President Barack Obama
The White House
Washington, DC 20502

June 19, 2014

Dear Mr. President,

We are pleased to send you this report, which provides a summary of five regional workshops held across the U.S. in the third year of the Materials Genome Initiative (MGI). A primary goal of the MGI is to catalyze greater collaboration amongst key stakeholders in the field of advanced materials. As the open sharing of DNA sequence data accelerated the Human Genome Project and enabled significant economic advances in biomedical applications, the MGI aims to speed the development and deployment of new materials to benefit a wide range of industry applications. The MGI workshops described in this report included key stakeholders from academia, industry, government, and national laboratories, who convened to address a range of issues related to MGI including models for collaboration, scientific progress, facilities and infrastructure, data sharing, and education, with key aims of increasing collaboration in the community and providing input to Federal MGI leaders on future directions for the initiative.

Across the workshops there was strong support for the Administration's MGI activity and we would like to take this opportunity to thank you for championing this important initiative. MGI is closely related to other Administration priorities including Advanced Manufacturing and Spurring Innovation; continued support for these activities by the federal government is vital to ensure the U.S. remains the global leader in science and innovation across these fields to benefit the U.S. economy.

The attached report summarizes the outcomes and recommendations from across the five workshops that we believe should be addressed in order to make progress with MGI. Key themes and issues identified include: the vital role of public-private collaboration to advance the key aims of the MGI; education and workforce development; computational and experimental research challenges; and mechanisms to spur interdisciplinary collaboration and enable data sharing.

We thank you again for your support and leadership on this initiative and hope that you find this report useful.

Best regards,

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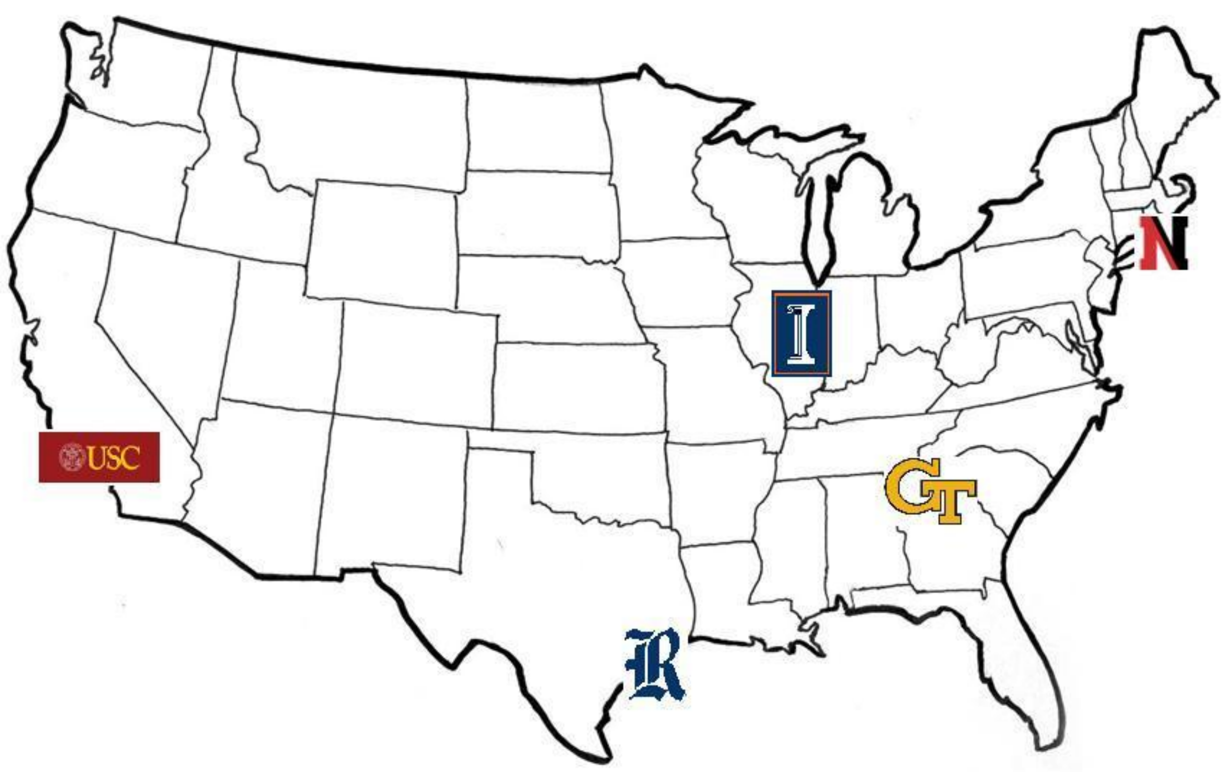
Summary of Materials Genome Initiative Regional Workshops

Introduction

During the third year of the Materials Genome Initiative (MGI), five universities from across the U.S. held a series of regional workshops that brought together academic researchers, materials research and development leaders from industry, representatives from national laboratories, and government science and technology officials to advance the goals of MGI. The meetings spurred regional discussions and partnerships and addressed a range of issues related to MGI including models for collaboration, scientific progress, facilities and infrastructure, data sharing, and education, to provide input to Federal MGI leaders on future directions for the initiative. This report presents a summary of those meetings and highlights the key outcomes and recommendations to advance the MGI.

Overview of Workshops and Attendees

Regional meetings were held in five regions of the U.S: the Northeast Regional Meeting at Northeastern University, the Western Regional Meeting at the University of Southern California, the Southwest Regional Meeting at Rice University, the Southeast Regional Meeting at Georgia Institute of Technology, and the Midwest Regional Meeting at the University of Illinois at Urbana-Champaign. Over 350 individuals attended the workshops, including 51 universities, 12 national laboratories from three federal agencies, and 59 different companies. Industry representation across the workshops included 23 Fortune 500 and Global 500 companies, of which 15 were top 100. Overall, 62 percent of attendees were from universities, 28 percent were from industry, 7 percent were from national labs, and the remainder were from non-profit groups, the federal government, or local government.



Key Outcomes

Across the workshops there was strong support from all stakeholders for the Administration's MGI activities. Participants highlighted the need for sustained effort from the federal government in terms of driving, coordinating, and funding MGI activities to ensure maximum impact. Efforts invested to develop and refine foci, establish roadmaps and metrics, and to put in place enabling structures and policies have the potential to advance the state of computational materials science, enhance high throughput materials synthesis, processing, and experiments, realize important value for industry, and provide multiple benefits to the U.S. economy.

The workshops provided a forum to increase community understanding of the goals of MGI and to explore opportunities for connectivity within regions to work together more closely on this challenge. Clearer definition of MGI along with defined goals for the initiative would be helpful to the community; the forthcoming MGI strategic plan should address these issues. Stakeholders agreed that the MGI can lead to new and important breakthroughs in materials and manufacturing, while leading to a rethinking of the disciplines of materials science and materials engineering. The changes in infrastructure (experimental tools, computational methods, data analysis, workforce development) and engineering thinking (moving from materials discovery and development to collaborative, systems-level approaches that bridge fundamental and applied research) are achievable with sustained effort from all stakeholders, and continued engagement and support at the federal level.

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[1] Word Cloud produced with Word It Out, http://worditout.com

Key themes discussed across the workshops include:

1. Models of partnership – innovation to facilitate public-private partnership

Workshop participants highlighted the vital role of effective partnerships between academia, industry, and government as key to the success of MGI. A range of issues from industrial experience for students and early stage collaboration, through to policy recommendations related to regulation and intellectual property were discussed across the workshops. For MGI to be successful, materials development must be a component of a complex systems approach rather than isolated activity. Early stage partnerships between industry, academia, and government research labs must occur to link materials research to desired applications so that all participants can best understand the real challenges and potential opportunities for progress. To ensure better industry buy-in to MGI, projects must demonstrate how the outcomes will make users more successful in the competitive industrial environment, for example through relevance, timeliness, openness (constraints on data use and ease of access), and dedicated facilitators.

Opportunities to encourage public/private partnerships for MGI include: work on large scale challenges or benchmarking problems; annual conferences; more focused objectives and activities for MGI, possibly around application domains, such as battery materials, structural materials, or material classes such as metals, ceramics, polymers, beginning with pilot activities; or production of a technology roadmap for industry or a set of industries. Regional centers of excellence were discussed as good models to encourage collaboration and support innovation. Examples of successful collaborations highlighted included semiconductors and the auto industry. The Industry University Collaborative Research Centers of the National Science Foundation (NSF) were also noted as a successful mechanism to catalyze industry-academic partnerships. The creation of test beds was similarly identified as key to success for MGI.

Participants agreed that the MGI must address the validation challenge – the time it takes for new materials to be validated for commercial application, either as a standalone product, or as a component of devices or platforms – in order to deliver on its strategic goals. This was identified as a particular challenge for aviation materials and materials used by the oil and gas industries. The need for new business models and IP sharing frameworks were also highlighted.

Key Recommendations to OSTP:

- *Implement materials development through complex systems approach.*
- *Establish Industry-University partnerships early in the process to collaboratively define challenges and opportunities.*
- *Base projects around grand materials challenges or more focused objectives related to application domains, material classes, or industry areas.*
- *Address issues related to material certification regulations and intellectual property.*

2. Education and workforce development

As for all major research and development topics, education and workforce development was identified as a key theme within MGI to ensure the U.S. has the best trained people to advance the initiative. Given the interdisciplinary nature of MGI and its close ties to industry, a number of workshop recommendations related to broadening student experiences to provide collaborative skills and opportunities for engagement with diverse communities and research problems. There is a need for broad, foundational education in science, technology, engineering, and mathematics (STEM) as well as holistic training that combines computation, experiment, data mining, and manufacturing facets. Students should be trained to work well in interdisciplinary teams that blend complementary skill sets and include project based learning. At the graduate level, there is a need to foster education in key areas such as materials / parts manufacturing. Universities should be encouraged to develop curricula for material scientists that include more problem solving, better appreciation of industrial practice, computational sciences and engineering, simulation methods, data analytics, uncertainty quantification, modeling and software development. Industrial experience was identified as being important for MGI such as internships and student participation in innovation activities. One specific policy recommendation was to provide tax incentives for industry-sponsored graduate fellowships. Students should be encouraged to go beyond curiosity-driven science, and develop an appreciation for current manufacturing practice and market forces. The need for continuing education and the development of new kinds of short courses and training for the existing materials workforce was also discussed at a number of workshops.

Key Recommendations to OSTP:

- *Continue strong support for STEM education.*
- *Encourage education and training that embraces a systems approach to materials development and includes computational skills for material scientists and engineers.*
- *Encourage interdisciplinary team work at all levels of education.*
- *Facilitate industry experience and involvement for students, for example through tax incentives for industry sponsored fellowships.*

3. Computational and Experimental Research Challenges

Participants discussed a number of research challenges to achieve MGI. Participants across the workshops agreed that advances in data analytics, data management, and computational methods are essential to realize the full power of MGI to transform materials design and advanced manufacturing. Many of the observations and recommendations at the workshops focused on bolstering investments in the development of new data and modeling tools. Critical challenges identified spanned a large range of computational issues, including developing better fundamental theories to predict physical properties, models and tools that can predict physical and dynamic properties over multiple scales, tools that can automatically incorporate past modeling and experimental data and capture future data, data mining tools to enable searches for particular properties, and methods for fusing experimental and computational data sets. At the Southwest Regional workshop, participants discussed particular challenges for materials that will be used in extreme environments for the aerospace and oil and natural gas industries. For these classes of materials, major advances are needed in predictive lifetime modeling to adequately model and test materials that will endure extreme conditions and must remain robust and durable over long time scales. At the Midwest workshop, participants emphasized the need for tools to be usable on new computer architectures and for efforts to focus on commodity computing used by industry, not just pursuing exascale.

Participants agreed that experimental challenges are heavily tied to specific materials classes and engineering systems. For example, at the Southwest Regional workshop, participants discussed the unique challenges related to achieving MGI for materials that must survive extreme environments while at the Northeast Regional workshop participants discussed the need for tools related to multi-scale manufacturing of composite materials. At the Western Regional workshop, participants recommended an effort on metrology as well as the development of in-situ approaches to measure nanoscale to mesoscale structure of defect compositions and their contributions to key material properties. At several workshops participants noted the need to support the development of tools and protocols for high throughput materials synthesis, processing, characterization and property measurement.

Key Recommendations to OSTP:

- *Ensure sustained support for and investment in data analytics, data management, modeling, and computational methods.*
- *Target investment in facilities for high throughput synthesis, processing, characterization and property measurement for screening materials to complement computational modeling and simulation.*
- *Support research to overcome experimental challenges related to MGI, considering the diverse needs of particular industries and material classes.*

4. Interdisciplinary Collaboration and Data Sharing.

Participants agreed that bringing together experimental and computational techniques to drive material design will require a change in culture towards enhanced collaboration across fields. However, many participants called for more focus in MGI, with some suggesting that effective collaboration would be promoted through encouraging smaller teams to learn initial best practices while others encouraged a focus on specific materials, properties, or methods. Some participants suggested holding a competition to choose pilot topics for research; these could be organized by industry sector, regionally, or by material class. An additional suggestion was to advance interdisciplinary work through the creation of shared user facilities that link synthesis, characterization, modeling, and data science. Many participants across workshops cited DARPA as an example of how to promote challenge-driven transformative research, although others noted that the sustained effort needed for MGI would not be well suited to the DARPA model.

At the Southeast Regional workshop, participants emphasized the need for interdisciplinary teams to come together at the beginning of a challenge and address scale-up and validation issues early in development. They also noted that at a basic level, standardized descriptions and definitions would enable better cross-disciplinary collaborations. The need for a materials innovation infrastructure was identified, including shared facilities and cyber-infrastructure for materials data, analytics, and decision support, with emphasis on high throughput methodologies.

In addition to advances in computational infrastructure and methods, participants emphasized the importance of data sharing and identified a number of models to incentivize sharing among researchers and industry and create tools to make such sharing easier. Many of the workshops recommended support for a central data repository or another kind of information-sharing entity. Participants emphasized the importance of usability for any data sharing tools and thought that there should be a broad range of data and tools included such as simulations and experimental data, analysis software, and experimental validation information. Some participants also added that dedicated personnel are needed to manage data and computing infrastructure. Participants also noted the importance of developing data sharing standards and establishing standard data formats to enable interoperability of data sets and encourage data sharing across materials fields.

Key Recommendations to OSTP:

- *Identify key priority areas for MGI.*
- *Establish shared facilities managed by expert personnel that link synthesis, characterization, property measurements, modeling, and data sciences*
- *Data sharing between and across academia and industry is key.*

Conclusion

The five regional workshops held on MGI spurred discussion among diverse stakeholders on the value of MGI and recommendations to advance its goals. Conversations among stakeholders have continued, including discussions on creating a national network for accelerating materials discovery, development and deployment that occurred at Georgia Tech during their national accelerator workshop held June 5-6, 2014, co-organized with the University of Wisconsin-Madison, and the University of Michigan. In the Midwest, collaborations are being enhanced through the Digital Manufacturing and Design Innovation Institute announced on February 25, 2014. Continued discussions and investments are critical for the U.S. to achieve its goal of accelerating advanced materials discovery and deployment, reinvent existing and fuel new industries, and address critical societal and economic challenges.