



Our vision is to connect academia, industry and government stakeholders to fulfill the goals of the Materials Genome and Manufacturing Initiatives.

*Summary of June 2014
Workshop Report: Building a
Materials Accelerator Network*

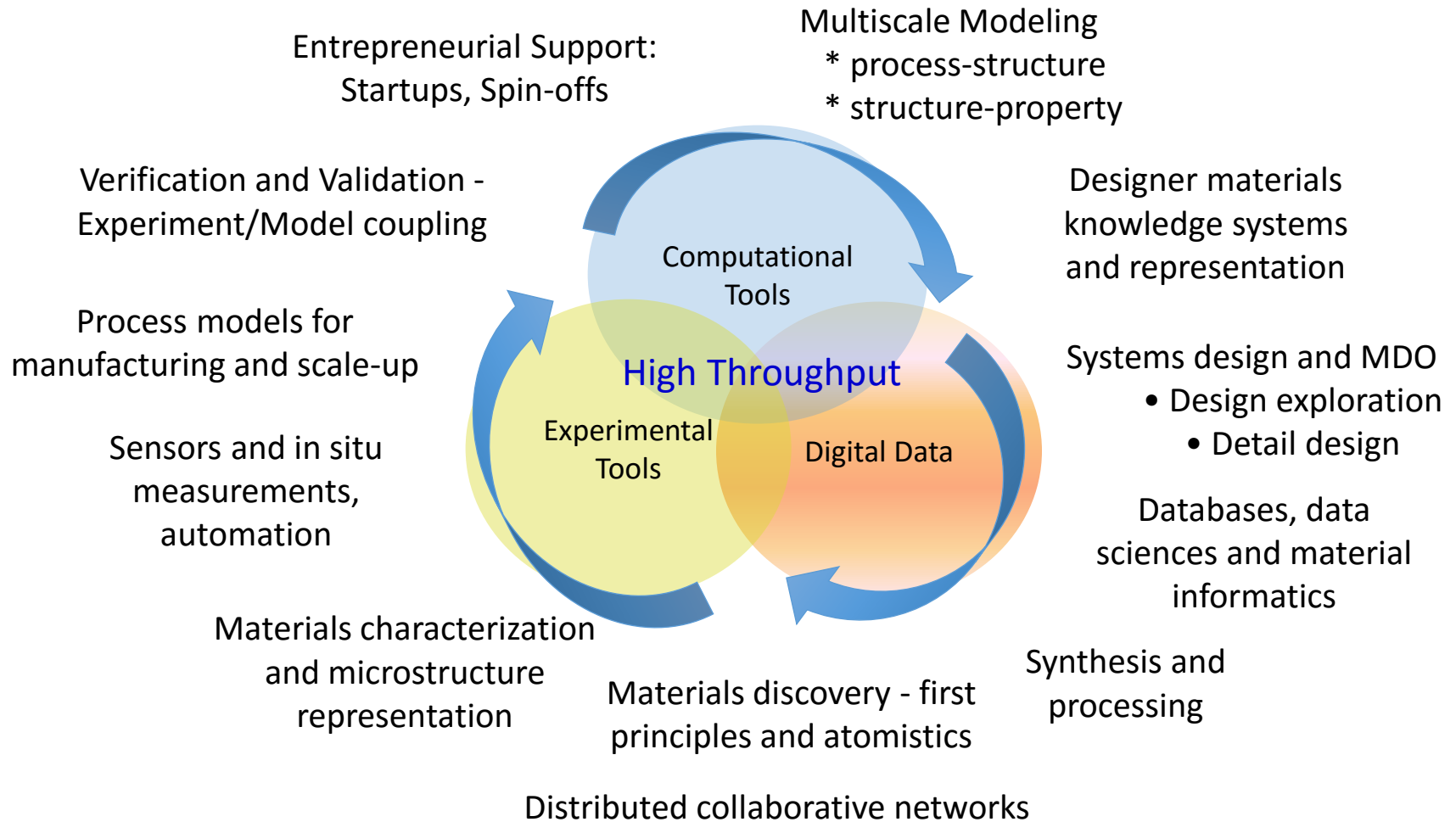
**Dave McDowell, Executive Director
GT Institute for Materials**

**UMC Meeting, MS&T 2015
October 7, 2015**



**Georgia Institute
of Technology**

The Materials Innovation Ecosystem



Expanded by DLM from OSTP Materials Genome Communication



WELCOME



Georgia Institute of Technology Launches New Institute for Materials

Georgia Tech is announcing the launch of a new Institute for Materials (IMat), an interdisciplinary research institute designed to foster a materials innovation ecosystem for research and education. This new institute is part of a \$10 million commitment over the next

<http://materials.gatech.edu/>

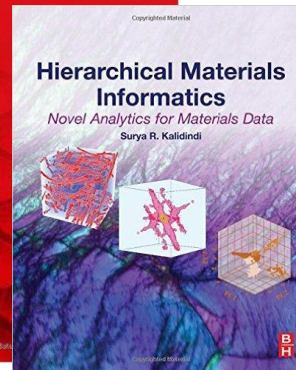
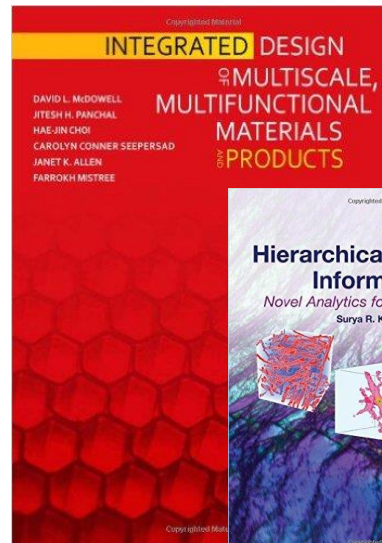
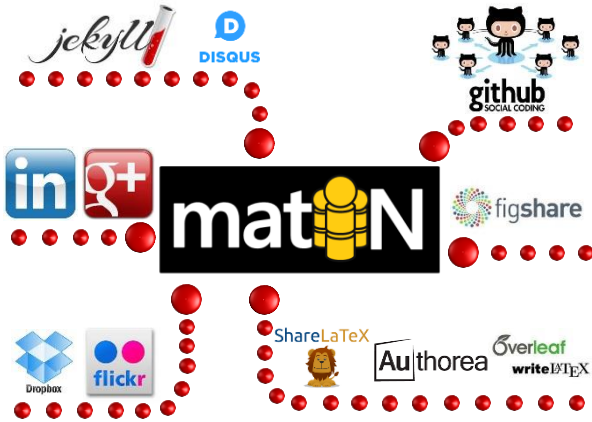
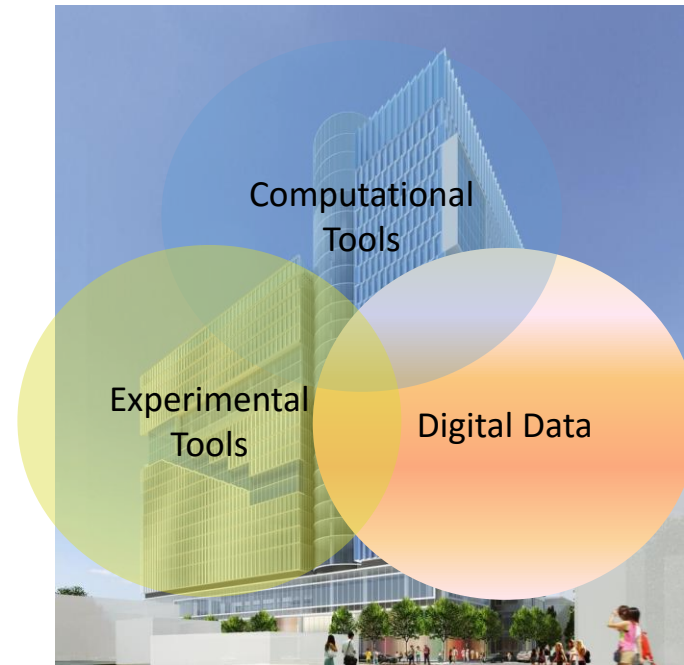


Georgia Tech: model university materials innovation ecosystem

- **Accelerating materials discovery, design, and development**
- **Materials + X**
- **Novel approaches to materials data sciences and informatics**
- **Preparing the future workforce for materials discovery and development**



IMat and Materials Data Sciences at Georgia Tech



High Performance Computing Center for Modeling and Simulation

24-story, 695,000 SF private and public development



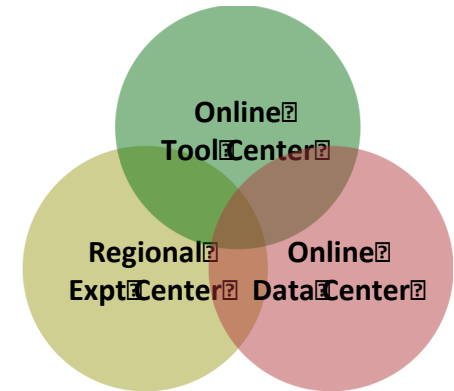


The Wisconsin Materials Institute

**Accelerating materials innovation through
integrated development of equipment, computation, and data.**

June 24th, 2013 the White House named UW-Madison a partner institution, with Georgia Tech and Univ. of Michigan, in its *Materials Genome Initiative for Global Competitiveness*.

UW established WMI with \$5M support from UW College of Engineering to lead this partnership.



Major Activities

- Drive productivity in Wisconsin and beyond by helping establish a Materials Genome Initiative inspired Regional Materials Network.
- Lead the materials community through transformative integrated physical and cyber-infrastructure for materials research.
- Establish the Materials Accelerator Network with University of Michigan, Georgia Tech, and others.

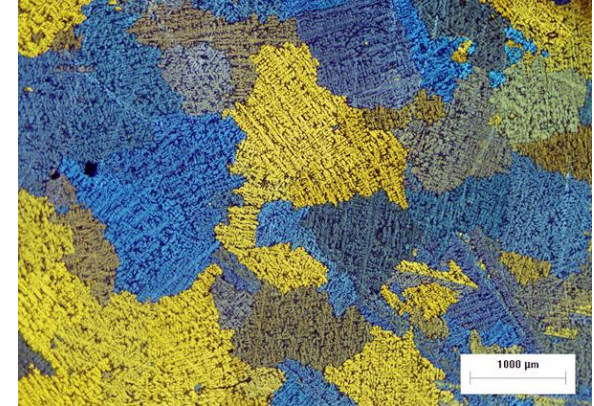
DOE PRISMS at University of Michigan

PI/PD J. Allison

DOE Software Innovation Center for Integrated Multi-Scale Modeling of Structural Metals. (PRedictive Integrated Structural Materials Science).

Goals:

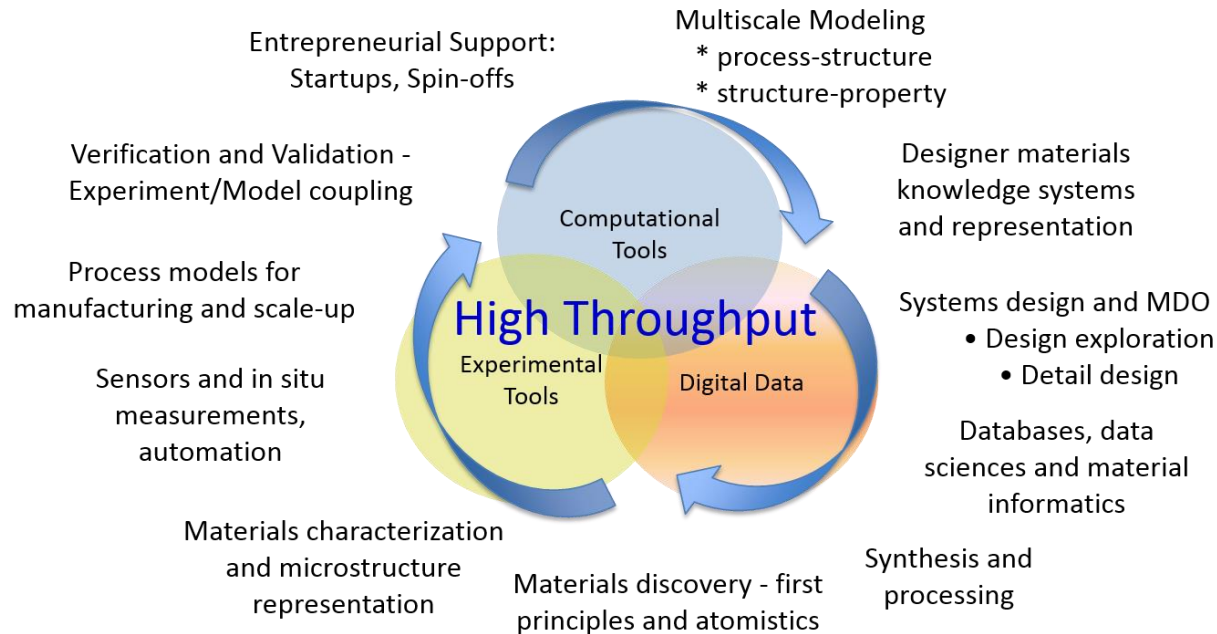
1. Establish an Integrated Multi-Scale Modeling Framework and Open Source Software (PRISMS)
2. Develop Advanced Open Source Computational Methods
3. Tightly Couple Experiments and Models
4. Application and Validation – PRISMS Demonstrator: Magnesium, Fatigue & Ductility
5. Establish the Materials Commons: An Open Source Knowledge Repository and Virtual Collaboration Platform for the PRISMS Community



Five year \$11M grant from DOE BES, with \$1.5M in cost-shared from UM, College of Engineering and the faculty and departments involved. The funding comes from the [Materials Genome Initiative](#).

Importance of US Academic Investment in MGI

- Key to future workforce development → must evolve curricula to reflect needs of the innovation ecosystem



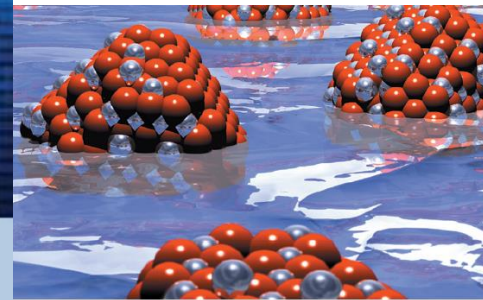
- Science of high throughput, including instrumentation, measurements, UQ/V&V, data sciences/analytics, and linkages to modeling and simulation

Not just \$\$, but also intellectual capital

How Might a Materials Accelerator Network Look?



National Nanotechnology Infrastructure Network



Data Readiness Levels, modelled on NASA's Technology Readiness Levels, to provide a basis for communicating the quality and maturity of materials data.

The MGI could also join the partnership between the NNI and the European Commission to support a transatlantic dialogue on the nuts and bolts of data sharing: informatics, consensus-derived ontologies, data representation and archiving.

Data sharing is an inherently collaborative activity that has the potential to propel materials science forward more rapidly. The MGI can invigorate existing efforts and serve as a hub for sharing information on materials at all scales.

<http://www.nnin.org/>

There is no need for the Materials Accelerator Network to mimic the NNIN – different times, different needs

Sharing data in materials science

Two years on from the launch of the US Materials Genome Initiative, five experts highlight how materials scientists still need to work differently.

SALLY TINKLE Learn from other initiatives

Policy analyst at the Science and Technology Policy Institute, Washington DC

The US Materials Genome Initiative (MGI), launched in June 2011 by President Barack Obama, aims to halve the time and cost of developing advanced materials for

applications such as energy, transport and security. Two years in, hundreds of millions of dollars have been invested in academic, industry and federal-agency projects.

Sharing data and developing computational tools are crucial to the MGI's success. Advanced materials have complex physical and chemical properties that can be manipulated for different applications, and these can change during synthesis, manufacture and use. The tracking of these properties is a formidable task, and the MGI includes efforts to standardize terminology, data-archiving formats and reporting guidelines.

Fortunately, much can be learned from

DAVID L. MCDOWELL Incentivize sharing

Executive director of the Institute for Materials, Georgia Institute of Technology, Atlanta

The MGI must avoid a 'build it and they will come' attitude. Incentives are needed for scientists and engineers to collaborate and share their data and skills. There has to be something in it for everyone.

The data-sharing environment must invite collaboration as well as facilitate it. Stakeholders have broad interests that go beyond retrieving existing data — they want to discover materials and forecast enhanced products. An intuitive and robust online environment, and cyber-infrastructure growth that is distributed and organic, rather than centralized, will encourage contributions from diverse users.

Social-networking strategies can connect users with varied expertise to pursue common interests. Win-win approaches should be encouraged. For example, uploading experimental data sets in return



Building an Integrated Materials Accelerator Network

- Organic electronics
- Structural materials
- Energy storage and conversion
- Catalysis and separations
- Biomaterials and bio-enabled materials
- Inorganic optical and electronic materials

Organizational Collaborators:

Dave McDowell & Jud Ready, GT

John Allison and Katsuyo Thornton, UM

Dane Morgan and Tom Kuech, UW



Georgia Institute for
Tech Materials

June 5-6, 2014



Coordinated with White House OSTP

Sponsors





MGI national accelerator workshop report, released January 2015



Office of Science and Technology Policy
Executive Office of the President
Eisenhower Executive Office Building
Washington, DC 20502

FOR IMMEDIATE RELEASE
June 24, 2013

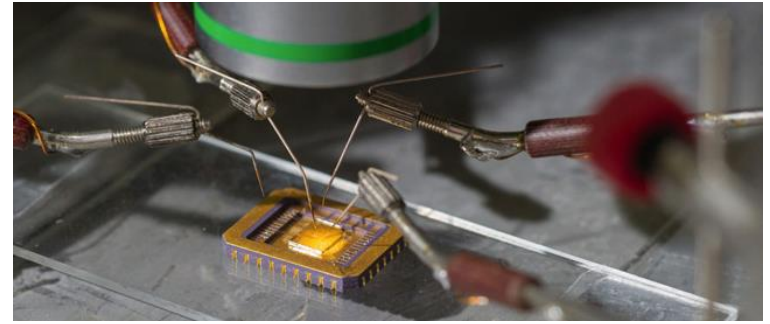
Contact: Rick Weiss
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"Materials Genome Initiative" Commitments Announced

Today the Obama Administration and academic and industry partners announced a series of commitments in support of the Materials Genome Initiative, a public-private endeavor that aims to cut in half the time it takes to develop novel materials that can fuel advanced manufacturing and bolster the 21st century American economy.

Universities to Build a Materials Innovation Accelerator Network: In support of MGI goals, the University of Wisconsin, Madison, and the Georgia Institute of Technology are creating new Institutes in materials innovation with collective investments totaling ~\$15 million while the

[http://acceleratorenetwork.org/wp-uploads/2015/01/PRELIMN MAN-REPORTV1-1_12_15.pdf](http://acceleratorenetwork.org/wp-uploads/2015/01/PRELIMN_MAN-REPORTV1-1_12_15.pdf)



Key Recommendations

- Education and training to prepare the **future MGI workforce** and build the necessary culture of collaboration across its elements.
- Invest in **high throughput tools and facilities** for materials processing and development, accessible to industry, linking computation, experiments, data sciences and materials information infrastructure more tightly.
- Establish **networks/working groups** within and across materials application domains in academia, industry, and national labs.
- Identify effective **Foundational Engineering Problems** (FEPs) for key materials applications domains to couple computation, experiments, and data infrastructure, build tools of common interest and utility, and achieve connectivity to industry.
- Build a **national physical- and cyber- materials innovation infrastructure** to address domain specific needs and ensure connectivity of academic, industry, and government stakeholders.

Commonly Identified Scientific Gaps

- **Materials information infrastructure** - more than just databases - web-based environments for e-collaboration and data sciences.
- **High throughput strategies for screening and development** that consider capabilities and constraints on available synthesis and processing routes, including fast acting modeling tools to assess probability of meeting requirements.
- **Future workforce** with integrated perspective on coupling of experiments, computation, and data sciences.
- **Fundamental understanding of the relations between structure at different length scales and properties/performance.**
- **Advanced diagnostic methods**, particularly in situ/in operando.

Continued...

Commonly Identified Scientific Gaps

- **Consideration of long term stability** under service conditions, environmental stability, degradation and performance lifetime at early stages of discovery and development.
- **Predictive simulation of metastable states and non-equilibrium trajectories** of evolution under service conditions for applications, enabling parametric exploration of candidate material systems for product applications.
- **Measurement science and modeling and simulation of synthesis and processing.**
- **Principles of kinetic and thermodynamic control of process route/structure relations.** Exert reliable control of structure over various length-scales (nano-macro) during processing, including up to large scales.



New kinds of user facilities are necessary

Possible Infrastructure for the Materials Accelerator Network: Future Workforce Integration

- High throughput science and research experiences at universities
- Summer courses
- Short courses in elements of MGI
- Cross-cutting graduate certificate programs
- Integration with two year and community college programs, veterans, etc.
- MS degree programs/professional degrees

Some MGI Activities Targeting Workforce Development

- **Examples of Degree/Training Programs**

- Masters in Materials Science and Simulation at the Ruhr University Bochum - <http://www.icams.de/content/mss/mss-start.html>
- Computational Engineering program centered in CAVS at Mississippi State
- ICME Masters certificate in ICME focused on design at Northwestern - http://matsci.northwestern.edu/docs/ICME_Brochure%205-27-11.pdf
- Georgia Tech FLAMEL (NSF IGERT) - <http://www.flamel.gatech.edu/>

- **Examples of Summer Schools**

- Texas A&M Summer School on Computational Materials Science - <http://msen.tamu.edu/images/IIMEC%20School%20Application%202014.pdf>
- University of Michigan Summer School on Integrated Computational Materials Education - <http://icmed.engin.umich.edu/orgcomm.html>
- LLNL Computational Chemistry and Materials Science Summer Institute - https://www-pls.llnl.gov/?url=jobs_and_internships-internships-ccms
- Summer Schools from University of Florida Cyberinfrastructure for Atomistic Materials Science center - <http://cams.mse.ufl.edu/>

Possible Infrastructure for the Materials Accelerator Network: High Throughput User Facilities

- Regional beamlines with computation and data science coupling (e.g., at ANL, BNL, SLAC, ORNL, ...)
- In situ, in operando facilities to understand kinetics and evolution of structure (key weakness in materials discovery and development) – e.g., NREL, NSF Materials Innovation Platform (MIP) competition – linked with computation.
- Facilities for synthesis and characterization of structure over various length-scales (nano-macro), including up to large scales relevant to applications – scale-up.

Possible Infrastructure for the Materials Accelerator Network: Data Sciences and Software

- e-collaborative platforms
 - MGI workflows (experiment, computation, data)
 - Flexible team formation and communication
 - Data visualization and decision support
 - Web-enabled agent-based strategies for data and modeling tools
- MGI software institute(s) – codes, tools, workflows
- Federated data curation and integration

Some MGI-related M&S and Data Sciences Efforts

- The Materials Project at LBNL - <https://www.materialsproject.org/>
- OpenKIM project on interatomic potentials (curating knowledge base) by E. Tadmor at Univ. Minnesota (really important) - <https://openkim.org/about/>
- Georgia Tech FLAMEL (NSF IGERT) - <http://www.flamel.gatech.edu/>
- NWU/Univ. Chicago/ANL/NIST Center for Hierarchical Materials Design (CHiMaD) - <http://chimad.northwestern.edu/>
- PRISMS Center, Univ. Michigan - <http://prisms.engin.umich.edu/#/prisms>

A nationwide partnership that accelerates the discovery, development and manufacturing of new materials.

Please visit our [page of links to data and informatics resources](#) supporting the [Materials Science and Engineering Data Challenge](#).



About Us

We're launching a nationwide dialogue to connect academia, industry and government stakeholders to fulfill the goals of the Materials Genome Initiative.

Partners include: Georgia Tech, University of Michigan, and the University of Wisconsin.

[Learn More](#)

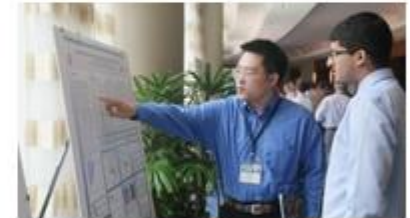


The Materials Genome Initiative

The Materials Genome Initiative (MGI) was announced by President Barack Obama on June 2011 to accelerate the development and deployment of new materials with the rallying phrase

"half the time at half the cost."

[Learn More](#)



Building an Integrated MGI Accelerator Network Workshop

150 leaders and stakeholders from academia, industry and government explored how distributed experimental, computational, and materials information might be networked to realize the MGI vision.

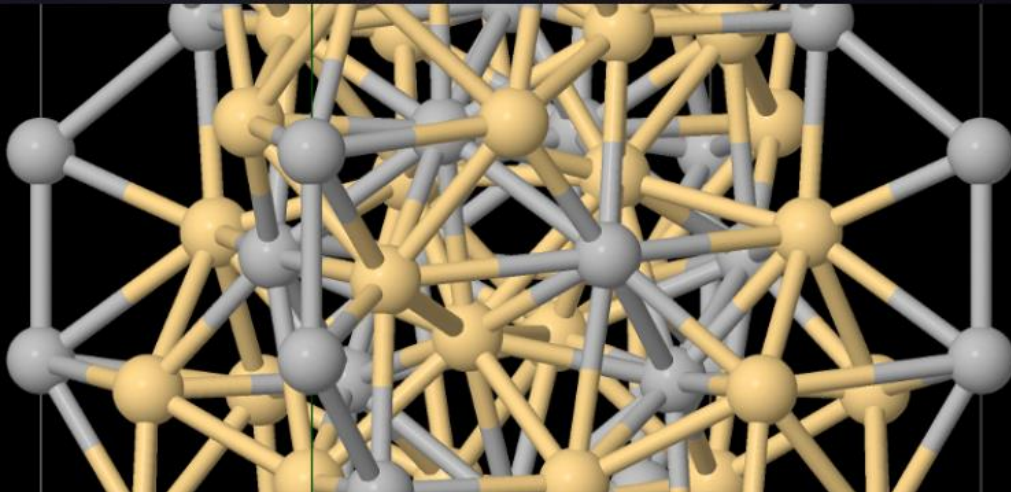
[Learn More](#)

Materials Genome Initiative

WWW.MGI.GOV

Home About Follow

<http://www.mgi.gov>



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[Subcommittee of the Materials Genome Initiative \(SMGI\)](#)

Welcome to the information portal of the Subcommittee of the Materials Genome Initiative (SMGI). The SMGI is a subcommittee of the National Science and Technology Council (NSTC) Committee on Technology. For more information, visit [NSTC](#). This portal will act as a clearinghouse for information on the US government's activities in support of the Materials Genome Initiative.

[Read more](#)

[About the Materials Genome Initiative](#)

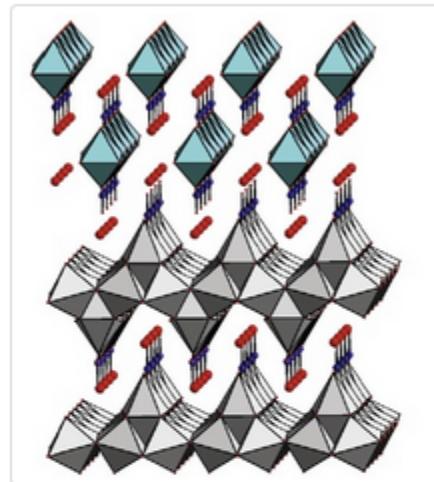
The **Materials Genome Initiative** is a multi-agency initiative designed to create a new era of policy, resources, and infrastructure that support U.S. institutions in the effort to discover, manufacture, and deploy advanced materials twice as fast, at a fraction of the cost.

MSE Data Challenge

<https://www.challenge.gov/challenge/materials-science-and-engineering-data-challenge/>

Materials Science and Engineering Data Challenge

 Air Force Research Lab



Challenge Details

Discussions 13

Solutions 0

Rules

Submit Solution

Challenge Followers 1

About the Challenge

We are seeking novel uses of accessible digital data to advance Materials Science and Engineering knowledge to accelerate the transition to industrial applications

Posted By: [Air Force Research Lab](#)
 Category: [Scientific/Engineering](#)
 Partnership With: [Access Board](#)
[National Science Foundation](#)

Submission Dates : Jul 01, 2015 - Mar 31, 2016

Judging Dates : Apr 01, 2016 - May 11, 2016

Winners Announced: May 11, 2016

People have successfully applied advanced analysis techniques to 'big data' and have solved significant challenges in several areas of society including business, biology, and astronomy. Using these techniques has provided people with new and valuable information from the data that was not readily available by other means. However, materials science and engineering data has not yet been exploited to its full potential because of its complexity. This complexity also stands to provide rich insights if the mysteries the data hold can be unraveled.

To advance the National goals of the Materials Genome Initiative (MGI), we are soliciting innovative approaches to solve materials science and engineering problems primarily through the analysis of publicly accessible digital data. Areas of particular interest include discovery of new materials to meet an application need, or development of a new model describing

[Follow this challenge](#)

Prizes



Materials Genome Initiative Prize

\$50,000.00

The awards will be paid to the best submission(s) as solely determined by the review committee. The US Government intends to make multiple awards with the top award being \$25,000 and no award being smaller than \$5,000.

• In addition to the monetary awards, winning Solvers will be invited to participate (present their research and engage the audience in a question and answer session) in a conference session at Materials Science & Technology 2016, to be held October 24-27, 2016, Salt Lake City, Utah. Travel



<http://acceleratornetwork.org/mse-challenge/>

Accelerator Network Data Support Site for the MSE Data Challenge

[HOME](#)[ABOUT](#)[INITIATIVES ▾](#)[EVENTS ▾](#)[EDUCATION](#)[NEWS ▾](#)[CONTACT](#)

MATERIALS SCIENCE AND ENGINEERING DATA CHALLENGE RESOURCES

This page provides links to data, informatics tools, and related information to support participation in the [Materials Science and Engineering Data Challenge](#). Thank you to the many supportive colleagues who have helped us develop this list - it continues to be a team effort. Please note that due to practical limitations these resources have not been reviewed by us and are provided without any assurances of accuracy, quality, performance, or value for your particular project.

About the Materials Science and Engineering Data Challenge

The Air Force Research Lab (AFRL), National Institute of Standards and Technology (NIST), and National Science Foundation (NSF) are sponsoring a contest to pursue the goals of the [Materials Genome Initiative](#). The focus is to seek novel uses of accessible digital data to advance Materials Science and Engineering knowledge, and accelerate the transition to industrial applications.

[Competition Link](#)

Submission Dates: Jul 01, 2015 - Mar 31, 2016

For any comments or suggestions for removal/addition of links, please [contact us](#).

Data Resources

Computed Data

[AFLOW database](#)

[Computational Materials Data \(CMD\)](#)

Data Mining Tools

[Best Data Mining Tools by Quora](#)

[Citrine](#). See also their blog posts on machine learning for the materials scientist [part 1](#) and [part 2](#).

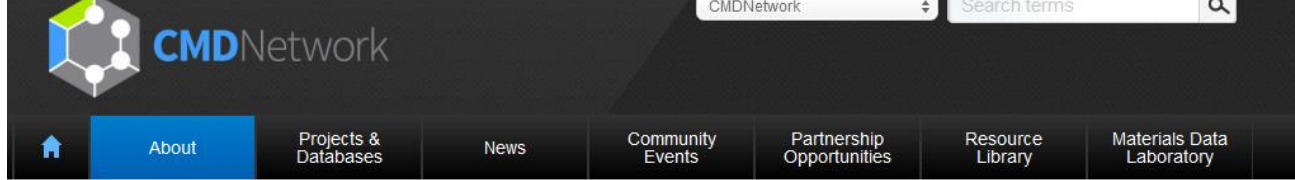
Places to Publish, Share (and Find) Data

Journals with Data Focus

[Data in Brief \(DiB\) \(Elsevier\)](#). See also Harvard



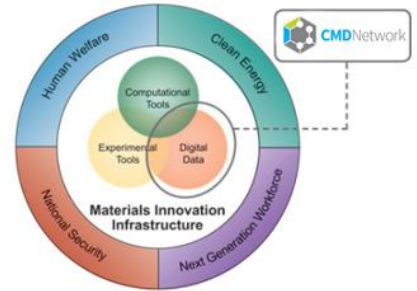
ASM



Supporting MGI

ASM International, a professional society dedicated to serving the information needs of the materials community, founded the CMD Network in response to the U.S. Materials Genome Initiative (MGI) mission to support the discovery, development, and deployment of advanced materials 'twice as fast at a fraction of the cost.' With the ability to convene materials scientists and engineering community and disseminate information technology and dissemination channels, the CMD Network is helping to accelerate the materials and processing industry of tomorrow.

The Materials Genome Initiative (MGI)



The Minerals, Metals & Materials Society (TMS) has established a network of respected leaders well versed in the Materials Genome Initiative (MGI) who serve as regional points of contact for public outreach and engagement regarding MGI-related events or inquiries. Ambassadors cover a diverse range of topics, sectors, industries, and geographic areas of interest to the materials community and are available to answer your inquiries related to the MGI. If you are unsure whom to contact or have a general question, please send an email to MGIambassadors@tms.org and your message will be directed to the appropriate ambassador(s).

MGI AMBASSADORS

TMS



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Vision and Membership

Our vision is to connect academia, industry and government stakeholders to fulfill the goals of the Materials Genome and Manufacturing Initiatives.

The Materials Accelerator Network is advocating for concerted in kind, federal, and industry support to network the materials innovation infrastructure:

- High throughput materials discovery and development
- Coupling of computational modeling with experiments and data sciences
- MGI-supportive future workforce development

We invite universities who share this vision for a federated physical- and cyber-infrastructure to support MGI and can offer their associated resources and capabilities to join us. Please contact us for further information.

**Georgia
Tech**



**Institute for
Materials**

Questions



**MATERIALS
ACCELERATOR
NETWORK**

