently trained workforce that accelerates advancements in materials through the MGI. Ultimately, all of these action plans are viewed as important to advancing the preparation of the current and future workforce to enable application of MGI methods and tools to accelerate the discovery, development, and deployment of new and improved materials. Where applicable, action plans include approximate timelines, milestones or metrics, stakeholder roles, and the critical resources required to ensure success. Table 5 summarizes the full list of action plans.

Reproduction of Table 5. Summary of Seven Recommended Action Plans.

Supply-Side Action Plans	
1	**Modernize academic curricula with MGI content** and reinforce concepts throughout undergraduate and graduate education; emphasize Research Experience for Undergraduates (REU) programs for undergraduates and fellowships for graduate students in areas that build MGI infrastructure and provide examples of fusion of computation, experiment, and data
2	**Identify, develop, and package instructional modules** that can be implemented in academic courses
3	**Develop targeted short courses, boot camps, and summer schools** to fill gaps not otherwise covered in traditional education and training modes; prepare the instructors (i.e., educate the educators) necessary for MGI workforce development
4	**Articulate foundational MGI moonshot objectives** and establish programs with societal impact to address the initiative's goals and broaden the communities that understand its implications
Demand-Side Action Plans	
5	**Solicit input from industry and government laboratories regarding necessary MGI workforce knowledge and skills** and capture a summary of MGI workforce knowledge and skills needed, helping them to articulate potential impact on their operations
6	**Develop a summit event for CTOs and executives, and communicate to the broader community** by making related resources easy to access
7	**Create a web-based registry to document MGI successes** and clearly define metrics for measuring enhanced competitiveness and impact of MGI methods and tools, along with web-based dissemination of advances by stakeholder organizations

I. Introduction

Materials innovation is essential to addressing society's greatest challenges. For example, advancements in broad societal and national objectives of improving healthcare, enhancing national security, and realizing gains in sustainable energy all require the discovery, development, and deployment of materials. Researchers are actively working to find alternatives for scarce yet essential minerals, to develop strong lightweight materials for fuel-efficient vehicles and protective gear, and to increase the efficiency of fuel cells and other energy conversion processes to lower the global carbon footprint, among other critical activities.[1]

The current timeline for materials development from concept to full-scale deployment is upwards of 10 to 20 years.[2] The long period between materials discovery and deployment has several contributing factors including the complexity arising from phenomena occurring at different length and time scales,[3] a lack of a cross-disciplinary culture of collaboration in materials innovation,[4] a mismatch between the materials development cycle and product development cycle,[5] and the misalignment of market needs and the value proposition of a new material.[6]

In 2011, the Materials Genome Initiative (MGI) was announced to transform the slow, relatively serial stages of materials development and qualification for use into a more rapid, parallelized process to improve the global competitiveness of the United States.[1] By supporting the development of a materials innovation infrastructure that seeks to combine computation, experiments, and digital data, the federal government seeks to drive industry, academia, and government laboratories to launch and develop ground-breaking technologies from discovery to production twice as fast and at a much lower cost. One of the four goals highlighted in the 2014 MGI strategic plan identifies the need to prepare the next-generation materials workforce to achieve the goals of the MGI.[7] As materials research and innovation continue to evolve and increasingly embrace advances in e-collaboration and digital information, the knowledge and skills of the future workforce must expand as well. The workforce needs to be able to integrate experiment, computation, and digital data to fully unlock the opportunities presented by the MGI.

Prior to the MGI, the integration of modeling and simulations was already emerging as a new discipline within the materials research and development community. A 2004 report from The National Academies thoroughly described this emerging area of integrated computational materials engineering (ICME) which involves "...the integration of materials information, captured in computational tools, with engineering product performance analysis and manufacturing-process simulation."[5]

While the MGI emphasizes the development of a materials innovation infrastructure to shape the tools and culture of the materials community, ICME is an approach that focuses on integrating the entire enterprise of materials development. Pursuing the goals of ICME will significantly reduce the time and cost of integrated materials and product development, which also moves toward achieving the goals of the MGI. Hence, ICME and MGI are congruent in their goals and impact on the materials R&D communities in academia, industry, and government.

Since the beginning of the MGI in 2011, progress has been made in updating the curricula of MSE programs, increasing the interdisciplinary nature of research projects, and increasing the availability of online resources that support the goals of the MGI,[8] as discussed in the Current State of MGI Curricula and Training section of this report. However, certain gaps still exist between the needs of employers and the capabilities of the existing and future workforce.

Project Goals and Process

To equip the broader materials community with the knowledge and resources necessary to fully address MGI goals, this project aimed to accomplish the following: (1) assess the current state of the academic curriculum and training approaches of the U.S. workforce to accomplish MGI goals; (2) identify the key MGI knowledge and skill requirements and needs for individuals entering the workforce; and (3) outline curricula development and training guidelines to improve readiness of current students and the existing professional workforce.

These objectives were addressed by assessing relevant curricula at U.S. universities; surveying MGI and ICME stakeholders regarding perceived gaps in education/curricula and workforce needs; benchmarking relevant MGI- and ICME-related reports and research programs to compile a comprehensive listing of past recommendations and efforts related to education, curricula, and workforce development; and identifying a clear set of gaps and needs, possible strategies for building and sustaining the MGI workforce, and overarching recommendations.

A team of 16 internationally renowned experts from various materials backgrounds across government, academia, and industry was assembled to lead this effort. As seen from the Acknowledgements section, this study team represents a variety of key stakeholder groups. The group's insights were collected virtually via online meetings and homework assignments as well as during two separate two-day, in-person workshops (held in February and July 2019) to address the objectives and goals. The outputs from these workshops along with the outcomes of related discussions and activities were captured and synthesized in this report. Input was also obtained from several other subject matter experts both through a satellite meeting and a survey has been incorporated into this document. In addition to iterative editing by the study team and TMS science and engineering staff, a draft of this report was also reviewed by an independent group of experts. Ultimately, this report is intended to broadly identify the knowledge and skills of a workforce that is needed to fully leverage the emerging materials innovation infrastructure and to provide actionable plans for improving the readiness of the next-generation materials workforce.

II. Background and Prior Efforts

This section will provide the reader with an understanding of the topics and disciplines included in MGI as well as the key stakeholders and their perspectives and motivations. It also summarizes the findings and recommendations provided by past studies.

Materials Genome Initiative Overview

The 2014 Materials Genome Initiative strategic plan identified four goals for the initiative: (1) lead a culture shift in materials research to encourage and facilitate an integrated team approach across the materials innovation ecosystem, (2) integrate experiment, computation, and theory in equipping the materials community with advanced tools and techniques, (3) make digital data accessible, and (4) create a world-class materials-science and engineering workforce that is trained for careers in academia, government labs, and industry.[7] Although this study focuses mainly on the fourth goal, it is important to discuss the overarching themes of the MGI.

A central theme to the MGI is a requirement for integration. The seamless integration of a variety of tools, disciplines, concepts, and human resources is essential to a successful MGI ecosystem. Goals 2 and 3 derive directly from the 2011 MGI white paper, *Materials Genome Initiative for Global Competitiveness*,[1] which describes a Materials Innovation Infrastructure that calls for the integration of advanced computation, experiment, and theory combined with digital data and related tools to fuel the successful discovery of new materials and their more rapid deployment and incorporation into manufactured products.

Derived in part from the MGI Strategic Plan,[7] computation, experiment, and theory can be defined as follows:

- **Computation**—the use of computational tools and methods, such as algorithms, models, and simulations, to visualize, design, and predict materials and their properties
- **Experiment**—the use of laboratory tools and procedures to capture data through physical tests, measurements, and characterization during synthesis and/or processing
- **Theory**—fundamental materials knowledge and first-principles concepts

The vast range of length and time scales addressed by materials research creates unique challenges for delivering quantitative and predictive scientific and engineering tools.[7] Therefore, it is important that a Materials Innovation Infrastructure utilizes an MGI-centered approach which draws simultaneously from computation, experiment, and theory, along with application of modern data science methods and tools, to develop advanced simulation tools that are both verified with theory and validated through experimental data. Moreover, this MGI approach would need to be incorporated into the entire materials development process. Thus, the tools, models, and techniques developed via basic scientific research, as well as the resulting data, must be integrated within the broader materials innovation ecosystem of scale-up manufacturing, systems design engineering, and methods for uncertainty quantification to contribute to the deployment of materials in pursuit of the MGI vision.

The MGI originated as a multi-agency effort, and today includes participation by many government agencies including the Department of Defense (DOD), Department of Energy (DOE), National Aeronautics and Space Administration (NASA), National Science Foundation (NSF), and Department of Commerce (DOC), among others.[b] Professional societies, universities, and other partners and institutions also play a key role in helping advance the initiative to meet its goals.

Materials Genome Initiative Workforce

For the purposes of this report, the MGI workforce is defined as the individuals responsible for implementing the activities of accelerating discovery, development, and deployment of new materials. These activities are naturally anchored in materials science and engineering but are inherently interdisciplinary and demand the engagement of a wide cross-section of knowledge and skills from other fields including various other engineering disciplines, chemistry, physics, biology, mathematics, computer science, data science, statistics, and information technology. Since materials science and engineering is at the core of the MGI, this community is a large focus of the report. However, multiple study team members and other contributors from outside of materials science and engineering also provided their perspectives on their role in the MGI workforce.

b A complete list of Materials Genome Initiative partner organizations from the federal government is available at https://www.mgi.gov/partners.

In addition to the range of disciplines that comprise the MGI workforce, it also includes members across academia, industry, and government. The MGI workforce encompasses university faculty, government laboratory researchers, and working professionals in industry, ranging from technicians to senior leaders in materials science and engineering and related fields (as listed previously). To provide a sense of scale for the size of the workforce that is most directly responsible for the MGI, data on the number of scientists and engineers employed in several related occupations is shown in Figure 1. According to the 2019 Science and Engineering Indicators, there were 31,000 "materials and metallurgical engineers" employed in 2017.[9] This number does not include "technicians," "engineering managers," or "teachers," which reside in other, general occupational categories that cannot be assigned to a specific science and engineering field. Nonetheless, this provides an approximate view of the number of existing workforce professionals who are increasingly likely to encounter elements of the MGI in their work, particularly in the case of "materials and metallurgical engineers."

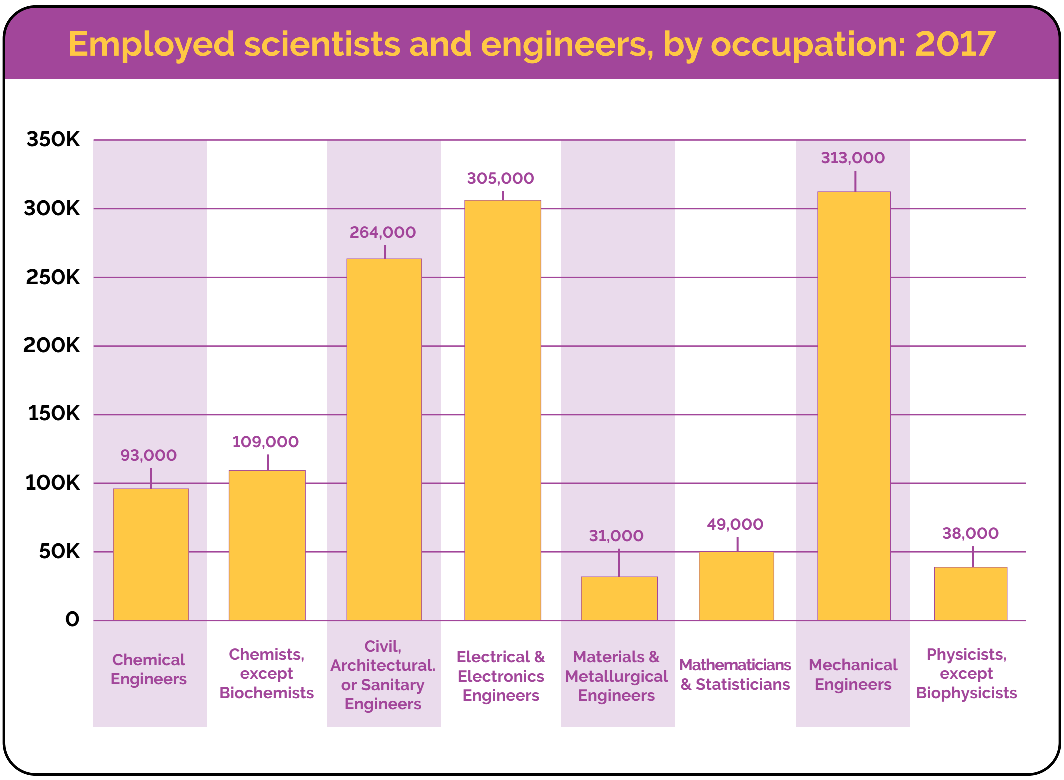


Figure 1. Total number of employed scientists and engineers in 2017 for several occupations that comprise part of the MGI workforce. (Source: 2019 Science and Engineering Indicators[9])

Another key group to consider when discussing the creation of the next-generation MGI workforce is the population of students in higher education enrolled in various disciplines that contribute to the materials innovation ecosystem. This population of individuals is effectively the supply that will meet the growing demand for the MGI workforce and must be properly educated and trained to accelerate the discovery, development, and deployment of new materials. To give a sense of the size of these populations, Figures 2–4 provide data on bachelor's, master's, and doctoral degrees granted, respectively, for several science and engineering fields that commonly contribute to the MGI workforce. In 2017, "materials engineering" added 1,968, 1,371, and 877 degrees at the bachelor's, master's, and Ph.D. level, respectively. Each of these numbers represents an increase compared to degrees granted in 2012. This aligns with an increasing trend in enrollment seen across a variety of materials science and engineering undergraduate departments.[10] It is expected that many science and engineering students will not enter the workforce in an occupation that directly matches their field of study. For example, they could go on to earn other degrees, choose to pursue a different field such as finance or law, or not enter the labor force. However, it is clear that the number of individuals who could be prepared to contribute to the MGI workforce is growing.

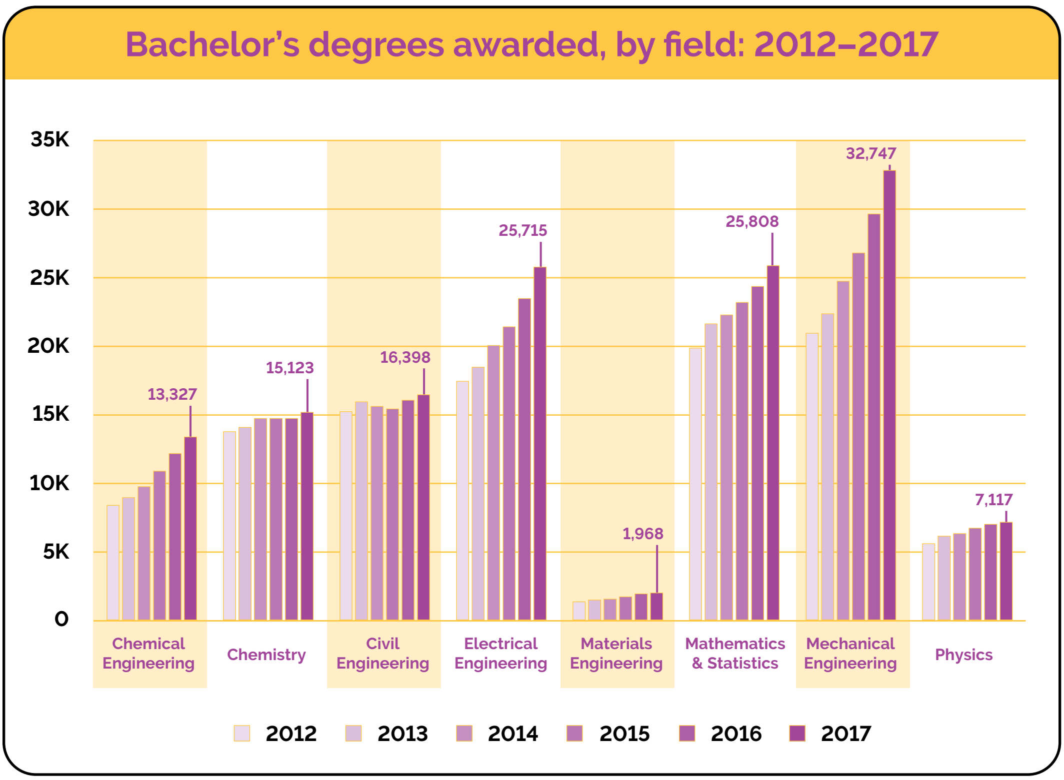


Figure 2. Total number of bachelor's degrees awarded from 2012–2017 for several science and engineering fields that impact the MGI workforce. Data labels indicate the total number of degrees awarded in 2017 for the corresponding field. (Source: 2019 Science and Engineering Indicators[9])

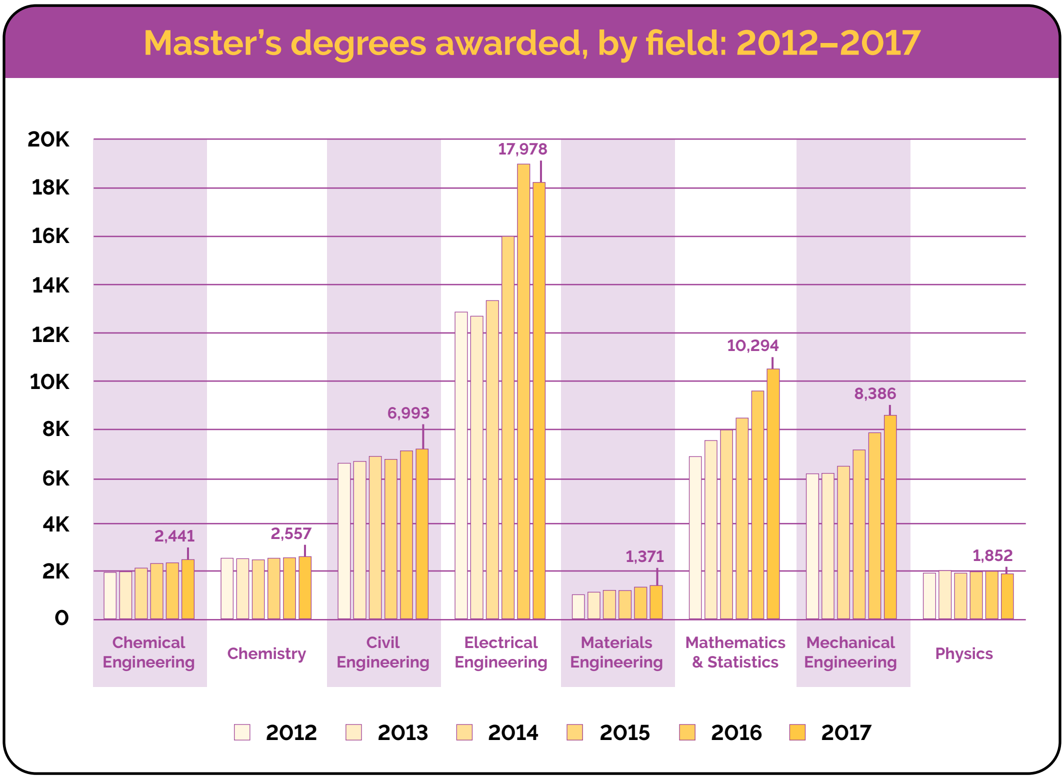


Figure 3. Total number of master's degrees awarded from 2012–2017 for several science and engineering fields that impact the MGI workforce. Data labels indicate the total number of degrees awarded in 2017 for the corresponding field. (Source: 2019 Science and Engineering Indicators[9])

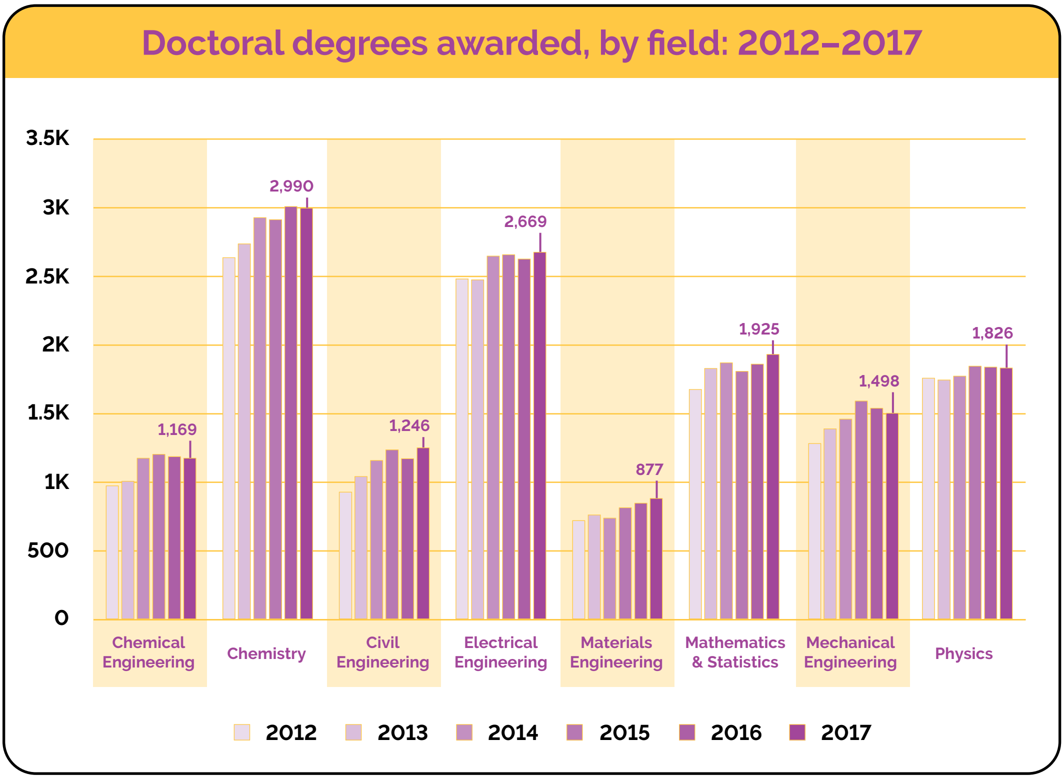


Figure 4. Total number of doctoral degrees awarded from 2012–2017 for several science and engineering fields that impact the MGI workforce. Data labels indicate the total number of degrees awarded in 2017 for the corresponding field. (Source: 2019 Science and Engineering Indicators[9])

Though K–12 students are part of the future workforce and essential for the MGI pipeline, to remain tractable, this report focuses primarily on education and training efforts involving undergraduate and graduate populations as well as the current workforce.

Role of Interdisciplinarity

The study team attempted to map various disciplinary contributions onto the MGI and its associated workforce. A total of 10 different common disciplinary themes or groupings were identified, along with examples of some contributions:

Biology/Biomedical Engineering

- Designs and synthesizes bio-inspired/biomimetic materials
- Applies knowledge of biomechanics to design prosthetics
- Utilizes bioinformatics to understand complex datasets and correlations
- Develops concepts for hierarchical, multiscale structures and associated phenomena
- Contributes applications such as programmed protein and DNA assemblies

Chemical/Biomolecular Engineering

- Applies principles in control of complex systems, reactors, and synthesis as well as optimization of process route and feedback control
- Develops high-throughput experimental methods
- Integrates materials [co-]design into engineering of systems; uses tools that inform the constitutive response of materials

Chemistry/Biochemistry

- Applies principles of thermodynamics, quantum chemistry, and quantum dynamics to materials development
- Builds quantitative structure activity relationship (QSAR) models in applications such as drug discovery
- Uses machine learning in retrosynthesis (e.g., identifying and prioritizing synthesis routes)
- Manages chemical complexity across length scales

Civil/Environmental, Mechanical, Aerospace, and Manufacturing Engineering

- Analyzes knowledge of cutting-edge/current materials problems and future trends (e.g., Industry 4.0; automation and robotics)
- Integrates materials in the [co-]design into engineering of systems
- Develops and applies methods of uncertainty quantification, verification, and validation to multiscale systems
- Develops constitutive equations of materials
- Develops methods for multiscale computational mechanics of materials
- Develops methods for systems engineering and design of materials and products
- Explores how next-generation materials can replace incumbent materials
- Recognizes/understands the potential impact of materials science on advanced manufacturing (e.g., additive manufacturing)

Computing and Information Sciences, Computer and Network Technologies

- Explores how the Internet of Things (IoT) can support the use of laboratory equipment
- Develops principles for data storage, sharing, schema, and ontologies that are critical to the materials innovation infrastructure
- Develops methods and tools of modern data science (e.g., analytics, advanced correlations, image processing, machine learning) that are key to future materials innovation infrastructure
- Provides examples of materials-relevant problems to automate the discovery processes
- Develops mathematics-based concepts for scaling computation for supercomputing resources
- Develops approaches for error estimation and uncertainty quantification
- Determines the reliability of predictive models
- Applies signal processing and pattern recognition to intelligent systems
- Analyzes distributed computing systems technologies

Electrical and Computer Engineering

- Addresses critical problems for electronic materials (e.g., solar photovoltaic, wide-bandgap semiconductors)
- Creates new standardized approaches for solving problems (e.g., simulation-based tools including multi-physics coupling)

Information and Intelligent Systems

- Explores how to use machine learning/artificial intelligence for intelligent systems
- Conducts information fusion from hierarchical, heterogeneous sources
- Identifies cybersecurity vulnerabilities in workflow processes

Materials Science and Engineering

- Explores processing-structure-property-performance relationships via linkages of computational, experiment, and data science approaches
- Simulates materials with specific and desired functions or properties from first principles
- Develops and exploits basic and advanced methods and tools to characterize structure and property of materials at length scales ranging from atomic scale to applications
- Contributes fundamental advances in computational materials science algorithms and codes and populates public databases with materials data

Mathematical Sciences and Statistics

- Translates prior knowledge into mathematical constraints that in turn can be integrated into machine learning tools
- Develops and applies methods for the design of experiments
- Provides a breadth of mathematical tools and communicates the needs to improve their 1) robustness, and 2) ability to deal with sparse, heterogeneous datasets and uncertainty
- Develops and advances mathematically rigorous approaches to inform uncertainty quantification and propagation

Physics

- Develops condensed matter theory
- Develops and exploits first principles methods in materials discovery
- Explores self-assembly and self-organization processes

Previous Materials Genome Initiative Workforce Recommendations

Over the past two decades, several studies and workshops have been conducted that examined the materials workforce as part of their objective. A brief summary of key outputs is provided in the following.

Prior to the announcement of the Materials Genome Initiative in 2011, several workshops and studies were held to develop recommendations on how to advance materials-related education that addresses materials design and development, leveraging computation and experiments. A 1998 workshop hosted at the Georgia Institute of Technology discussed how the emerging field of materials design might revolutionize the materials industry and virtual manufacturing. The resulting report, *New Directions in Materials Design Science and Engineering (MDS&E)*, concluded that a materials-design oriented workforce should be cultivated through development of undergraduate and graduate programs that integrate modeling and simulation tools, cross-disciplinary courses, and virtual instructional tools.[11] Later, the 2004 *Accelerating Technology Transition* study by the National Academies advocated for the creation of a modern design culture that emphasizes communication, collaboration, and flexibility.[12] Then, in 2008, the *Integrated Computational Materials Engineering: A Transformational Discipline for Improved Competitiveness and National Security* study recommended the training of both students and existing workforce in ICME-relevant topics such as computational modeling and simulation, as well as the development of databases and tools to support the growth of ICME.[5]

In 2011, the White House Office of Science and Technology built upon many of these prior reports and recommendations in the release of the MGI, which announced education and workforce development as a key focus of the initiative.[1] The follow-up MGI strategic plan released in 2014 outlined two main objectives to achieve the MGI goals: the development of new curricula and integrated research opportunities.[7] At the *Building an Integrated Materials Genome Initiative Accelerator* workshop that same year, attendees from various scientific domains and employment sectors organized into breakout sessions and discussed the future MGI workforce in the context of their particular fields, revealing overlapping needs.[13] Additionally, Stoebe, Cox, and Cossette studied the state of materials education with regards to manufacturing and engineering technicians and published their findings in the *Journal of Engineering Technology* in 2013.[14] More recently, workforce development has also been discussed as part of an Office of Economic Cooperation and Development Report on *The Next Production Revolution*, which includes a chapter focused on materials innovation.[15] The *Building a Materials Data Infrastructure* study conducted by The Minerals, Metals & Materials Society in 2017 also provided recommendations to prepare the MGI workforce to develop MDI technologies.[16]

The recommendations suggested by these studies, workshops, and experts can be summarized by the following three broad statements (additional detail on the full list of recommendations can be found in Appendix B):

1. **MGI-related topics should be integrated into existing undergraduate and graduate curricula.** For example, modeling and simulation modules can be integrated into core courses such as thermodynamics, kinetics, characterization, and laboratory courses. Additionally, new cross-disciplinary courses should be developed to expose students to the multidisciplinary nature of materials development.
2. Stand-alone offerings such as **short courses, workshops, online courses, and summer schools** should be developed and implemented to train the existing workforce in MGI-related skills. In addition, current and future faculty members should participate in educational programs that equip them with the knowledge and skills necessary to train the future workforce.
3. Industry, national laboratories, and academia should collaborate to implement **internships and research opportunities for students and postdoctoral researchers** which expose participants to real-world problems and cross-disciplinary teams. This will allow future workforce members to develop interdisciplinary collaboration skills and awareness of the entire set of methods, tools, and disciplines involved to support accelerated materials discovery and development. This should also encourage stronger integration between academia, industry, and national laboratories.

Related International Efforts

In addition to a strong and increasingly well-coordinated initiative in the United States, there are several concurrent activities going on around the globe that share a similar vision with the MGI. Though specific information on their contributions to education and workforce development is limited, a brief overview of noteworthy MGI-like activities in other countries is provided for additional context.

Horizon 2020 is an EU-based research and innovation program which has invested nearly €80 billion of funding available over 7 years (2014 to 2020) towards producing world-class science, removing barriers to innovation, and making it easier for the public and private sectors to work together in delivering innovation.[17] To this end, Horizon 2020 funds have supported the European Materials Modelling Council (EMMC) which has worked to strengthen existing materials modeling and data schemas as well as implement a collaborative and integrative approach to bring materials modeling benefits to manufacturers.[18] Some key ways of achieving this is through the development of the EMMC Marketplace, a digital European hub for all information and services on materials modeling including materials data repositories, translation, integrated workflows and training, and the Business Decision Support Systems (BDSS) which associates materials modeling with clear economic impacts and, thus, becoming an integral part of product life cycle management in European industry.

Japan's National Institute for Materials Science (NIMS) has formerly produced publicly available, high-quality data for years.[19] A recently announced Letter of Intent of Understanding on research exchange between NIST and NIMS will "promote Materials development globally by facilitating efficient Data Utilization."[20] NIMS also houses the Materials Research by Information Integration Initiative (MI2I), which aims to build government-industry-academia collaboration.

China has signaled a strong investment in new materials since its 2015 announcement of its "Made in China 2025" action plan to promote manufacturing, which included "new materials" as one of the 10 key sectors targeted.[21] Over the period from 2016-2020, the Ministry of Science and Technology and National Natural Science Foundation have together allocated approximately $3.6 billion USD for strategic electronic materials, key basic materials, biomedical materials and tissue replacement, nanometer science, additive manufacturing and laser manufacturing, material genetic engineering, metal materials, inorganic nonmetallic materials, and organic polymer materials.[22] Specifically, as part of their Materials Genome Engineering initiative, China has invested $150 million USD.[23] Its goal is to build a world-class MGI research platform by developing an infrastructure consisting of well-equipped laboratory facilities and outstanding faculty members. In addition, $86 million USD is being invested to construct a facility known as the Center for Materials Genome Initiative that is partly sponsored by the Chinese Academy of Sciences.[24] China's MGI has demonstrated a much more comprehensive integration between industry and academia than other MGI initiatives.

The German-based Novel Materials Discovery (NOMAD) Laboratory maintains the largest open-access, repository "for input and output files of all-important computational materials science codes."[25] NOMAD provides computer time to scientists to run calculations via online tools/platforms. Other international, MGI-related initiatives and tools worth noting exist at the Commonwealth Scientific and Industrial Research Organization (CSIRO) of Australia,[26] the Automated Interactive Infrastructure and Database (AiiDA) for Computational Science based in Switzerland,[27] and the European-based OpenCALPHAD,[28] which provides users with open access to phase diagrams based on free energy values from literature as well as the underlying code for the software.

While there has been significant progress around the world in the development of a comprehensive MGI ecosystem, a relatively small contingent of the greater MGI community has established the unique infrastructure to facilitate rapid materials innovation and the skilled workforce critical to that infrastructure's widespread implementation. In response to this challenge, various stakeholders have emerged to create a broad and diverse set of programs, training and educational platforms, schools, centers, and initiatives to champion the values and convey the methods and tools of the MGI. As impressive as these accomplishments are, however, there is still much work to be done to grow these individual nucleation sites for MGI infrastructure into a robust national and international networked infrastructure for accelerated materials discovery and development.

III. Current State of MGI Curricula and Training

In the last decade, academia, industry, and government agencies have developed and implemented a variety of programs that support the rising MGI workforce. Many of these efforts are aimed at addressing the recommendations highlighted by some of the key reports and workshops discussed in the foregoing.

Undergraduate and Graduate Education

Since the MGI was announced in 2011, there have been several substantive changes undertaken within colleges and universities across the country to align their curricula with MGI-relevant goals, such as expanded incorporation of computational and data science tools and educational offerings, a shift to more relevant programming languages, and strategic hiring of faculty with interdisciplinary backgrounds.

To learn more about the state of MGI education and training in undergraduate and graduate programs and current perspectives on its importance, a questionnaire was distributed to members of the University Materials Council (UMC).[c] In total, 24 responses were received and evaluated.[d]

c The University Materials Council (UMC) is composed of department heads, chairpersons, directors, and group leaders from approximately 114 academic programs in the materials field in U.S., Canadian, and Australian universities. Additional information including the current list of officers and members is available at https://umatcon.org/.

d A total of nine of the 24 respondents to the survey agreed to have their institution's name published as a participant. These institutions are: California Polytechnic State University (Cal Poly), Colorado School of Mines, Texas A&M University, University of Florida, University of Illinois Urbana-Champaign, University of Kentucky, University of North Texas, University of Texas at Arlington, University of Utah, Worcester Polytechnic Institute.

The first question in the survey asked respondents to rate the importance of teaching MGI principles to their undergraduate and graduate students. The distribution of answers is shown in Figure 5. In the case of undergraduate students, 79% of respondents agreed it was "Somewhat Important" or "Very Important." For graduate students, that number jumped to 96%, indicating that some view MGI as a more advanced set of concepts that are more essential to graduate training.

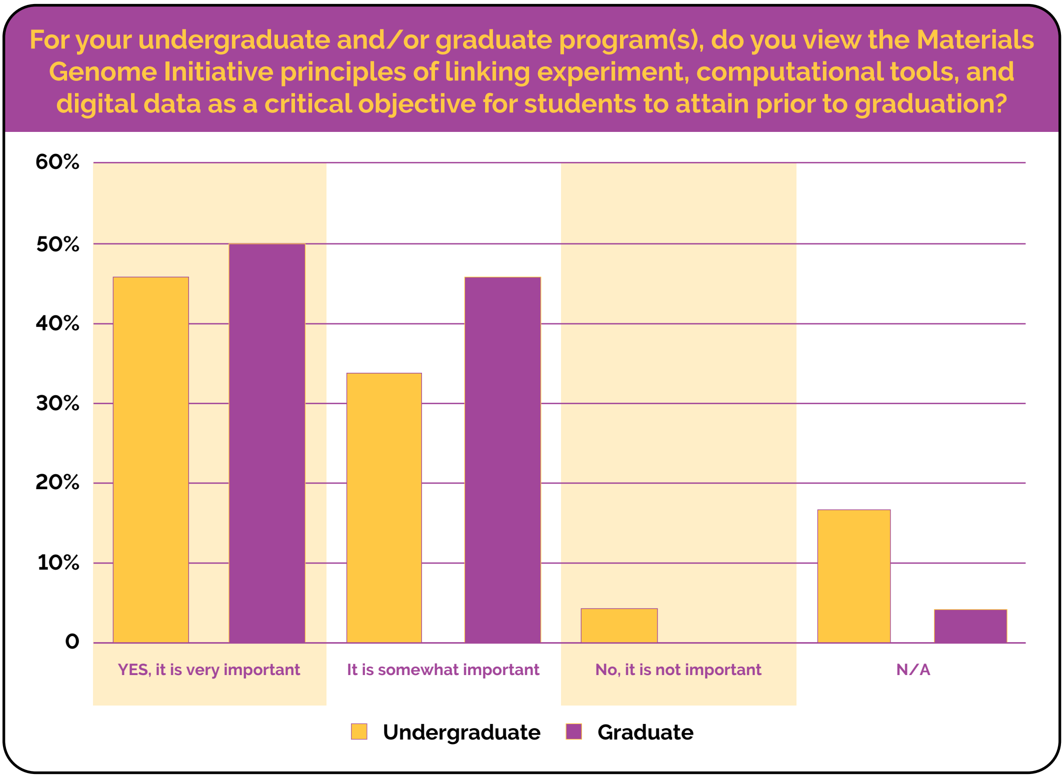


Figure 5. Survey respondents were asked for their opinion on including MGI in their undergraduate and/or graduate program(s).

Another question asked about the elements of the MGI that are embedded in their institution's undergraduate capstone design course. As expected, "experiment" was the most commonly found and was reported to be in 75% of the respondents' capstone courses. That number dropped to 54% for "computational tools" and was just 17% for "data science concepts." Nonetheless, 50% of respondents indicated that linking of experiment, computational tools, and/or data science concepts was integrated into their undergraduate capstone course, which is a key principle of the MGI. Thus, there is still room for more programs to introduce MGI components at the undergraduate level; approximately half are already doing so as part of the capstone design curriculum.

The questionnaire also posed separate questions for undergraduate and graduate programs regarding the number of courses offered that "...are dedicated to coupling of experiment, computation, and/or digital data." For undergraduate programs, 12 respondents indicated having at least one course offered. Of those 12, eight reported that all of the offered courses were required. For graduate programs, 15 respondents indicated having at least one course offered in their curriculum. Of those 15, only three reported requiring at least one of them as part of the curriculum. This availability of courses with MGI-oriented content aligns with the sentiment of respondents, who generally view MGI as more important at the graduate level. The lack of required courses that cover MGI content at the graduate level may simply reflect trends toward reducing the number of hours of required courses.

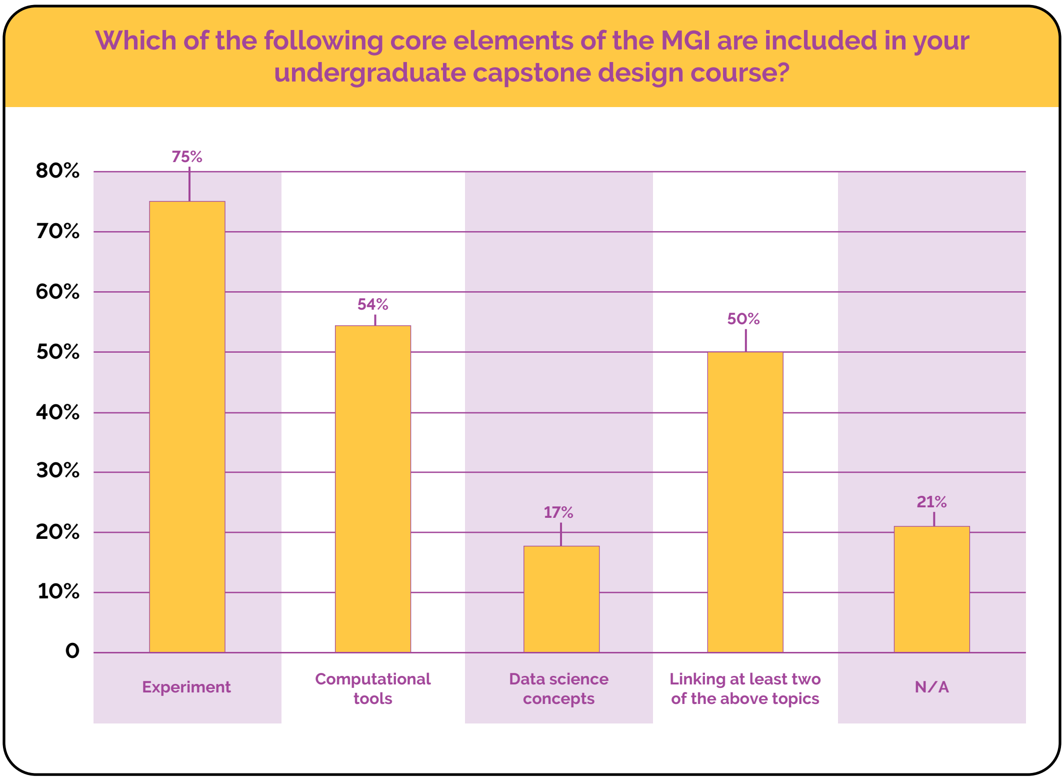


Figure 6. Results from question about topics included in undergraduate capstone design course.

When asked about the strategy they most favor for the potential integration of MGI into materials science and engineering curriculum, a majority of respondents (56%) preferred integration of concepts across one or more existing courses (see Figure 7). Nonetheless, some (28%) also preferred a mixture of integrating across many courses as well as offering stand-alone courses focused on MGI. A total of 17% of respondents to this question indicated they favored introduction of MGI through stand-alone elective courses.

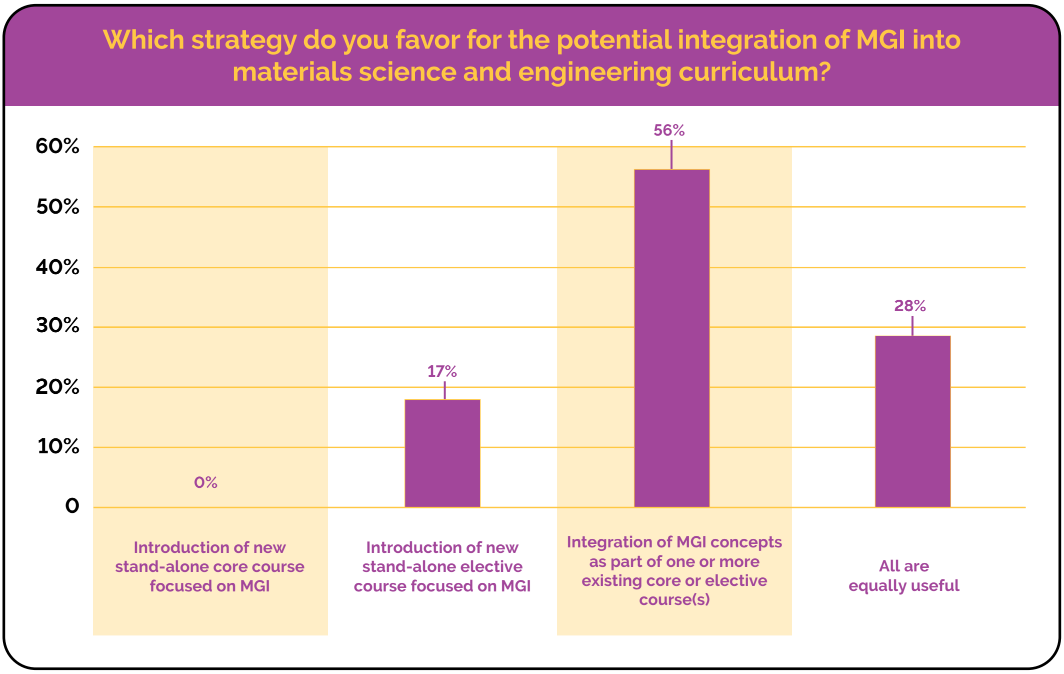


Figure 7. Results from question about preferences on how to introduce MGI into curriculum.

In addition to the questionnaire, a more detailed assessment of existing undergraduate and graduate MGI-related curricula in U.S. universities was also conducted. A total of 50 out of the approximately 114 U.S. programs were examined to assess the prevalence of coursework that meets the MGI's strategic plan goal to "equip the next-generation materials workforce." These programs were selected as a representative sample of MSE programs based on a wide range of research investment, geographic distribution, public vs. private institutions, and research focus areas. The following evaluation is meant to provide a reasonable snapshot of the degree to which the three foundational pillars of the MGI (experimental tools, computational tools, and digital data) are woven into current MSE curricula.

As expected, all 50 programs examined provide a wealth of course offerings that address a variety of experimental tools. In fact, many such courses have been offered in MSE departments for decades. Of the 50 universities sampled, 40 offer computational materials science and engineering (CMSE) related coursework at the undergraduate and/or graduate level, specifically courses that contain keywords such as "computational materials," "modeling," or "simulations" in the title and/or course description. The focused CMSE courses offered at the universities typically cover atomistic simulations, Monte Carlo-based statistical thermodynamics methods, computational thermodynamics and kinetics, density functional theory, phase field methods, and other modeling techniques. Moreover, core MSE coursework—such as thermodynamics, phase transformations, and kinetics—and laboratory classes in many programs may also include the instruction and usage of materials engineering software such as computational thermodynamics engines (e.g. Thermo-Calc, PANDAT, FactSage, JMatPro), atomistic modeling tools (CrystalMaker), and electronic structure calculations software (e.g. VASP, CASTEP, ABINIT, Quantum ESPRESSO). A number of the universities also had computer programming requirements in their undergraduate degree programs or required mathematical methods courses based on MATLAB or Python, further reinforcing the development and utilization of computational tools within their curricula. These findings are in good agreement with a 2018 study on the state of CMSE education in the United States,[8] which revealed that most of the materials departments included in the survey increased the amount of CMSE courses available since a previous study in 2009.[29] Similar to results found in this assessment of U.S. MSE programs, the 2018 study states that 84% of universities now offer at least one (stand-alone) course in CMSE, with several universities having incorporated computational modules into the core classes.[8]

However, the successes in incorporating CMSE concepts into MSE curricula have not yet extended to the third pillar of the MGI: data science. Only nine out of the 50 institutions included in the research sampling currently offer courses that reference "data science," "data handling," or the utilization of "databases." Of the programs that have introduced data science, the incorporation of data analytics, digital data representation, and digital data manufacturing into existing core curricula is overwhelmingly preferred to the addition of new, stand-alone data science courses. With increasing exposure to data science concepts, some capstone materials design courses are developing significant data and computational components by including projects involving machine learning and materials informatics. While there are some exemplars in this regard, the overall dearth of data-related MSE course offerings highlights the degree of investment of resources, time, and effort still needed to develop a modern MSE curriculum that exposes students to the tools and concepts that will be ubiquitous in the workplace of tomorrow.

In addition to offering specialty courses involving MGI principles, a true integration of this interdisciplinary way of thinking about and approaching materials innovation is needed to fully realize the benefits of curricula reform, both within materials-related academic units and with other engineering and science departments. Mansbach et al. conducted a case study on the revised MSE curriculum at the University of Illinois at Urbana Champaign, revealing that the curriculum changes successfully increased students' knowledge and capabilities of computational tools.[19] However, the survey revealed that there was no significant change in attitude of the students concerning the importance of computational tools for their careers. Likewise, a 2017 study on integrating a computational lab sequence in the undergraduate MSE curriculum at the Ohio State University noted that 13 of 35 graduating senior students indicated that the computational materials content was "not valuable" for career preparation.[30] This suggests an apparent disconnect between student perspectives and the desires of employers, whom when surveyed indicated the desire for more interdisciplinary training and awareness for materials graduates.[31] It is clear that changing the educational materials for the future workforce alone is not sufficient in preparing the students to embrace the changes needed within the workforce. Anecdotally, it appears that lack of reinforcement of use of computational methods and tools across the curriculum may negate the impact of stand-alone course offerings. Clearly, lack of courses in data science further frames the challenge in preparing the future workforce, whether data originates from experiment or computation.

Beyond adding relevant new content to existing courses, several universities now offer certificate programs that target individuals who are interested in building interdisciplinary skills that support the vision and goals of MGI and ICME to facilitate accelerated discovery and development of materials. These certificate programs are offered as specialty tracks to students currently matriculating through a given department. Typically, these programs are relatively rigorous and time-consuming. The curriculum often includes 3–4 courses, or their equivalent, and are intended to run in parallel with a standard degree program. As an example, Northwestern University offers two unique graduate programs: a Certificate Program in ICME for Masters' level MSE students and a Cluster Program in Predictive Science & Engineering Design (PSED) for Ph.D. engineering students.[32,33] Moreover, some universities are now providing multi-track offerings, with one prolonged, rigorous track aimed at students, and one shorter, content-rich track more appealing to existing workforce professionals who typically have strict time constraints. For example, Texas A&M University hosts an interdisciplinary program known as Data-Enabled Discovery and Design of Energy Materials (D^3EM), which offers graduate students the ability to become D^3EM Fellows or to participate in the Materials, Informatics, and Design Certificate Program.[34] (See sidebar on page 27 for more information.) Similarly, from 2014–2019 the Georgia Institute of Technology (Georgia Tech) housed an NSF Integrative Graduate Education and Research Traineeship (IGERT) Program that targeted MGI topics. This program, known as *From Learning, Analytics, and Materials to Entrepreneurship and Leadership Doctoral Traineeship (FLAMEL)*, trained Ph.D. students conducting materials research in engineering and science in data science through specialized additional coursework and collaboration on teams with computer scientists, driven by the objective to advance materials design and manufacturing.[35] Georgia Tech also offers a Modeling & Simulation Certificate program for individuals already in the workforce.[36] There are also some professional certifications offered through various universities such as the "Foundations of Data Science" professional certificate at the University of California, Berkeley. It is important to note that in order to be successful, these programs require active support from the host institution, including the strategic hiring of passionate, interdisciplinary faculty and appropriate support from teaching assistants.

Stand-Alone Courses and Training

Along with integrating computational and data-driven techniques into core curriculum of academic units involved in materials education, several stakeholders offer summer schools, online courses, and training opportunities on topics related to computational materials science and engineering in an effort to educate and train the current and future workforce. The examples listed below are not comprehensive but aim to be representative.

In addition to the certificate programs offered through universities, there are several focused summer schools and short courses that aim to provide participants with a particular knowledge base in a short period of time. These programs may target a wide variety of materials practitioners, from students or faculty to government or industrial employers, depending on the focus of the course. One such course is the Summer School for Integrated Computational Materials Education which is led by the University of Michigan, and has been sponsored by NSF.[37] It is a week-long, "educate the educator" program that prepares graduate students, post-doctorates, and faculty to teach and integrate CMSE into undergraduate MSE curriculum through a series of computational modules. Similarly, Texas A&M University has been offering an NSF-funded Computational Materials Science Summer School (CMS3).[38] Initially focused on theoretical/practical modules on multi-scale computational materials science, CMS3 has refocused a third of its modules toward materials informatics for the past four years. Another approach is utilized by Stanford University's Institute for Computational & Mathematical Engineering, which offers summer workshops on the fundamentals of data science.[39] It consists of 10 day-long workshops offered over the course of one week, which can be taken individually or combined to earn a certificate of completion if one participates in four or more workshops. By contrast, the 5-day Machine Learning for Materials Research bootcamp and workshop offered through NIST is intended to be attended in full with the goal of educating members of industry, academia, and government labs how to utilize machine learning techniques for a range of materials applications.[40] Moreover, federal agencies have been particularly active in sponsoring various forums for independently learning MGI principles, such as the NSF MATDAT18 Hackathon,[41] the Materials Science and Engineering Data Challenge sponsored by Air Force Research Laboratory (AFRL), NIST, and NSF[42] and the Materials Informatics workshop for industry hosted by NIST and the Center for Hierarchical Materials Design.[43] National laboratories, under the umbrella of the DOE, have been long-standing providers of not only research opportunities, but also workshops, bootcamps, and internships to expose students and the current workforce to industry-relevant manufacturing technologies and associated data-driven software suites. As an example, the Oak Ridge National Laboratory (ORNL) Manufacturing Demonstration Facility (MDF) holds workshops and internships focused on additive manufacturing applications.[44,45] Additionally, Lawrence Livermore National Laboratory hosts a Computational Chemistry and Materials Science summer institute that pairs graduate students with laboratory researchers working in areas such as *ab initio* electronic structure theory, quantum chemistry, molecular dynamics, and phase field modeling.[46] Professional societies have also proven to be a reliable source of MGI-centric short courses, workshops, webinars, and symposia over the years. A number of short courses, webinars, and symposia on computational- and data-driven methods and tools for materials science, such as the webinar series providing an "Overview of Materials Data Curation Tools"[47] have been offered through societies like TMS. These examples show the range of topics, timeframes, and target audiences that could be effectively reached using a short course or workshop model.

A wealth of online resources is available to anyone seeking to learn more about the MGI, including related concepts, methods, and tools. Several universities offer MGI-focused online instruction at no cost, such as Georgia Tech's massive open online courses on "Materials Data Sciences and Informatics" and "Introduction to High-Throughput Materials Development." Additionally, open source, university-hosted online tools and platforms help to teach MGI-based approaches. Orange, hosted by the University of Ljubljana, Slovenia, is an open source machine learning and data visualization platform with interactive data analysis workflows.[48] Weka is a Software "workbench" for standard ML techniques hosted by the University of Waikato in New Zealand.[49] The Network for Computational Nanotechnology (NCN) at Purdue University, through nanoHUB, offers both open source and closed source (i.e., by request) simulation tools and other MGI-based approaches for cataloging and sharing models/data.[50] Online nonprofit organizations, such as Data Carpentry and Software Carpentry,[51,52] also provide community-driven boot camps to assist users learning computing and artificial intelligence skills. Lastly, commercial software companies, such as Thermo-Calc, host user groups/conferences to demonstrate their tools for industry and/or provide free software packages and student versions to aid the workforce in building familiarity and comfort with new data-driven methods and tools.

This mix of various styles of stand-alone initiatives to address specific educational needs of the evolving materials innovation infrastructure is a vital supportive foundation in the development of the next-generation MGI workforce; however, these initiatives do come with some limitations: (1) dependence on passionate individuals who are willing to invest considerable time, effort, and resources to develop these new initiatives and content, and (2) the need for the knowledge gained to be reinforced through direct/practical experiences, as well as usage within other courses in the curriculum beyond a few computational course offerings.

Research Opportunities

Another critical way in which the materials community has trained generations of practitioners is through hands-on experience in research laboratories and on manufacturing plant floors. Though universities are tasked with the most prominent role in educating the next-generation workforce in terms of critical MGI concepts and fundamentals, it is often government organizations and industry that provide students with the support and opportunities needed to develop both the skills and interest in MGI- and ICME-relevant technologies.

With regard to government support, it is instructive to revisit the role of NSF's Designing Materials to Revolutionize and Engineer our Future (DMREF) program. Since its inception in 2012, DMREF has been one of the most consistent and impactful sources of funding for promoting MGI concepts, fundamentals, goals, methods, and tools. The program has funded more than 260 university research projects either in whole or in part, and has supported the training of more than 160 post-docs, 900 graduate students, and 150 undergraduate students in research that is centered on MGI-relevant approaches that couple experiment, computation, and data science. In addition, through DMREF, new courses have been developed that address methods to promote accelerated materials discovery and development, and MGI-related symposia have been organized at national conferences to educate the community on MGI strategies.

Moreover, DMREF also supports efforts aimed at community outreach to inform and engage underrepresented groups, K–12 students, and the general public regarding future workforce opportunities and possibilities offered by the MGI. For the better part of the last decade, this stable source of funding has substantively supported the growth of the MGI cohort of the materials workforce.

Moreover, several other NSF programs have missions that are synergistic with MGI principles and have been successfully leveraged. NSF's Division of Materials Research (DMR) established Materials Innovation Platforms (MIPs) for the purpose of developing new mid-scale user facilities at universities. MIPs are awarded over a five-year time period at a support level of $10,000,000 to $25,000,000 and are eligible for a one-time 5-year renewal program. Under this program, two MGI-related facilities have been stood up: (1) the 2-Dimensional Crystal Consortium (2DCC) hosted at Pennsylvania State University, which is "focused on the development of 2D chalcogenides for applications in next generation electronics,"[53] and (2) the Platform for the Accelerated Realization, Analysis, and Discovery of Interface Materials (PARADIM) facility at Cornell University, which is "dedicated to the discovery and fabrication of materials with unprecedented properties that do not exist in nature."[54] Both facilities are accessible to students, faculty, and external users, creating a community of researchers. Beyond the research conducted at these facilities, the MIP grants support a range of outreach and community-building activities such as summer schools, multiple Research Experience for Undergraduates (REU) programs, and a series of informational- and experiential-focused workshops convening individuals from across academia, industry, and government. In addition, the NSF Research Traineeship (NRT) Program has awarded nearly $6 million toward the development of training methods in data-enabled materials science and engineering and the Data Infrastructure Building Blocks (DIBBs) is a cross-directorate program, established in 2016, which is focused on addressing data challenges facing scientific and engineering communities.

Several other government agencies have supported the development of an MGI community and workforce. NASA and DOE's national laboratories offer several programs that grant undergraduate and graduate students opportunities to gain research experience, including the Pathways Internship Program, the Science Undergraduate Laboratory Internship (SULI) program, and the Science Graduate Student Research (SCGSR) program.[11,12] The DOD is preparing the lightweight materials manufacturing workforce by developing a manufacturing curriculum model and offering internships through the Lightweight Innovations for Tomorrow (LIFT) program.[13] NIST sponsors the Center for Hierarchical Materials Design (CHiMaD), which focuses on the development of new computational tools, databases, and experimental techniques to achieve the MGI goal of accelerating the design of novel materials, offers undergraduates research opportunities through the Summer Undergraduate Research Fellowship (SURF), and offers a Postdoctoral Fellowship for MGI related projects.[14]

Industry has also played an important role in training the MGI workforce. Many successful companies have incorporated MGI concepts of interdisciplinary materials innovation by leveraging computational advances into their culture and practice, thus training more MGI-related workers. However, some of these companies have taken even more purposeful steps toward developing the future MGI workforce. For example, the Simulation Innovation and Modeling Center (SIMCenter) housed within the Ohio State University College of Engineering was established as a result of a $5 million gift from Honda R&D Americas, Inc. This interdisciplinary, collaborative center allows users to conduct virtual simulation and modeling of product performance and manufacturing processes and offers a library of software licenses supporting work in computational fluid dynamics (CFD), finite element analysis, optimization, structural analysis, and systems modeling. Also, the federal government has created opportunities for industry and academia to work together to accomplish the goals of the MGI. The NSF Grant Opportunities for Academic Liaison with Industry (GOALI) project "promotes university-industry partnerships by making project funds or fellowships/traineeships available to support an eclectic mix of industry-university linkages." The joint Penn State-Georgia Tech collaborative Center for Computational Materials Design (CCMD) was funded directly out of the NSF Industry/University Cooperative Research Center (I/UCRC) program and developed long-term partnerships with industrial members who share the goal of promoting technology in computational materials design. These industry–academia partnerships allow industry to work directly with faculty and students to define challenge problems and to provide a pipeline for student internships and eventual employment.

Data-Enabled Discovery and Design of Energy Materials (D^{3}EM)

Figure 8. At left, a photo of D3EM trainees during a class exercise. At right, a schematic illustrating how data science enables the discovery of processing–structure–properties–performance relationships and engineering design enables their exploitation to accelerate materials development.

Program Overview

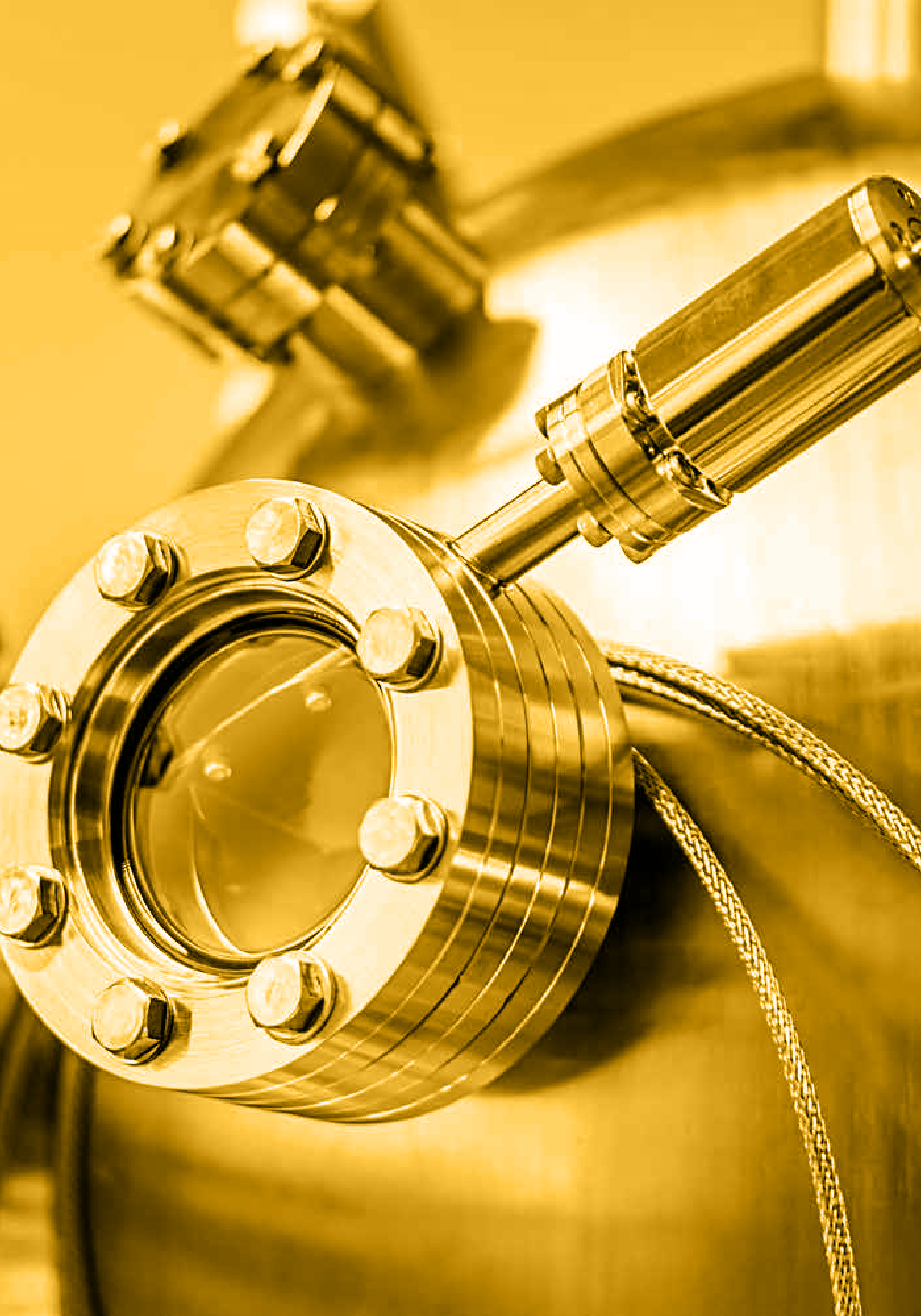
Initially funded by the NSF Research Traineeship (NRT) program, the Data-enabled Discovery and Design of Energy Materials (D^{3}EM) initiative at Texas A&M University has been institutionalized as an Interdisciplinary Graduate Certificate on Materials Science, Informatics, and Design.[34,55,56] D^{3}EM seeks to address the workforce development needs of the MGI by training M.S. and Ph.D. students with backgrounds in science or engineering to develop and deploy novel data-enabled frameworks to predict processing–structure–property relationships and to use advanced engineering design principles to invert such relationships to enable the goal-oriented design of materials. The program includes a cross-disciplinary curriculum including courses on materials science, informatics, and engineering design. The technical aspect of the program culminates with an interdisciplinary Materials Design Studio (MDS), modeled after undergraduate capstone design courses. The program includes a strong professional skill development component that provides training on interdisciplinary communication and collaboration, technical writing, team science, conflict resolution, and leadership. Participating faculty are organized through a community of scholars whose focus is the continuous improvement of the students' educational experience.

D^{3}EM has trained (or is in the process of training) four cohorts, corresponding to over 40 Ph.D. and M.S. students. All students have formally enrolled in the Interdisciplinary Graduate Certificate, with close to 30 students having completed all elements of the program. D^{3}EM seeks to prepare students for success in any career path of their choosing and thus has created a rigorous internship program through partnerships with industry and national laboratories. Furthermore, the program has served as a template for a new, Transformative Doctoral Education Model (TDEM) that seeks to revolutionize graduate education by emphasizing interdisciplinarity.[5]

Lessons learned

The following are some of the most important takeaways that have emerged in the first four years since D3EM was initiated:

- *Design-thinking is essential to realize the goals of the MGI*: While much can be accomplished by the use of data science frameworks to predict materials behavior, the goal-oriented design/discovery of materials requires practitioners to solve inverse problems through engineering design frameworks.
- *To educate students with an interdisciplinary mindset, it is imperative that the faculty leading similar programs embrace interdisciplinarity*: D^{3}EM faculty with expertise in machine learning and engineering design are key participants in the program.
- *Interdisciplinarity can only be achieved through strong communication and within a robust collaborative environment*: One of the first things that D^{3}EM students and faculty learn is how to communicate effectively with experts in disciplines other than their own.
- *Interdisciplinary approaches to materials science must be put into practice to reinforce skill acquisition*: The relative high success rate of the Materials Design Studio in converting class projects into peer-reviewed publications is only made possible because students are encouraged to deploy their skills to solve novel challenges worthy of publication.
- *Institutional buy-in is essential for sustainability*: D^{3}EM has been able to leverage existing programs within Texas A&M to provide the participating students with professional development opportunities that are beyond what a small group of faculty can offer.



IV. Defining the Future MGI Workforce

The subject matter experts in this project, with supplementary input from industry, government, and academic perspectives, identified and prioritized the knowledge and skills that are essential to preparing the next-generation MGI workforce. They are organized into the three foundational pillars that map onto the MGI: data, computation, and experiment. For each of the pillars, a group of subtopics is listed that represent the associated key competencies. An overview of this structure is presented in Table 1. A set of core knowledge and skills, as well as advanced/specialty knowledge and skills, are provided for each key competency area, along with examples in Tables 2–4. In general, it is helpful to think of the *core* knowledge and skills as most applicable to undergraduate curriculum and new workforce, whereas *advanced/specialty* knowledge and skills are typically a better fit for graduate curriculum or training opportunities for existing professionals.

The knowledge and skills described herein are in addition to the typical core requirements in materials science and engineering, such as basic thermodynamics, kinetics, and materials characterization. In many cases, there are additional MGI elements that could be integrated into such core courses. For example, theory and practical software related to calculation of phase diagrams (CALPHAD) could be introduced as part of a thermodynamics course at the undergraduate level. This is helpful since it is widely acknowledged that there are few options to introduce new concepts into already crowded curriculum. Instead of shrinking the technical core, faculty are encouraged to identify synergistic approaches to embed data and computational lessons and demonstrations within existing instructional content. This integrative approach has in fact been shown to foster deeper understanding of complex engineering problems.[58,59]

While it is not necessary for someone to become an expert in all of the knowledge and skills areas described in the table, it is important for students—both undergraduate and graduate—to develop awareness of these concepts and to be conversant in multiple topical areas such as data handling and measurement tools. It is also important to acknowledge that the linkage of these core knowledge and skills underpin the MGI, so there is some overlap. For example, data management, analysis, and interpretation are threads that run through each of the foundational MGI pillars.

Soft skills (such as professional networking, communication skills, and technical writing) were also acknowledged by the study team as important for advancing the MGI. Full implementation of an MGI approach will require an increased focus on effective communication, among other soft skills, as a result of the required culture change. Like the typical materials science core requirements mentioned previously, soft skills are broadly essential and, to varying degrees, addressed in today's curricula so this study instead emphasizes unique MGI methods, tools, and skills beyond those regularly taught today.

Table 1. Summary of Foundational Pillars and Key Competency Areas for the MGI Workforce.

Foundational Pillars	Key Competency Areas
Data	• Data handling • Modeling and simulation visualization • Software and codes to manage MG workflows
Computation	• Quantum and atomistic modeling methods • Microstructure evolution and material response • Multiscale and continuum modeling methods • Integrated workflows for computational tools
Experiments	• Multi-objective design and decision-making under uncertainty • Measurement methods and tools • Sensor fusion, high-throughput methods, and automation

The following three tables present the detailed MGI knowledge and skills along with examples for each of the three MGI workforce areas: data, computation, and experiment.

DATA

Table 2. Required Data-Related Knowledge and Skills for the MGI Workforce, with Examples.

Key Competency Areas	CORE		ADVANCED/SPECIALTY	
	Knowledge and Skills	Examples	Knowledge and Skills	Examples
Data Handling	• Data storage and archiving • Best practices in provenance and versioning • Data curation and cleaning	*Tracing provenance; understanding and appropriately representing metadata; data cleaning*	• Ontology and schema • Data fusion • Working with legacy data • Big data handling • Data mining	*Working with data from heterogeneous sources; developing data management plans; version control*
Modeling and Simulation Visualization	• Data modeling • Digital representation of material structure • Data visualization and representation • Information and knowledge extraction	*Statistics/modeling; use of existing machine learning tools/algorithms; principles and common methods for uncertainty quantification*	• Development and application of tools for machine learning and computer vision • Principles of optimization to maximize utility of information in the presence of uncertainty	*Materials discovery with heterogeneous data analytics (i.e., process–structure–property relationships); image segmentation and tomographic techniques; feature learning; anomaly detection; principal component analysis*
Software and Codes to Manage MGI Workflows	• Scripting scientific workflows with data from several sources • Integration of software modules and experimental data	*Jupyter Notebooks (and similar tools); Python; JavaScript; MATLAB; R; Julia; C++; working knowledge of materials libraries in these languages*	• Advanced programming • Heterogeneous code/ data environments • Batch processing and parallel execution • Methods to fuse computational and experimental data	*Advanced applications of Python and Java; use of high-performance computing resources; optimization of iterative workflows to provide decision support for materials development; automatic learning.*

COMPUTATION

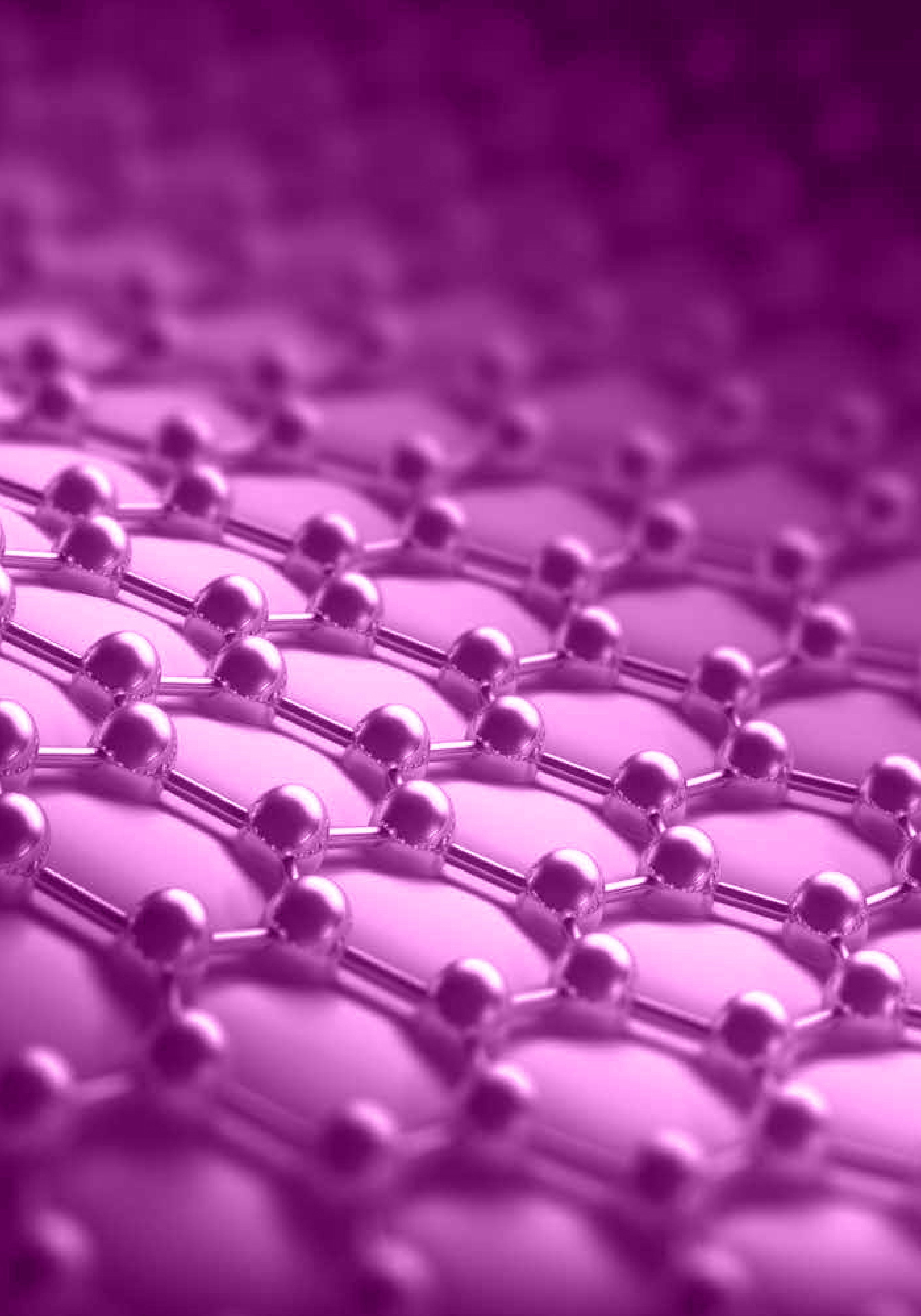
Table 3. Required Computation-Related Knowledge and Skills for the MGI Workforce, with Examples.

Key Competency Areas	CORE		ADVANCED/SPECIALTY	
	Knowledge and Skills	Examples	Knowledge and Skills	Examples
Quantum & Atomistic Modeling Methods	• Density functional theory (DFT), atomistic modeling via molecular dynamics (MD) with empirical potentials, quantum Monte Carlo (QMC) methods	*Specific software and tools for executing: DFT calculations, QMC simulations; atomistic modeling via MD*	• Electronic Structure Theory (quantum mechanics and solid-state statistical mechanics) • Development of interatomic potentials • Transition state theory and reaction pathways	*Quantum chemistry and DFT approximations; MD; kinetic and statistical Monte Carlo methods (KMC/SMC); nudged elastic band method;*
Microstructure Evolution and Material Response	• Computational thermodynamics • Basic kinetics and materials processing models	*Computational thermodynamics and kinetics tools: Thermo-Calc, DICTRA, AFLOW*	• Uncertainty quantification (UQ) and propagation in multiscale (i.e., length and time scale) material models • Developing/modifying thermodynamic and kinetic databases	*UQ in scientific workflows; kinetic Monte Carlo (KMC); phase field modeling (e.g. MARMOT code); PARROT module in Thermo-Calc*
Multiscale & Continuum Modeling Methods	• Awareness of methods for upscaling models across length and time scales • Numerical methods for continuum behavior	*Finite element method tools*	• Reduced-order and coarse-grained modeling approaches	*Development and calibration of constitutive laws for material behavior; model selection; parameterization of empirical atomistic potentials; digital microstructure representation*

EXPERIMENTS

Table 4. Required Experiment-Related Knowledge and Skills for the MGI Workforce, with Examples.

Key Competency Areas	CORE		ADVANCED/SPECIALTY	
	Knowledge and Skills	Examples	Knowledge and Skills	Examples
Multi-objective Design and Decision-Making Under Uncertainty	• Design of experiments methods and relevant statistics • Design and selection of processing and synthesis routes	*Factorial design of experiments; material response and failure mechanisms for multiple competing performance objectives; methods for robust design; Pareto optimality*	• Optimized experimental design principles • Digital representation of hierarchical structures • Application of critical datasets to relevant theories and models	*Bayesian methods; active learning; Pareto optimal designs for multiple property/ response targets*
Measurement Methods and Tools	• Awareness of techniques, tools, and derivative output information • Error and uncertainty in experimental measurements; Instrument precision, misalignment, sensor resolution, signal processing and temporal signal acquisition	*Interaction with common equipment and instrumentation such as atomic force microscopy, optical microscopes, diffraction and scattering methods, scanning electron microscopes, and mechanical and thermal testing equipment; LabVIEW*	• Advanced characterization methods • UQ and uncertainty propagation in interpreting experimental measurements • In-situ vs. ex-situ methods • Time-resolved data	*Understanding critical nucleation processes via in situ measurements; combined/ integrated measurement modalities; evaluation of dominant mechanisms governing kinetics of microstructure evolution*
Sensor Fusion, High-Throughput Methods, and Automation	• Data management to support scientific workflows • Application of statistical methods to datasets	*Statistical UQ methods for measured quantities of interest; digital signal processing for data compression and parsing*	• Multi-model data collection • Methods for data fusion • Automation of experiments and data acquisition • High-throughput synthesis and/or characterization methods	*Controlling composition gradients in thin film co-deposition; formatting data and workflows to facilitate reuse; combined/ integrated interrogation modalities; rapid assessment of process parameters on microstructure; autonomous materials discovery*



V. Barriers to Implementation

This study examined how curricula and training implementation barriers specifically apply to three groups: (i) students and early-career professionals, (ii) mid-career professionals, and (iii) educators and leadership/management. When considering common barriers that limit the rate of implementation of new MGI education and training opportunities for these groups, four key themes emerged, as described in the paragraphs that follow.

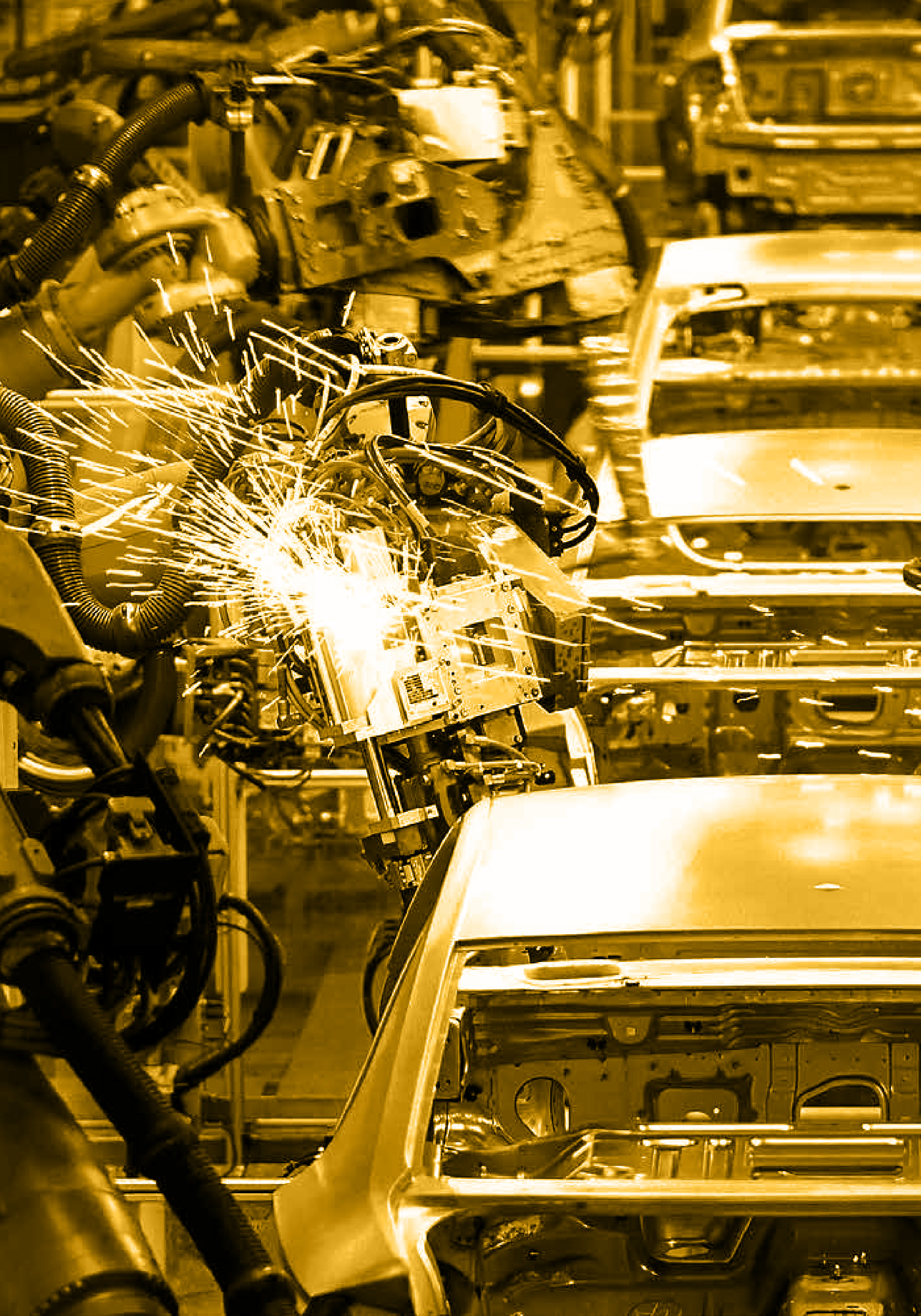
Inadequate number of available, qualified educators. In the case of students and early-career individuals, there is limited availability of qualified instructors who are familiar with the goals and technologies underlying the MGI. Mid-career professionals are less likely to be familiar with emerging concepts in computation and data science, yet they are often involved in management activities and/or execution of significant R&D programs, and thus have limited availability for sustained education and training. Moreover, many in this group are also somewhat less likely to have knowledge of current topics in statistics and programming, which were not as pervasive when they were undergraduate and/or graduate students. They often have in-depth disciplinary knowledge in specific domains. As a result, mid-career professionals may require significant additional introductory education and training via short courses or other focused learning experiences to be able to develop a functioning knowledge of MGI-relevant technologies. This further contributes to the need for qualified educators in the MGI arena. Senior leaders/managers and educators face similar challenges to the mid-career group. In addition, they could benefit from "MGI sabbatical" opportunities that facilitate more in-depth experiences in applying MGI approaches. However, there is a lack of such opportunities. At the same time, senior career professionals are also more interested in learning about the application and benefits of a new technology or approach (instead of the details surrounding utilization of the tools), but there are few resources and available educators to provide this type of information.

Overall, there is a relatively small cadre of senior MGI leaders who could serve as exemplars and train others in the value and utility of MGI approaches. This perspective is now broadly acknowledged and leads to bandwidth challenges in educating the future MGI workforce.

Lack of existing educational content and modules for learning MGI approaches. For early-career professionals, there is limited availability of easy-to-digest and classroom-friendly educational materials for individuals seeking self-guided or modular training. At the same time, there is limited access to relevant software and tools, depending on the academic institution, which often incur significant costs, faculty champions, or limited trial periods associated with their use. Additionally, there are few venues on which early-career professionals can focus to learn more about MGI-related codes and software. While some activities like the Materials Resource Registry at NIST are making data registry, software, and codes more readily available,[60] there is still a lack of self-contained modules that train students and/or professionals on how to leverage these elements within the context of the MGI. In the case of mid-career professionals, there are few existing online resources and short courses that enable one to pick up knowledge and skills pertinent to employing MGI tools and methodologies. Most companies involved in materials R&D also have limited bandwidth to implement MGI methods into established, ongoing workflows, so there is often limited opportunity for on-the-job training in MGI. At the level of senior leaders and educators, a key barrier is the absence of readily available modules/instructional materials that can be inserted and employed in their own institution or workplace. Since they are intimately involved in making decisions regarding allocation of resources and emphasis of education programs, a lack of exposure to methods and tools of the MGI is a concern.

Insufficient awareness of MGI or its value proposition. Many early-career individuals are recent graduates who may be unaware of the MGI, as they were focused on completing required courses that typically did not introduce the importance of linking experiment, computation, and data science. Mid-career executives, especially those lacking formal education in materials or related disciplines, may also not be aware of MGI benefits and therefore will not make available the funding or time needed for training. This group may also have an incomplete understanding of challenges and opportunities in the MGI, due to a lack of experiential knowledge and may remain hesitant to consider MGI principles and methodologies. Senior leaders and educators likely don't receive any direct outreach regarding the MGI unless they have been directly involved in the initiative. Since the MGI is not necessarily a high-profile technology concept brought up in senior-level discussions (in contrast to additive manufacturing, digital twins, or industry 4.0), it is often not considered a valued part of their toolbox. Yet, perhaps more than any of these other technologies, MGI is a key integrative foundation for modern materials science and engineering that will impact both basic research and its translation to products and applications. Since most senior leaders and educators were trained decades ago, their understanding of the value proposition of MGI is likely limited to second-hand knowledge. Even senior academic leaders may consider the MGI to be a computing-oriented initiative rather than fully integrative as intended. Additionally, since corporate leaders are often reluctant to share the impact of proprietary advances realized by embracing elements of the MGI, broader awareness of its value may be limited.

Cultural resistance to modernizing curriculum and training. Many early-career professionals and students are unlikely to have exposure to MGI concepts, in part due to the slow pace of change in education and training at universities, industry, and government laboratories. While some departments and companies are introducing more opportunities to learn about MGI principles, many institutions and organizations have only introduced them within the last 3–5 years. Ultimately, it is quite difficult to change curriculum at universities, which is already saturated with required courses. Mid- to senior-career faculty may have limited interest in changing the composition of a traditional materials curriculum, and not see room for data science, for example. Additionally, once they have settled into teaching a set of core courses, educators have little time to improve existing classes or create new ones that would introduce MGI concepts. This is exacerbated by limited expertise in elements of MGI (data fusion, data science, uncertainty quantification, systems engineering, etc.). Because the MGI has also been around for less than a decade, there is also resistance to accept it as a long-term methodology that will still be around in another 10 years. Though lifelong learning is critical to career advancement, some early-career professionals may be challenged by having recently completed degrees and needing to make their mark for tenure and promotion processes in areas that will be deemed as substantive by senior faculty. Mid-career professionals in industry are typically embedded within a business unit, and many are likely already so busy with current projects and deadlines that they don't have time to even consider the need for new knowledge and skills associated with the MGI. Additionally, it is likely that their projects are driven by a top-down approach that does not consider the value that exercising MGI principles might bring. In the case of mid-career educators, there is also likely skepticism or resistance to introduce new content in old courses due to Accreditation Board for Engineering and Technology (ABET) constraints, and discomfort with teaching topics they may not know as much about. Since pursuit of the MGI is inherently interdisciplinary, it may also present a challenge in ways of measuring credit for individual contributions, which is something that is especially important to early- to mid-career individuals in industry and academia. Some senior leaders and educators are reluctant to fully embrace certain megatrends such as big data and data science, in conjunction with rapidly increasing computing power and cloud storage capabilities, which are key elements of the MGI, believing that they have seen prior waves of research that introduce these elements but have somehow dissipated. As such, many senior leaders and educators may be more likely to label the MGI as hype and instead focus their education and training efforts more toward more traditional views that do not necessarily fuse experiments with computation and data science.



VI. Action Plans

Based on in-depth study and discussion regarding the current state of education and training as well as the needs for the future MGI workforce, the study team identified a total of seven recommended action plans. These action plans are intended to serve as guidance for next steps the community should take that will lead to significant progress in creating the next-generation MGI workforce. The action plans are organized into two categories of recommendations: supply side and demand side. In the case of supply-side recommendations, there is an immediate impact on near-term workforce readiness and the supply of trained scientists and engineers who are prepared to address MGI challenges and opportunities. In the case of demand-side action plans, focus is placed primarily on acknowledging the inexorable impact of data science in materials research and development and building the demand for a sufficiently trained workforce that helps accelerate advancements in materials through the MGI. In other words, the supply side is the "push" and the demand side is the "pull." Both are essential to foster in view of the foregoing discussion of barriers. Ultimately, all of these action plans are important to advance the preparation of the current and future workforce to tackle critical problems using cross-disciplinary teams, methods, and tools within the material innovation ecosystem of the MGI.

Each action plan includes a set of key tasks that are organized by timeframe of completion. However, some key tasks could be completed in parallel or reordered according to resource constraints. In addition to these key tasks, approximate timelines and milestones (and/or metrics) are provided where applicable, to help in measuring progress toward achieving the stated goals. The roles of various stakeholders are also articulated, along with the critical resources that are needed to ensure success. Several potential next steps are provided to catalyze near-term action and advancement of the varied action plans. Table 7 summarizes the full list of action plans.

Table 5. Summary of Seven Recommended Action Plans.

Supply-Side Action Plans	
1	**Modernize academic curricula with MGI content** and reinforce concepts throughout undergraduate and graduate education; emphasize Research Experience for Undergraduates (REU) programs for undergraduates and fellowships for graduate students in areas that build MGI infrastructure and provide examples of fusion of computation, experiment, and data
2	**Identify, develop, and package instructional modules** that can be implemented in academic courses
3	**Develop targeted short courses, boot camps, and summer schools** to fill gaps not otherwise covered in traditional education and training modes; prepare the instructors (i.e., educate the educators) necessary for MGI workforce development
4	**Articulate foundational MGI moonshot objectives** and establish programs with societal impact to address the initiative's goals and broaden the communities that understand its implications
Demand-Side Action Plans	
5	**Solicit input from industry and government laboratories regarding necessary MGI workforce knowledge and skills** and capture a summary of MGI workforce knowledge and skills needed, helping them to articulate potential impact on their operations
6	**Develop a summit event for CTOs and executives, and communicate to the broader community** by making related resources easy to access
7	**Create a web-based registry to document MGI successes** and clearly define metrics for measuring enhanced competitiveness and impact of MGI methods and tools, along with web-based dissemination of advances by stakeholder organizations

Action Plan 1:
Modernize academic curricula with MGI content

A key outcome of the study team's deliberations was the recognition that the underpinning elements and integrative aspects of the MGI should be embedded within a modern materials science and engineering curriculum. Those who do not embrace the critical importance of the MGI within their curriculum will not only be missing an opportunity but will also effectively be leaving their students at a disadvantage while other departments innovate. It is important to note that an enormous amount of work remains on fleshing out the MGI and modes of connecting its key elements, and these efforts will invariably interplay with advances in robotics, machine learning, systems engineering and design optimization, and so forth. Accordingly, the MGI in many respects offers a "blank slate" of potential tools and methods that are yet to be developed by new generations of researchers. The importance of student fellowships and internships in this regard cannot be overstated. The infusion of the MGI into capstone design projects should also be strongly emphasized.

Universities that embrace active development of MGI integration of experiment, computation, and data science are apt to gain significant advantages in large-scale materials proposals that rely on cumulative materials innovation infrastructure development. Moreover, as a part of the materials innovation ecosystem that particularly supports materials discovery, the sciences (e.g., physics, chemistry) should be engaged in cross-cutting curricula, introducing elective courses as possible to augment their education and training, and collaborating in cross-cutting certificate programs in the MGI.

Some universities and academic units are already advancing on this action plan. Yet, it is important to note that these changes do not have to happen only at individual department or program levels. The process could potentially be accelerated by also involving larger, multi-stakeholder organizations such as the University Materials Council and professional societies, which could focus activities on modernizing curricula to better prepare students to develop and employ MGI concepts.

Task 1.1: Assemble a group of diverse faculty and academic institutions dedicated to embedding MGI into curricula

A key step in embedding MGI content into curricula is to identify a faculty cohort who can champion the development or enhancement of curricula and develop suitable strategies to appropriately recognize their contributions. Such faculty teams might collaborate within or across universities to survey recent graduates and existing workforce to refine and prioritize elements of the modernized MGI-relevant curricula. Simultaneously, it is suggested that such groups also map existing curricula within a given academic unit or program to identify where specific problem sets or additional methods/tools with a stronger MGI emphasis could be introduced. For example, laboratory projects could begin introducing concepts such as scripting, utilizing digital notebooks, and employing basic visualization tools, as part of a move toward training an MGI-capable workforce. Similarly, e-collaboration tools (e.g., the Integrated Collaborative Environment, Materials Commons, nanoHUB, Materials Innovation Network (MATIN), and Timely and Trusted Curation/Coordination (T2C2)) could be introduced in an early, introductory course and then reinforced by use throughout the curriculum as another mechanism to train students in MGI-supportive tools they are likely to utilize after graduation.

There may also be other opportunities to lower the barrier for insertion of topics that may not require comprehensive revisions of existing courses, such as insertion of demonstration modules that reinforce user experience. Such opportunities should be explored over the next 1–3 years as they will reinforce the importance of MGI as more than just a standalone, isolated topic in the curriculum advanced by computational materials scientists and engineers.

It also must be acknowledged that department heads and center/institute directors play a key leadership role. If they are not fluent in and supportive of the MGI vision, then it is much less likely to be successful.

Task 1.2: Develop new MGI-related content and integrate into existing courses
After priority targets are identified for updating or revising course content, faculty leading this effort should identify leadership with accountability to develop the updated content and/or revise courses as appropriate. This could include revising some core courses, but in the near term is more likely to involve introduction of educational modules within such core courses or by introducing new MGI-related elective courses. The development of this content is an important task that could take up to a year, depending on the extent of new material needed. This activity should not be restricted to only undergraduate courses. It should also include the identification and reworking of new or revised curriculum at the graduate level. For instance, topics such as high throughput synthesis and characterization would be especially impactful if integrated into graduate courses, and could differentiate and better prepare students graduating from a department or program with a materials focus. We recommend devoting competitive federal funding to support cooperative course development activities across academic institutions that may form the basis for open source, modular elements of curriculum that can be adopted across a broad range of education and training stakeholders.

As mentioned previously, undergraduate capstone design courses present a critical opportunity to blend teaching and application of the fusion of experiment, computation, and data science in materials design and development; therefore, they should be viewed as a key opportunity for teaching and reinforcing MGI concepts. For example, problem-based learning methods might be employed to expose undergraduate students to various aspects of the MGI starting in freshman and sophomore years. Collaboration with other departments or industry partners as necessary in areas such as data science, manufacturing, design, and other fields should be encouraged to the extent feasible. Building on this idea, the introduction of graduate-level MGI capstone courses could integrate expertise across academic colleges and departments. Such courses could also introduce opportunities to learn and work across disciplines in a way that is not as well defined at the outset compared to undergraduate programs—something that is not typically available in the standard classroom environment. Capstone courses at undergraduate and graduate levels would also present an opportunity to have industry partner with universities to work on actual products and applications. Some universities already offer graduate capstone projects, though most of these are commonly part of a master's-level research project. In addition, Ph.D. students should be encouraged to participate in experiences that seek to apply MGI integration of experiments, computational simulations, and data science in solving problems of practical interest, with a goal of accelerating the process.

This task would clearly benefit from financial resources provided by one's department, university, or through a federal agency with a strong interest in materials education and workforce development, such as NSF. DOE and DOD laboratories are critically dependent on the future MGI workforce and would benefit from the support of cross-cutting student research and development experiences in the MGI context. As mentioned previously, such support could also be leveraged to make course materials more widely available to other universities, possibly through a shared repository (e.g., NIST repository) or via support for an educator's workshop that convenes several experts and facilitates the development of a network that addresses curriculum updates and modernization.

Finally, this task will integrate well with NSF broader impacts requirements and data management plans, particularly in DMREF programs, but also in various other MGI-related programs and calls (e.g., mid-scale infrastructure). The National Science Foundation (and other agencies such as DOE Basic Energy Sciences) could encourage researchers to include plans to incorporate their MGI-integration activities and results, including data and scientific/engineering workflows, into modules for courses and online data and code registries that would be broadly available for conveying MGI advancements and supporting MGI instruction across the United States.

Task 1.3: Launch new courses and content

After developing the associated content, the new or revised tools, modules, and courses should be launched. Feedback and evaluation from students should be an important component, especially during the early phases of instruction, to ensure that the concepts are being properly introduced and to facilitate rapid improvement during future iterations. If multiple courses are launched, a department could also seek to identify common themes for degree minors or certificates. In some cases, the courses could introduce information from other departments (e.g., statistics, computer science) and thus would not require the development of a full progression of courses.

In addition to the concept of registries and open curricular tools and modules, faculty who develop a significant amount of content for their departments or programs might be encouraged to write instructional textbooks on relevant MGI topics. Such books could ultimately reduce the barriers faced by faculty members when introducing MGI content and courses, and could be customized in electronic form to suit the needs of each particular academic unit and its course offerings.

Task 1.4 Coordinate with accreditation bodies

Accreditation Board for Engineering and Technology (ABET) leadership may not be aware of the transformational impact of MGI on materials research and education in the next 10–20 years. Thus, concurrent with the other tasks identified in this action plan, it is also incumbent upon department and program leaders to provide advice and guidance to the representatives from the materials community on the ABET commissions to ensure there is sufficient awareness as well as flexibility in the accreditation criteria for a department to begin introducing MGI concepts as part of the modernization of a materials science and engineering curriculum.

Action Plan 2: Identify, develop, and package instructional modules

There are several widely recognized barriers that make it especially challenging to introduce new concepts into existing curricula for undergraduate or graduate engineering and science academic programs. A key recommendation from this work is to identify, develop, and deploy portable, accessible, instructional modules that can introduce MGI-relevant instructional materials as part of existing core and elective courses over a broad range of institutions. This will lower the barrier to entry for a variety of departments and programs that might not otherwise have the resources or support to create their own modules representing MGI integrative concepts, methods, and tools.

Task 2.1: Identify funding support

To complement already developed MGI-relevant educational materials that may be broadly available to integrate into academic courses, competitive funding should be provided for faculty teams and experts (Instructional Modules and Materials [IMM] teams) at or across academic institutions. This also includes collaboration as appropriate with industry and government laboratories to ensure that relevant exemplary applications are considered. This task could take up to one year, as competitive white papers would be desirable as a first step in the development of modules that are complementary to existing materials and have a targeted value proposition across materials classes, applications, and MGI principles. The value proposition would focus on the critical nature of the proposed educational materials to the MGI workforce, consistent with this study, and would favor those topics having the lowest barrier to integrate into existing courses in materials science and engineering or related programs.

Task 2.2: Develop focused modules

Examples of topics for modules that selected IMM teams would develop might include one or more of the following:

- Computational thermodynamics (e.g., CALPHAD)
- Computational kinetics (e.g., DICTRA, KMC)
- Digital workflows manipulating data and sequences of operations in simulations and data analysis
- Image processing for segmentation, visualization, and analysis of microscopy data (e.g., optical microscopy, scanning and/or transmission electron microscopy)
- Quantitative analysis of microscopy images, including multiple spatial fields and time-resolved data
- Design of experiments methodologies applied to simulations and laboratory experiments
- Constrained optimization, utility of information, and Pareto optimality
- Combinatorial search of polymer synthesis routes to achieve target structures and properties
- Digital notebooks, tracking provenance, metadata, and e-collaboration
- Visualization of simulations
- Uncertainty quantification, verification and validation of experiments, computation, and workflows
- A video/webinar on a MGI project (e.g., integration of computational and experimental data, enabled by data science methods)

- Principal component analysis (PCA) and regression models for structure-property relations leveraging data science methods
- Machine learning (e.g., for process–path and process–structure relationships)
- High-throughput computing and automatic learning strategies.

IMM teams will develop detailed curricula for a given module, ensuring through collaboration that pertinent examples are provided to link principles to applications. Prior successful modules arising, for example, from the NIST Software and Data Carpentry initiative, could be studied in advance to scope new module development. Modules should make liberal use of open-source software tools and resources that are acknowledged and used within the MGI community, an important component to consider in awarding of competitive funding. This development phase for modular curricula could culminate 12–24 months after funding is in place.

Task 2.3: Deploy the modules

To maximize deployment, it is recommended that a central registry of modules be created, potentially via a federal agency (e.g., NIST), professional society, and/or a university with a long-term commitment to maintaining the resources. Some funding should be allocated to maintain these registries to ensure they remain sustainable and are able to track usage and student and instructor feedback, and to provide any updates. A successful prior example of a repository along these lines is housed at MatEdU,[61] which is primarily intended for a community college audience. Another example is the Materials Explorers™ website, which is focused on topics appropriate for high school students.[62]

Task 2.4: Obtain and act on feedback

Once deployed, it is strongly encouraged that the IMM team remain engaged in soliciting feedback from students and instructors regarding module content and effectiveness. The modules can then be updated and refined accordingly to ensure they are delivering content effectively. Broad dissemination of the resources and deployment of the modules will follow successful initial deployment over a timeframe of 1–2 years following initial introduction of the modules.

Action Plan 3: Develop targeted short courses, boot camps, and summer schools

Additional opportunities for MGI education and training beyond the typical classroom environment are strongly recommended as a means of educating and training practicing professionals, as well as faculty who might not otherwise have had much exposure to MGI concepts, methods, and tools. Examples could include short courses (e.g., less than 4–5 days), boot camps (e.g., extended, intensive learning experiences lasting one week or more), and summer schools (e.g., providing upwards of two weeks of content).

While these approaches are especially well suited for practicing professionals and faculty members who can return to the classroom to teach MGI-related topics, they can also be utilized by advanced undergraduate or graduate students who are interested and may not have access to MGI-relevant knowledge and skills through their own academic institution. Accordingly, these learning opportunities are critical to exposing a diverse set of stakeholders to MGI concepts. Moreover, the notion of educating the educators is a key strategy addressed by this action plan.

Task 3.1: Develop programs and funding incentives for educational opportunities beyond the traditional classroom

Funding agencies, universities, and professional societies should design incentives and offer funding to foster collaborative responses of university-led teams to define the audience, develop learning objectives, and metrics for assessment and impact on MGI workforce development. The portfolio over a set of teams should address the interplay of MGI elements of experiments, computation, and data science, either self-contained or in a well-designed, complementary set of short courses, summer schools, and boot camps. Example outcomes might include familiarity with data science methods to integrate experiments and computational simulations, increased understanding of methods to use computational modeling along with data science and high-throughput methods to rapidly explore viability of new and improved materials, standard methods for scripting digital workflows in managing computations and analysis of data, and so on. Clearly, these course development teams should focus on key MGI workforce needs, with instructors having experience in MGI-relevant research and development. As was the case in the task on instructional modules, these short courses, summer schools, and boot camps should maximize exposure of students to open-source software codes and tools that can be adopted in the classroom as a logical follow-on, promoting widespread adoption of MGI-relevant instruction in universities and training in industry and national labs.

Examples of existing educational opportunities include the Summer School for Integrated Computational Materials Education, which has now been held eight times with support from NSF, the University of Michigan, and others. NIST has also hosted a Machine Learning for Materials Research Bootcamp for the past four years with support from the Department of Materials Science and Engineering at the University of Maryland and others. Texas A&M continues offering the Computational Materials Science Summer School, which includes a substantial number of modules on materials informatics and machine learning-assisted materials discovery and design. Professional societies also play an important role in this task as many host short courses and bootcamps that reach a large, international audience.

Task 3.2: Survey participants and continuously improve the short course, boot camp, or summer school

Pre- and post-course surveys of students should be used to obtain feedback to ensure continuous improvement in course content and delivery, as well as MGI-relevance and impact on professional practice and preparation of educators.

Task 3.3: Identify mechanisms for sustainable delivery and evolution of instruction

In addition to developing and executing these short courses, boot camps, and summer schools, mechanisms should be introduced to evaluate, update and sustain those activities necessary to maximize continued impact on the momentum of MGI workforce preparation.

These efforts might include evaluation of dissemination to a large number of MGI workforce stakeholders, and plans to update, modify, combine or expand these offers to facilitate desired impact on MGI workforce and university-based MGI instruction over a 3–6 year time period, including community adoption and citation of short-course materials.

Action Plan 4: Articulate foundational MGI moonshot objectives

As a mechanism for catalyzing broader societal interest in the MGI and to inspire new entries into the materials workforce in various MGI-related disciplines, articulation of a set of foundational moonshot programs is recommended. Analogy is made to such powerful and broadly compelling objectives as landing a man on the moon in the Apollo program, curing cancer, providing clean drinking water in underdeveloped nations, and reducing global infant mortality. We emphasize that new capabilities to rapidly discover and design/develop new materials that will come with realizing the vision of the MGI are just as bold as these analogies in the sense of their tremendous, transformative impact on grand challenges such as renewable energy, sustainable mobility solutions, communications, and security. In fact, solutions for many of these already articulated grand challenges hinge critically on having capabilities of tailored materials with new functionalities. Hence, the materials R&D community must go beyond what may appear to others as incremental advances in increasing productivity to framing MGI moonshot objectives at the intersection of new and improved materials with candidate solutions broadly acknowledged in grand challenges. Devoting energy and intellect to defining bold objectives should offer a creative and innovative outlet to communicate the power and promise of the MGI in a broader societal context. The challenge of framing approaches that address these moonshot objectives will lie in the development of associated roadmaps for strategic development of methods, tools, and integration of emergent data science approaches with advances in materials computation, synthesis, processing, and various experimental tools, including autonomous materials research and development routes. Such roadmaps can provide substantial benefit to framing long-term research agendas for basic and applied research in federal funding agencies and can interplay with the core missions of national laboratories, as well as spurring new start-up companies and commercial development ventures. A good example to build on is the current emphasis of SpaceX in designing new materials tailored specifically for exploring and inhabiting the Martian environment in the next 20–50 years.[63] Another example is that of new materials that facilitate nuclear fusion as a transformative energy source.

Task 4.1: Convene a strategic leadership effort to engage the broader community, scope, and vision moonshot objectives

A first step will be convening a broad and highly interdisciplinary advocacy group or leadership team with an expansive view of potential opportunities for new materials. Such a team should also have a well-developed understanding and vision for the future of the MGI. This team should represent all stakeholders, academic, industry and federal agency participants. This may include one or more members of the National Science and Technology Council Subcommittee on the MGI to ensure consistency with the goals and trajectory of the MGI. The team should identify candidate MGI moonshot objectives and articulate the value proposition and goals clearly at a high level.

Contemporary emergent research in areas such as quantum computing and artificial intelligence may play a key role. For this task, The National Academies, professional societies, and university organizations might play a role in convening the effort and providing forums for input from a broad audience.

Task 4.2: Further define and vet candidate moonshot objectives
As part of an information-gathering stage, this effort should scope the existing landscape of materials research and development for which the MGI theme of accelerated discovery can play a transformational role in realizing enabling advances. It should target identification of multiple (i.e., 3–4) candidate MGI moonshot objectives to be further explored in more depth regarding potential for broad societal impact and ability to articulate to a general audience. Long time horizons for achievement of objectives, ca. 20–25 years in the future, will lend credence to the magnitude of the challenges involved and potential for transformational impact. Clearly, these advances will be expected to lie at the convergence of disparate disciplines, even beyond the current vision for the MGI. For example, it is expected that these challenges will incentivize engagement of the broad multidisciplinary design optimization community in engineering (materials, aerospace, mechanical, chemical, aerospace, industrial, systems) to address MGI-relevant integration of experiment, computation, and data science.

Groups of leaders in candidate moonshot themes could organize and host workshops to refine the vision and engage thematic visionaries, experts, additional convergent disciplines, including socio-economic stakeholders, as well as the broad MGI community, to select major moonshot objectives and articulate goals to facilitate follow-on roadmapping activities. Outcomes from these workshops, which should be easy to articulate to the general public, are expected to serve as actionable agendas to define support of relevant federal agencies and industry to support roadmap development efforts that will assist in the formulation of major MGI research agendas for the next 10–20 years. In this way, the momentum of MGI in the past decade will be amplified and will be enhanced by adopting transformative goals with strong public buy-in and awareness.

Task 4.3: Develop roadmaps and recommended plans for funding moonshot objectives
The process should culminate in the development of roadmaps for 2–3 moonshot objectives in distinct development efforts. There is no need for a common template beyond the need for a clear mapping of parallel efforts that are required, types of research and development activities, and the role of future workforce development. These roadmaps should emphasize clarity of investment priorities on the path toward framing the MGI materials innovation infrastructure to pursue these objectives. This includes application of existing technologies with particular emphasis on identification of gaps and how they can be closed with investment. It is expected that these roadmaps will be helpful to funding agencies, industry, and government labs in prioritizing investments in further MGI development, and to gain societal and political support for the broad purpose of advancing MGI to new generations of integration, technologies and future workforce.

Action Plan 5:
Solicit input from industry and government laboratories regarding necessary MGI workforce knowledge and skills

Feedback and guidance regarding industry and government laboratory needs will be essential as input to the development and integration of MGI content in curricula, short courses, and other instructional platforms.

Task 5.1: Reach out to industry and government laboratories for input on high-demand knowledge and skills for the MGI
Using the outcomes in Section IV of this report as a foundation, industry perspectives and views regarding necessary MGI-relevant knowledge and skills should be sought. A team of experts could be convened with financial support from a federal agency or could work in coordination with a professional society to develop a plan for outreach that will ensure broad but relevant input. A key task for the team of experts will be to identify appropriate industry segments. This segmentation should be used to facilitate broad sampling of perspectives and eventual reporting of results.

Task 5.2: Conduct a formal survey of industry perspectives
A formal survey should be conducted to gather comprehensive industry perspectives. This includes identification of key audiences and participants who are in a position to answer the questions posed in the survey.

Task 5.3: Issue a summary report
Issue a summary report in a journal with high visibility (ideally open-access). Consider updating the survey on a regular basis for a period of up to five years as a complement to other action plans regarding curriculum development, short courses, and other activities.

Action Plan 6:
Develop a summit event for CTOs and executives, and communicate to the broader community

The transition toward concurrent MGI approaches in industry will require a significant cultural shift. It is therefore important to promote understanding and buy-in of leadership regarding the value proposition of the MGI. The urgency of the need to build MGI methods and tools into engineering and production workflows for global competitiveness should be reinforced by quantitative arguments.

For large corporations as well as many small and medium-sized enterprises, it can be challenging for an individual or small group to make the case for incorporating elements of the MGI and the particular need for MGI education of the workforce to leadership, especially when many of these corporate leaders are not familiar with the complex nature of developing and deploying materials systems. For this reason, a summit event for CTOs and similar executives is recommended as one mechanism to build interest in the MGI and to create demand for the associated workforce. It may also be helpful to work on related modules for those who are not able to attend the summit but could learn more about the MGI in condensed webinars or via other resources suitable for lay audiences and decision-makers in the public arena.

The strategy of such a summit could focus on leveraging the NIST Economic Impact Study, which estimates the potential economic benefit of an improved Materials Innovation Infrastructure to be between $123 billion and $270 billion per year.[2] An organizing committee led by key industry MGI stakeholders working alongside academic counterparts would also be responsible for identifying a list of potential attendees to target for participation at such a summit. In particular, candidates who are more materials centric with demonstrated interest in investing in MGI approaches can play a role as an ambassador to the broader attendance pool.

When developing the summit program, the organizing group should identify key business/technology opportunities presented by introducing MGI concepts. Ideally, there will be documented examples that can be presented on the metrics of greatest interest to the CTO community. The anticipated timeframe for organizing an event like this is 18 to 24 months. It is recommended that a professional society that bridges academia and industry secure funding and organize this summit event.

In addition to organizing the CTO summit, it also recommended that additional resources be assembled to introduce and demonstrate the value of MGI. This could include the development of articles tailored for publications like *Harvard Business Review* and the *Wall Street Journal*. Additionally, webinars, podcasts, and other online venues (e.g., TED talks) could be actively considered and cultivated.

If successful, the CTO summit and additional resources should also be accompanied by a deployment toolkit that will help CTOs implement MGI approaches within their companies. Such a toolkit could build on the ICME toolkits developed as part of a 2013 study, *Implementing ICME in the Aerospace, Automotive, and Maritime Industries*.[64]

Action Plan 7: Create a web-based registry to document MGI successes

Success stories and case studies are powerful mechanisms for demonstrating the value of embracing the integrative materials innovation ecosystem approach of the MGI. However, clearly documented success stories from the MGI are still evolving, and are not commonly or broadly disseminated. Therefore, we recommend the development of an easily accessible registry or catalog of MGI successes with examples of quantitative metrics for improvement.

Task 7.1: Canvass industry for example success stories

An interagency group, a professional society, or a coalition of academics from various departments could canvass industry for examples of MGI successes that demonstrate the benefits of deploying an MGI materials innovation infrastructure within one's company. Time, cost, and additional metrics of interest to industry (such as return on investment [ROI]) that can articulate the benefits of the MGI should be considered and included as part of any capture of success stories. This includes identifying success stories not just from a technical perspective but also from a financial perspective that illustrate the value of the MGI with respect to research productivity. For example, even if a new material is not developed from an MGI-oriented effort, it is still possible to explore a much larger design space than would otherwise be possible from traditional materials development approaches that occur largely within disciplinary silos.

Hence, success stories regarding enhanced and accelerated basic materials research capabilities and infrastructure from universities and federal funding sources such as the NSF would also be important to include.

To date, the acquisition of success stories from industry has been especially challenging because corporate culture is risk-averse when it comes to potentially sharing information that may be helpful to a competitor. However, there is a strong need to share these success stories and articulate the demand for a capable MGI workforce that continues to push these companies to fully utilize the capabilities of a modern materials innovation infrastructure. Without demonstrated success, existing and new employees are not likely to obtain the skills needed to leverage and advance the MGI and the pace of innovation may be slowed in discovering, developing, and deploying new materials. This effort to capture success stories could take place over the next 12–24 months.

Task 7.2: Disseminate success stories via publications, easy-to-access registries, and other channels
After obtaining a set of detailed success stories, the information should be shared via journals (e.g., review articles) and posted to a central clearinghouse such as one of the federally managed Materials Genome Initiative websites.[65,66] At present, there are already success story examples such as commercialized alloys developed via an MGI approach. This includes high-strength aluminum alloys for 3D printing, which were identified in part by using a software tool that helped down select from more than 4,500 combinations, and performing experiments on a subset of these that best matched the desired design and performance constraints.[67,68] In addition, The Materials Project, launched in 2011, is another good example of how the MGI can enable the prediction of new materials and properties through data mining. It has already been applied to an array of new materials including Li-ion batteries, photocatalysts, thermoelectrics, piezoelectrics, and other functional materials.[69] Examples of the emerging area of autonomous materials research may even help showcase some of the cutting-edge opportunities enabled by the MGI. In this area, the Air Force Research Laboratory has successfully demonstrated the use of closed-loop autonomous approaches for discovery of carbon nanomaterials.[70] There have already been multiple articles that focus on innovations in academic environments; instead, it is essential to draw from industry to demonstrate that MGI advances are powerful in their ability to scale to an industrial processing or manufacturing environment. It is anticipated that if the right stakeholders and resources are leveraged, within 2–3 years there could be a robust registry with many success stories.

In addition to sharing success stories, interested groups might further disseminate information via webinars or videos to communicate the value of the MGI to a broad audience. Such videos might reduce the barrier for industry to share information because the commitment is somewhat lower as compared to authoring an article or peer-reviewed manuscript. At the same time, professional society conferences could provide a similar low-barrier pathway for convening panels that are focused on recent MGI success stories.

Other Recommendations

In addition to the action plans detailed previously, the study team also generated several other recommendations considered important to preparing the next-generation MGI workforce.

- Create an MGI award to recognize researchers for exemplary efforts
- Create MGI network fellowships and sabbaticals to promote interactive experiences at various educational institutions
- Establish dedicated symposia for sharing educational efforts in MGI
- Foster a culture of sharing by integrating data and code registries within MGI-related courses
- Embrace sharing of failures to accelerate learning and build support for adopting new MGI-based approaches
- Prioritize hiring of MSE faculty members who *integrate* modern data science methods and tools with computational materials science and/or materials experiments
- Incentivize development of training/retraining protocols for automation and data science principles that prepare operators, technicians, etc. for operating in data-intensive (e.g., industry 4.0, MGI) workforce
- Various academic units involved in materials education and research should clearly articulate their MGI-related education and research initiatives

VII. Conclusion

The MGI remains a foundational opportunity to achieve systemically accelerated discovery, development, and deployment of advanced materials in manufactured systems that will address the challenges and opportunities of tomorrow. Despite technical progress in advancing the underlying experimental, computational, and data science pillars of the MGI, there remains a strong need to improve the education and training of the existing and future workforce in materials research and development to better integrate these three pillars. Because educational curricula is slow to change, progress will require a sustained and multifaceted effort from the community.

This report aims to advance understanding and provide recommendations pertaining to development of the next-generation workforce, an often overlooked yet key goal of the MGI. In addition to providing a detailed vision for the necessary knowledge and skills of the future MGI workforce, seven action plans are provided to promote the culture shift that is needed to speed the implementation of MGI approaches.

Readers of this report are asked to reflect on their role in the materials innovation infrastructure and how they can contribute to advancing the MGI education and training objectives discussed here.

Now is the time to begin implementing action plans, as we know that many will take time to realize the full benefits. With the MGI in place now for the majority of a decade, it is becoming embedded as a theme for accelerated materials R&D in both academic basic research and industrially applied R&D. It is clear that the major emergent R&D themes such as additive manufacturing and artificial intelligence in materials discovery and development resonate strongly with the MGI, and in fact it is difficult to see how to move forward in these directions without the MGI. It is our hope that this report serves as a guide for articulating and motivating near-term actions that ultimately will have long-term impact on advancing the various elements of the materials innovation ecosystem, with prime focus on education of materials-related researchers and educators toward preparing a future workforce that will realize the goals of the MGI.

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Appendix A: Acronyms & Abbreviations

2DCC	2-Dimensional Crystal Consortium
ABET	Accreditation Board for Engineering and Technology
AFLOW	Automatic Flow
AFRL	Air Force Research Laboratory
AI	artificial intelligence
AiiDA	Automated Interactive Infrastructure and Database
BDSS	Business Decision Support Systems
CALPHAD	CALculation of PHAse Diagrams
CASTEP	CAmbridge Serial Total Energy Package
CCMD	Center for Computational Materials Design
CFD	Computational Fluid Dynamics
CHiMaD	Center for HIeararchical MAterials Design
CMSE	Computational Materials Science and Engineering
CSIRO	Commonwealth Scientific and Industrial Research Organization
CTO	Chief Technology Officer
D^3EM	Data-Enabled Discovery and Design of Energy Materials
DFT	Density Functional Theory
DIBBs	Data Infrastructure Building Blocks

DMR	Divison of Maerials Research
DMREF	Designing Materials to Revolutionize and Engineer our Future
DOC	Department of Commerce
DOD	Department of Defense
DOE	Department of Energy
EMMC	European Materials Modelling Council
ESPRESSO	opEn-Source Package for Research in Electronic Structure, Simulation, and Optimization
EU	European Union
FLAMEL	From Learning, Analytics, and Materials to Entrepreneurship and Leadership Doctoral Traineeship
GOALI	Grant Opportunities for Academic Liaison with Industry
I/UCRC	Industry/University Cooperative Research Center
ICME	Integrated Computational Materials Engineering
IGERT	Integrative Graduate Education and Research Traineeship
IMM	Instructional Modules and Materials
KMC	kinetic Monte Carlo
LBNL	Lawrence Berkeley National Laboratory
LIFT	Lightweight Innovations for Tomorrow
MATDAT	MATerial properties DATabase
MATIN	MATerials Innovation Network
MD	Molecular Dynamics
MDF	Manufacturing Demonstration Facility
MDI	Materials Data Infrastructure
MDS	Materials Design Studio
MGI	Materials Genome Initiative
MIP	Materials Innovation Platform
ML	machine learning
MSE	Materials Science and Engineering
NASA	National Aeronautics and Space Administration
NIMS	National Institute for Materials Science
NIST	National Institute of Standards and Technology
NOMAD	NOvel MAterials Discovery
NRT	NSF Research Traineeship

NSF	National Science Foundation
ORNL	Oak Ridge National Laboratory
PARADIM	Platform for the Accelerated Realization, Analysis, and Discovery of Interface Materials
PCA	Principal Component Analysis
PSED	Predictive Science & Engineering Design
QMC	quantum Monte Carlo
QSAR	quantitative structure activity relationship
REU	Research Experience for Undergraduates
ROI	Return on Investment
SCGSR	SCience Graduate Student Research
SMC	statistical Monte Carlo
SULI	Science Undergraduate Laboratory Internship
SURF	Summer Undergraduate Research Fellowship
TDEM	Transformative Doctoral Education Model
TMS	The Minerals, Metals & Materials Society
UMC	University Materials Council
UQ	uncertainty quantification
VASP	Vienna Ab initio Simulation Package

Appendix B: Summary of Past Recommendations for MGI Workforce Development

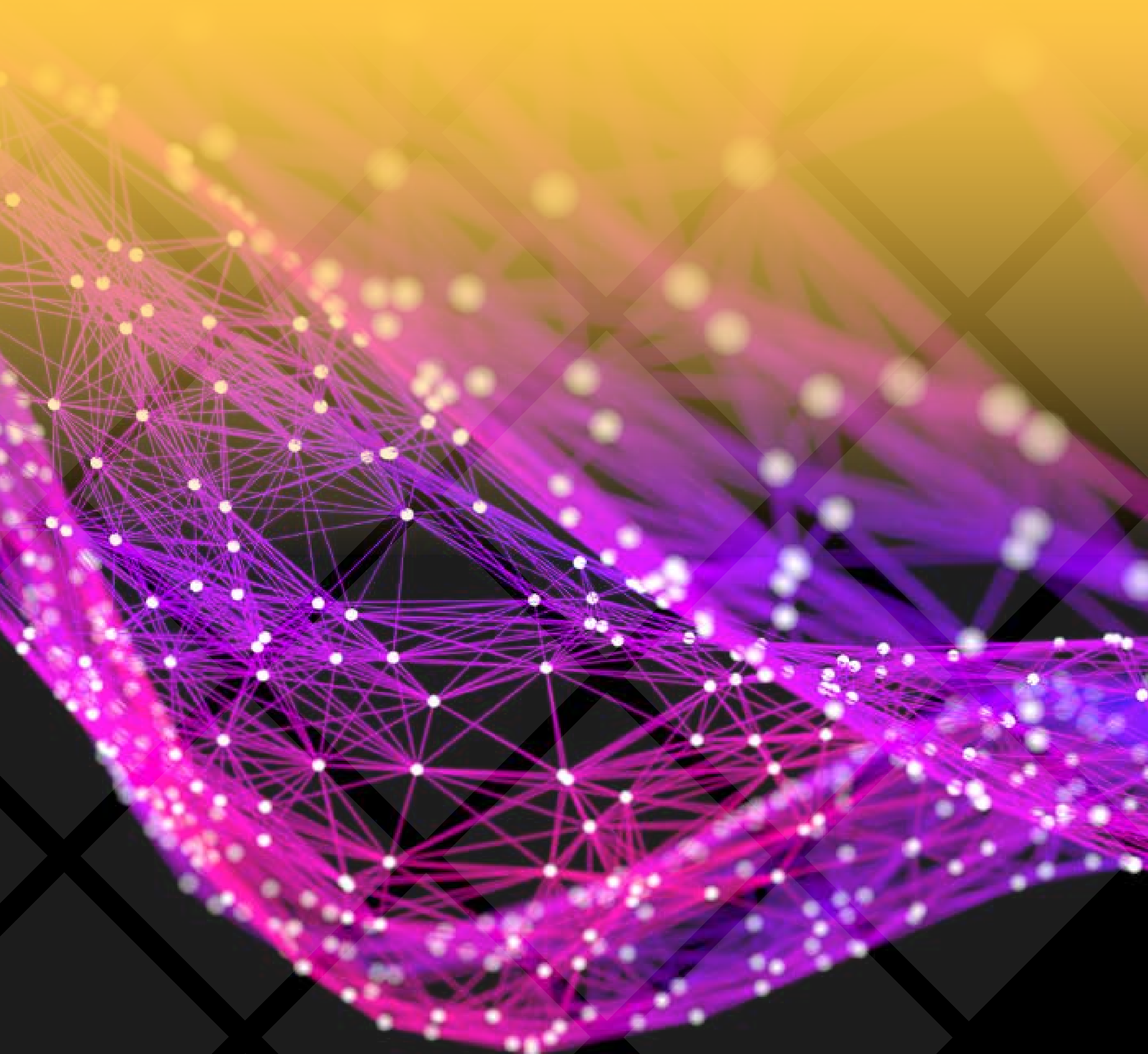
The tables below provide a detailed list of recommendations regarding MGI workforce development from past workshops, studies, and related activities. The recommendations have been organized by the topics of education (E) and professional development (P). In each table, the first column includes a code for identifying the specific recommendation, such as E.1 for a recommendation regarding education (E). The number simply identifies the specific recommendation, with no association with priority. The second column describes the recommendation, and the third column includes the source(s) of the statement.

Education		
ID	**Recommendation**	**Refs**
E.1	**Incorporate cross-disciplinary topics and skills into existing courses.** Before developing new courses, a first step would be to improve existing curriculum. Computational modules can be integrated into core curriculum to allow students to learn modeling and simulation skills in the context of fundamental coursework. For example, a mechanical behavior of materials course could introduce finite-element calculations so students can predict the response of a structure before performing a physical test.	5, 11, 13, 14, 16
E.2	**Introduce new cross-disciplinary courses in undergraduate and graduate curricula.** Standalone cross-disciplinary courses should be developed on special topics such as atomistic modeling, density functional theory, and materials data analysis. These courses can be developed and taught by multidisciplinary teams.	1, 7, 11, 13, 16

E.3	**Expand senior capstone design courses to capture integrated materials design approach.** Capstone design courses are already required in most MSE programs; the challenge will be to integrate realistic materials computational skills into solving a challenging problem. These courses should require students to work collaboratively in a group of materials students, or more ambitiously, in a multidisciplinary group of students from different backgrounds.	5, 11
E.4	**Provide minor program of study options to encourage cross-disciplinary education.** Materials science and engineering programs can offer minor options to allow students in other majors to develop materials skills. Additionally, cross-disciplinary minor options can be developed within multiple departments, such as electronic materials or computational materials science, to offer students more flexibility.	11
E.5	**Establish graduate specializations in ICME and/or MGI.** While some universities have specializations in computational materials science, few programs offer specializations or certificates specifically in ICME.	5
E.6	**Convene different university departments engaged in materials research.** MGI goals are multidisciplinary. Different departments within academic institutions should convene to identify methods for promoting interdisciplinary research as well as opportunities to more effectively integrate theory, modeling, experimental, and data analytics training for materials students.	4, 7
E.7	**Cultivate a modern design culture at universities.** Students should be exposed to materials design experiences that emphasize teamwork and collaboration, risk-taking, and innovation. For example, inquiry-based labs can be included in the curricula to give students more responsibility over projects.	4, 11, 12
E.8	**Facilitate collaboration among universities.** Leaders from the UMC should convene to identify effective educational practices and develop a model for incorporating ICME into a wide range of MSE courses. The effectiveness of these curriculum modifications should then be assessed according to ABET criteria.	5
E.9	**Facilitate discussions among federal agencies, academia, and industry.** Identify necessary skills for recent graduates entering the workforce and determine methods of prioritizing the development of such skills at academic institutions.	7
E.10	**Educate faculty about the goals of the MGI.** To encourage practices which help further the goals of the MGI in university departments (curricula, research, etc.) it is important that faculty members are aware of these goals.	7

E.11	**Offer educational programs for instructors to broaden the background and skill set of current and future faculty.** To facilitate the integration of MGI-related topics into curricula, educational programs such as summer schools and workshops should be created and provided to professors, graduate students, and post-doctoral researchers who are interested in becoming instructors.	13, 14
E.12	**Develop and host digital instructional materials on a centralized, commonly accessible database.** Virtual instructional tools and modules should be created and offered through open-access means to expose students to materials design concepts and practices. These online modules can easily be implemented by faculty into courses, reducing the need to develop new course content.	11, 16
E.13	**Establish alliances between the small businesses who are developers of software tools and MSE teaching institutions.** Alliances may encourage businesses to provide software at a reduced cost and/or offer training workshops to university researchers (faculty, postdoctoral researchers, and students) to facilitate proficiency in using software.	5
E.14	**Provide students with access to freely available research codes.** In many other engineering disciplines, developers of computational tools often provide software to educational institutions at a free or reduced cost. Implementing this practice in materials programs would allow more students to access and become trained in using computational software prior to entering the workforce.	5
E.15	**Create funding programs to assist universities in establishing a "critical mass" necessary to embed materials design within their curricula.** The development of new courses and research opportunities will require additional funding to accomplish. Government can also use the funding as an incentive to encourage more cross-disciplinary developments. The awards should be offered through a competitive, peer-reviewed proposal process.	11

Professional Development		
ID	**Recommendation**	**Refs**
P.1	**Create more opportunities for integrated research experiences for students and postdoctoral researchers.** Undergraduate/graduate students and postdoctoral researchers should practice MGI-related techniques in academic, government, and/or industrial labs as a standard part of their training. Participating in research with faculty or industrial internships helps to supplement students' coursework and expand postdocs' network of collaborators.	7, 14
P.2	**Provide workshops, short courses, and tutorials in MGI-related skills such as modern MSE computation for existing workforce members.** Educational training programs can serve to enhance the skills of professionals who are already in the workforce. These programs can be in the form of online offerings such as webinars and discussion forums as well as in-person activities such as short courses and boot camps. Materials professional societies can collaborate with members of industry, academia, and government to develop workshops, courses, and tutorials.	1, 5, 13, 16
P.3	**Stimulate new partnerships between manufacturers and software developers.** Partnerships can facilitate a more rapid conversion of science-based materials computational tools into engineering tools, providing basic research opportunities to educate researchers.	1, 4
P.4	**Encourage researchers to work closely with professionals from disparate backgrounds.** Experimentalists must understand the capabilities of modeling, whereas theorists and modelers must understand the processes and limitations of experimental methods.	7
P.5	**Facilitate a more integrated, collaborative MSE community** Collaboration among academic, industrial, and government participants is crucial to effectively achieve the goals of the MGI. Personnel can be exchanged among the three sectors within larger-scale MGI projects to encourage a collaborative approach. Professional societies can help facilitate communication and development of collaborative networks.	1, 5, 13



TMS

The Minerals, Metals & Materials Society

Promoting the global science and engineering professions concerned with minerals, metals and materials