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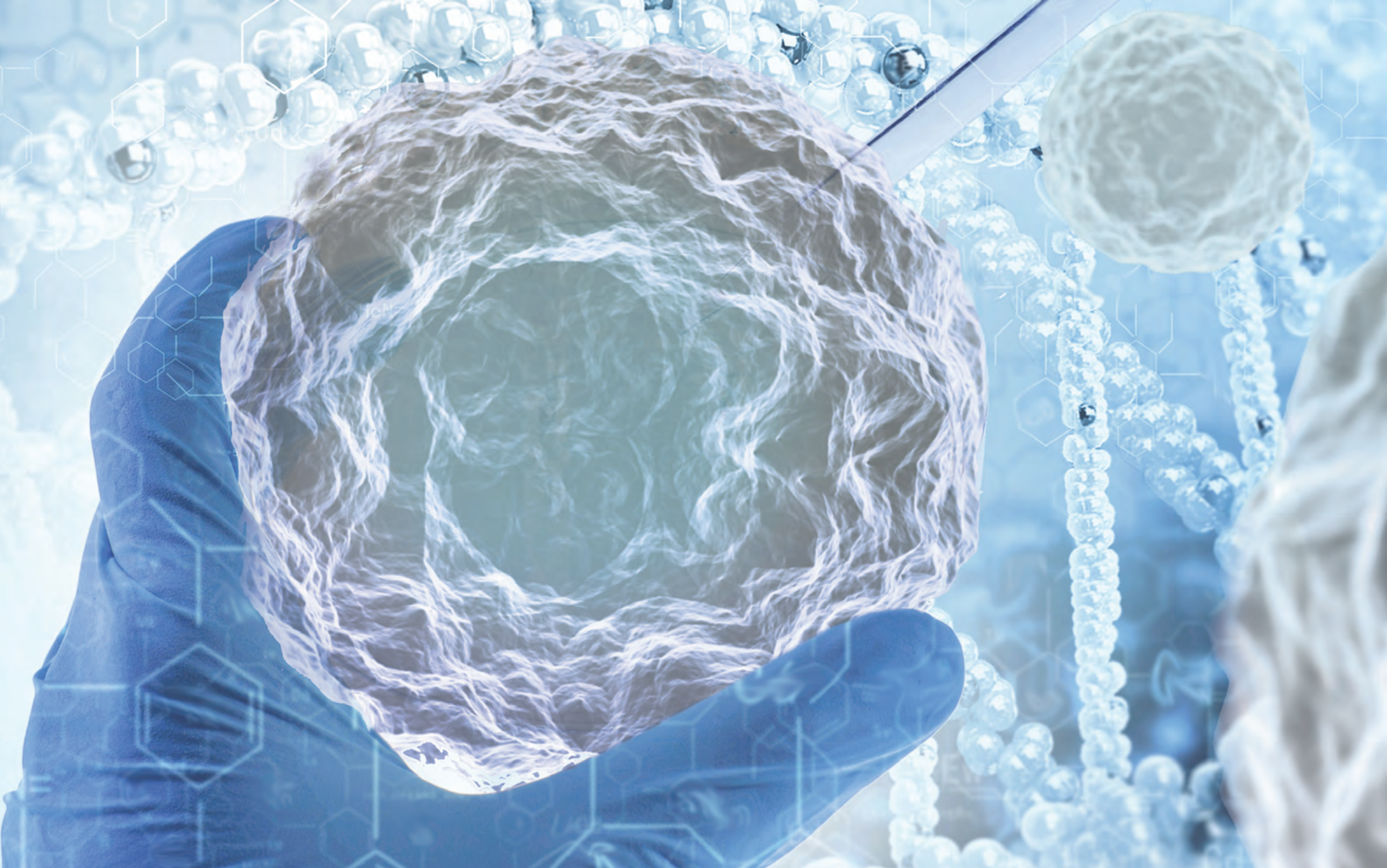
www.acceleratornetwork.org

Workshop Report:
Building an
Integrated Materials Genome Initiative
Accelerator Network

Georgia Institute of Technology
University of Wisconsin
University of Michigan



Workshop Report: Building an Integrated Materials Genome Initiative Accelerator Network

Workshop held June 5-6, 2014
Georgia Tech Hotel and Conference Center
Atlanta, Georgia

Co-Organizers

Georgia Institute of Technology

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Executive Summary

The workshop **Building an Integrated MGI Accelerator Network** brought together 150 thought leaders and stakeholders from across the nation in areas of academia, industry, and government to explore how distributed experimental, computational, and materials information infrastructure might be further developed and collaboratively networked to most efficiently realize the vision of the Materials Genome Initiative (MGI). Co-organized by the Georgia Institute of Technology, the University of Wisconsin-Madison, and the University of Michigan, the workshop was hosted June 5-6, 2014, by Georgia Tech. The event initiated a national dialogue regarding the Materials Accelerator Network concept, as highlighted in the OSTP press release on the second anniversary of MGI, June 24, 2013. A set of opening plenary talks outlined the government MGI strategy and shared industry and academic perspectives on accelerating materials discovery, development, and deployment. The plenary talks were followed by breakout sessions organized in a range of application domains, including: materials for organic and inorganic electronics; structural materials; materials for energy storage and conversion; biomaterials and bio-enabled materials; and materials and interfaces for catalysis and separations. Breakout sessions explored and discussed three specific themes: critical issues and technology gaps; infrastructure for MGI integration; and strategy for road mapping a materials accelerator network.

High priority recommendations included:

- Focusing on education and training of the future MGI workforce;
- Compiling a knowledge base of existing federally funded MGI-related efforts;
- Linking physical- and cyber-infrastructure that cuts across materials classes and application domains;
- Establishing working groups and networks in and across these domains;
- Defining effective foundational engineering problems for each application domain to rally MGI stakeholder collaboration and networking; and
- Establishing a distributed materials information infrastructure.

Information regarding this workshop and the materials accelerator network concept can be found at *www.acceleratornetwork.org*.

Summary of Workshop Objectives

The U.S. Materials Genome Initiative has launched a broad discussion among industry, government, and university stakeholders regarding the computational tools, experiments, and digital data that comprise the Materials Innovation Infrastructure. These elements are necessary to accelerate the discovery, development, and deployment of materials into products. However, related efforts are often localized in specific institutions, and we face a major challenge in integrating efforts to achieve synergies, identifying and utilizing best practices, and avoiding unnecessary duplication.

Regional MGI workshops held from fall 2013 through spring 2014 across the United States explored specific interests and regional connectivity of MGI stakeholders, with an eye toward understanding complementary capabilities of academia, industry, and government laboratories. Building an Integrated MGI Accelerator Network followed these regional workshops with the intent to initiate a broad national discussion between stakeholders regarding priorities of a nationwide network for accelerating materials discovery, development, and deployment in pursuit of the MGI vision. Representatives from government, universities, and industry engaged in the discussion regarding ongoing significant MGI efforts and ideas for how an integrated MGI effort can be established, with national and international dimensions. Breakout sessions were designed to further explore opportunities for integration and to suggest concrete steps for its realization. Those engaged in MGI activities will use the results of this workshop to more effectively network, integrate their activities, and provide guidance for funding agencies in developing a comprehensive and efficient effort. Identification of working groups and a path forward to road mapping an accelerator network were also key results of this workshop.

Workshop Agenda

June 5, 2014

Introduction and Workshop Goals, GT/UM/UW Organizing Team

Dave McDowell

Executive Director, Georgia Tech Institute for Materials

The Materials Genome Initiative for Global Competitiveness

Julie Christodoulou

Director, Naval Materials S&T Division

U.S. Office of Naval Research

Arlington, Virginia

Enabling Materials Innovation for Future Economic Growth

Rick Barto

Senior Manager, Applied Sciences Lab

Lockheed Martin, Advanced Technology Laboratories

Cherry Hill, New Jersey

Toward a Distributed Network for Nanofabrication and Characterization: Lessons Learned from the NNIN

Roger Howe

Director, National Nanotechnology Infrastructure Network (NNIN)

William E. Ayer Professor of Engineering, Dept. of Electrical Engineering

Stanford University, Stanford, California

The Materials Genome: Shortening the Iteration Cycle in Materials Development

Gerbrand Ceder

R.P. Simmons Professor of Materials Science and Engineering

Massachusetts Institute of Technology

Cambridge, Massachusetts

Networking Materials Data

Ian Foster

Distinguished Fellow, Argonne National Laboratory

Professor of Computer Science, The University of Chicago

Director, Computation Institute

Chicago, Illinois

From Discovery to Deployment: Opportunities for Big Data in Materials R&D

Jed W. Pitera

Manager, Computational Chemistry and Materials Modeling

IBM Research - Almaden - San Jose, California

Julie Christodoulou

Rick Barto

Roger Howe

Gerbrand Ceder

Breakout Sessions

Suggested Discussion Topics

1. Critical Issues and Technology Gaps — First Hour

Identify critical issues and technology gaps that should be addressed by a road map relevant to MGI goals for accelerating discovery and development of new and improved materials

2. Infrastructure Needs for MGI — Second Hour

List essential elements of the accelerator network critical in achieving the MGI vision of discovery, development and deployment of materials at half the cost in half the time

3. Positioning and Outreach — Third Hour

Leadership strategy for road mapping MGI accelerator network among stakeholders (industry, academia, government)

Ian Foster

Jed W. Pitera

Session 1: Organic Electronics

Co-Leaders:

Peter Green

Professor and Chair, MSE

Vincent T. and Gloria M. Gorguze Professor of Engineering ▪ University of Michigan

Elsa Reichmanis

Professor

School of Chemical and Biomolecular Engineering ▪ Georgia Tech

Session 2: Structural Materials

Co-Leaders:

Vasisht Venkatesh

Materials and Modeling Engineering ▪ Pratt & Whitney

Mei Li

Technical Expert and Group Leader for Light Metals Research

Ford Motor Company

Session 3: Energy Storage and Conversion

Co-Leaders:

Gerbrand Ceder

R.P. Simmons Professor of Materials Science and Engineering

Massachusetts Institute of Technology (MIT)

Esther Takeuchi

Distinguished Professor

Department of Chemistry ▪ Stony Brook University

Breakout Sessions

Session 4: Catalysis and Separations

Co-Leaders:

Cathy Tway

R&D Director

Inorganic Materials and Heterogeneous Catalysis

The DOW Chemical Company

David Sholl

School Chair, Michael E. Tennenbaum Family Chair

GRA Eminent Scholar for Energy Sustainability

School of Chemical and Biomolecular Engineering

Georgia Tech

Session 5: Biomaterials and Bio-enabled Materials

Co-Leaders:

Carl Simon

Biologist in Biosystems & Biomaterials Division

Biomaterials Group

National Institute of Standards and Technology (NIST)

Joachim Kohn

Director of the New Jersey Center for Biomaterials

Board of Governors Professor of Chemistry

Department of Chemistry and Chemical Biology

Rutgers School of Arts and Sciences

Session 6: Inorganic Optical and Electronic Materials

Co-Leaders:

Julia Phillips

Vice President and Chief Technology Officer

Sandia National Laboratories

Louis Terminello

Fundamental & Computational Sciences Directorate

Chief Science & Technology Officer

Pacific Northwest National Laboratory (PNNL)

June 6, 2014

Reports from Breakout Session Leaders

Nominally 15-minute presentation, 15-minute Q&A for each breakout group

Moderator: John Allison, University of Michigan

Sessions 1-3

Moderator: Dave McDowell, Georgia Tech

Sessions 4-6

Summary and Next Steps

Dane Morgan, University of Wisconsin-Madison

Above, co-leaders of the session on Organic Electronics lead a spirited discussion.
From left, Peter Green of the University of Michigan and Elsa Reichmanis from Georgia Tech.

Charge to Breakout Sessions

The groups were asked to discuss and compile recommendations, focusing on their individual materials class or application domain, with regard to the three areas listed below. Their goal was to identify steps toward building a road map for integrating existing and forthcoming efforts.

1. Critical Issue and Technology Gaps — First Hour

Identify critical issues and technology gaps that should be addressed by a road map relevant to MGI goals for accelerating discovery and development of new and improved materials.

Items to consider and identify during this discussion include:

- Key science and technology gaps and opportunities.
- Key integration and networking gaps and opportunities.
- Status and opportunities in areas of integration, high-throughput synthesis, and characterization; data sciences and information infrastructure; and integration of computational and modeling activities with experiments and digital data in your materials class/grouping.

2. Infrastructure Needs for MGI Integration — Second Hour

List essential elements of the accelerator network critical in achieving the MGI vision of discovery, development and deployment of materials at half the cost in half the time.

Items to consider and identify during this discussion include:

- Lists of high-throughput synthesis, processing, fabrication, characterization, modeling and simulation tools, data resources, and other initiatives essential to meet our goals.
- Lists of major infrastructure items (e.g., high-throughput facilities, cyber-infrastructure, user facilities, centers, initiatives), existing or proposed, that could serve the needs of the MGI accelerator network.
- Focus problems that might be targeted as a basis to flesh out useful demonstration case studies in building an accelerator network.
- Educational and future workforce issues that should be addressed as part of MGI infrastructure.

3. Positioning and Outreach — Third Hour

Leadership strategy for road mapping MGI accelerator network among stakeholders (industry, academia, government).

Items to consider and identify during this discussion include:

- Key organizations, participants, and individuals to formulate and initiate the accelerator network.
- Designing a working group structure and outlining its charge for road mapping an integrated accelerator network that addresses elements of synthesis and processing, characterization, modeling and simulation, data sciences, and materials information infrastructure. For example, a task force comprised of representatives from a variety of materials classes that might formulate a road map for targeted investments.
- Mechanism for establishing and developing appropriate working groups (e.g., national or regional workshops, webinars, discussion forums), including how subgroups might be established (e.g., open sign ups or major initiative leaders).
- Possible role for a network of MGI representatives around the U.S.

Summary of Cross-Cutting Recommendations from Break-Out Sessions

1. More focus is needed on education and training to prepare the future MGI workforce and build the necessary culture of collaboration across its elements.

2. The National Science and Technology Committee (NSTC) Subcommittee for MGI, composed of federal agency representatives, should compile an online database of stakeholders and participants in existing federally funded MGI-related efforts in academia, industry, and government laboratories.

a. Provide opportunities for MGI-related projects not identified in the federal agency database to self-identify, including grass roots projects and industry funded MGI efforts.

b. There is a need to organize distributed efforts in digital data and materials information infrastructure. This could perhaps be addressed through follow-up workshops and/or working groups.

3. Computational modeling, experimental and data sciences, and materials information communities need to be coupled more tightly. The need to link physical and cyber infrastructure is common among all materials classes.

a. Real-time in-situ measurement (4D, time resolved) of evolving material structure is necessary to understand mechanisms (reactions, processes).

b. Reproducibility and uncertainty are critical aspects of the network that should be addressed in its implementation.

c. Methods for improved rate of discovery need to be developed (both high-throughput modeling and high-throughput synthesis, processing and/or characterization).

d. Funding for experiments to construct, validate, and extend/augment models is needed.

4. Networks and working groups need to be identified within and across materials application domains in academia, industry, and national labs.

a. To accelerate development of the MGI network, the NSTC Subcommittee for MGI should sponsor a major multi-agency workshop of all MGI-funded activities within the next 12 months.

b. Networks and opportunities for engagement should be posted on the OSTP and MGI accelerator network websites.

c. Connectivity should be enhanced with existing MGI relevant activities.

d. Support for networking and connectivity must be provided.

5. Effective Foundational Engineering Problems (FEPs) for key materials application domains must be identified to provide focus areas that couple computation, experiments and data infrastructure, build tools of common interest and utility, and achieve connectivity to industry.

a. Early stage discovery and exploration should be linked to downstream manufacturing and service requirements to the greatest possible extent to enhance concurrency.

b. Address TRL 3-7 transition by considering scale-up more explicitly in the screening stages of materials discovery and preliminary exploration (prior to process/property optimization).

c. Product certification is a critical stage (e.g., 30,000 hours required for qualification of airplanes) and needs increased emphasis on accelerated testing and reliability predictions (in-service degradation/failure modes, failure models coupled with estimates of uncertainty), as well as involvement of legal and certification communities.

6. A stronger materials innovation infrastructure should be developed.

a. There is a pressing need for new information infrastructure in sharing and archiving materials data and ensuring collaborative connectivity of academic, industry, and government stakeholders. Structuring data and scientific workflows for materials discovery and development is a new endeavor for the materials community and the approaches are far from settled. These activities must have strong collaborative character, integrate tightly between academic and industry users, and will likely be domain/application-specific. Each application domain has its own critical obstacles in achieving MGI objectives (e.g., reproducibility for biomaterials, mesoscale morphology for organics, high purity for inorganic electronic materials, etc.) with a few high-level cross cutting themes. Investment in web-enabled collaborative platforms should augment ongoing efforts in data structures, databases, and high performance computing.

b. Additions to existing infrastructure should be augmented by facilities with high-throughput emphasis (e.g., distributed synthesis, processing, characterization, property measurements, cyber-infrastructure) to effectively realize MGI goals with targeted federal investment.

Domain-Specific Recommendations

Session 1: Organic Electronics

I. Critical Issues and Technology Gaps

1. Technologies and performance metrics

- Materials: Small molecule or polymeric.
- Performance Requirements:
  - Electronic properties, environmental stability, optical absorption, control of morphology, biocompatibility, diverse performance metrics (efficiency), mechanical properties (flexible, stretchable).
  - Interfacial compatibility: wetting, electronic structure, chemical/molecular structure.
  - Properties are "tunable."

2. Challenges that limit widespread applications

- Lack of fundamental understanding of the connection between structure, at different length-scales and performance.
- High efficiencies achieved with newly discovered exotic materials.
- Difficulty processing high efficiency exotic materials.
- Lack of materials composed of widely available chemical constituents that are capable of high performance.
- Culturally breaking away from the paradigm of publishing only the most efficient device results.
- Lack of documentation of specific, detailed protocols.
- Lack of reliable reference data.

3. Predictability, processing, and reliability challenges

- Long-term environmental stability.
- Integration into devices for high efficiency.
- Reliable control of structure over various length-scales (nano-macro) during processing.
- Modeling role of interfaces (including organic/inorganic) with regard to materials integration and device performance.
- Optimization of molecular structure vs. solubility vs. processing.
- Theory/computation (predicting morphologies for efficiency, properties at interfaces, etc.)

4. Manufacturing challenges

- Design and control of structure over various length-scales (nano-, meso-, and macroscopic scale) over large areas.
- Large-scale synthesis of materials.
- Manufacturability of the entire device.
- Environmental impact (green manufacturing, sustainability).

5. Issues and gaps

- Design and synthesis (computational and empirical/experimental) of new materials to achieve critical morphologies (over relevant length-scales) and properties using readily available chemical constituents, which are cost effective, sustainable, and green.
- Scale-up and manufacturing of materials for devices (development of new manufacturing processes).
- New materials and processes that satisfy criteria for design/synthesis and scale-up.
- Integration into devices (device integration, dissimilar materials, hybrid devices).

II. Infrastructure Gaps

- Existing Infrastructure:
  - Soft material characterization facilities are available (e.g., DOE labs, NIST).
  - Simulation tools to predict the behavior of new materials (e.g., NREL program and database).

1. Infrastructure Issues/Gaps

- Molecular design (computational), synthesis (computational or empirical), and databases.
- Prediction of morphology (new models to predict the morphology at different length scales nano, meso-macro); processing strategies to achieve specific morphological structures.
- Manufacturing protocols (integration into devices with different interfaces, i.e. structural and electronic).

2. What are the infrastructure needs for large-scale integration?

- Viability of same location scale-up should be investigated by synthesis and processing facilities.
- Widespread availability of state-of-the art shared facilities for structural characterization.
- In-line characterization methods.
- Computational (software and models, methodologies, multiscale modeling).
- High quality experimental data for optimization of computational models.
- More sophisticated computer models to predict the effects of morphology at the mesoscale.

III. Strategy for Road Mapping the Accelerator Network

Six working groups are proposed:

- Group 1: Quality assurance and sustainability.
- Group 2: Materials identification (design and synthesis, databases for materials).
- Group 3: Characterization and metrology.
- Group 4: Processing laboratory scale and large manufacturing scale (materials and morphologies, computation, in-line monitoring, morphology control, manufacturing methods, data storage standards).
- Group 5: Devices (manufacturing methodologies, characterization, metrology, life cycle, and sustainability).
- Group 6: Facilitation and integration of working groups (high level) and policy (membership — liaisons from each group, academia, government, and industry).

Session 2: Structural Materials

I. Critical Issues and Technology Gaps

- Predict rare event properties (Stochastic description of material behavior).
  - Processing, material, and property/response variability.
- Fast-acting modeling tools to evaluate process capabilities/constraints to meet required final properties — microstructure/texture.
- Create, develop, and operate federated databases covering multiple length scales and database tools for easy access:
  - Tools and standards for data exchange and links among databases.
  - Priorities: thermodynamics, kinetics, elastic constants, CTE, crystal structure, electric and thermal conductivity, plastic properties.
- Pervasive and linked computational tool set for materials design: Link domains quantitatively and develop workflows (computational and experimental):
  - Thermodynamics, diffusion.
  - Process simulation.
  - Microstructure length scales and domains.
  - Property domains.
  - Product/component performance.
  - Experimental information as required.

II. Infrastructure Gaps

- Experimental infrastructure:
  - Tracking current capability, needs for unique requirements.
  - Data to build databases — thermodynamics, kinetics.
  - 3D/4D datasets with statistical distribution.

II. Infrastructure Gaps *(continued)*

- Verification and validation in UQ framework:
  - Maturity requirements based on end use.
  - Standards for use in materials community.
- NDE tools and methods:
  - Advanced non-destructive techniques for quality control and damage assessment.
  - Need for in-situ characterization during processing.
- Develop a skilled workforce:
  - Materials engineers with new skills and tools.
  - Data scientists/analysts.
  - On-line courses and short courses.

III. Strategy for Road Mapping the Accelerator Network

- Develop the current and future MGI workforce:
  - Provide professional education opportunities in the missing skills.
  - Develop interdisciplinary courses and instructional methods for MGI.
  - Fund undergraduate and graduate students to work on industry-oriented projects using their learned skills.
- Funding approach to creating new platforms:
  - Develop linkage program to integrate algorithms, models, and software.
  - Facilitate the transitioning of advanced algorithms, models, and programs developed at universities.
  - More accessible user facilities to expensive or unique instruments (training, joint projects).
- Establish working groups for pre-competitive technologies and new FEPs:
  - USCAR/MAI programs are good models for an overall collaborative approach (industry, academia, national labs, software companies, measurement labs).
  - Identify new FEPs to accelerate the development and integration of theory, experiments, and models (thermal protection system materials, corrosion, and corrosion fatigue, etc.).
  - Examples identified from Grand Challenges MGI Workshop in 2013.
  - On-going review of existing FEPs to identify the gap and formulate new programs.

Session 3: Energy Storage and Conversion

I. Critical Issues and Technology Gaps

There is a need to address technical issues of:

- Reactivity at solid-solid, solid-liquid, and solid-gas interfaces.
- Degradation and lifetime estimation.
- Synthesis cartography (guiding synthetic approaches and identify possible products from starting reagents (kinetic vs. thermodynamic control)).
- Identification and generation of experimental data needed by the computational community.

II. Infrastructure Gaps

- Advanced diagnostic methods to generate needed data sets, particularly for interfaces.
- Correlation of synthetic approaches for materials:
  - Use data mining approaches for synthesis.
  - Advanced diagnostic methods, particularly in-situ/in-operando.
- Facilities and web-based infrastructure.
  - MGI-dedicated computing and data facilities.
  - Web-enabled databases.

III. Strategy for Road Mapping the Accelerator Network

- Create working groups to focus on the identified MGI challenges:
  - Gain crosstalk and interaction among groups working in MGI.
- Address key issues of cost and reliability:
  - Challenges important to deployment and commercial success.
  - Recognize difference between material screening for function and scale-up of implementation into a product.
- Address academic, national laboratory, and industry interests:
  - Processing, manufacturing, and cost are important for industry.
- Address issues that apply to multiple application areas:
  - Broad applicability of methodology developed should be consistent with MGI approach.

Session 4: Catalysis and Separations

I. Critical Issues and Technology Gaps

Catalytic and separation processes operate over a wide range of conditions (temperature, pressure, chemical environment), but individual processes typically operate over a much narrower range of parameters (that may not be defined a priori). The active sites themselves can transform due to their working environment.

- There is a need for data repositories of catalyst and separation material structure processing-property relationships. How does one recover data obtained from a century of catalysis and separations research? This requires an institutional/organizational setup.
- There is a need to collect, develop, and standardize easily usable tools for mining data to develop data-driven correlations and descriptors.
- In-situ characterization of a catalyst or separation material during its actual function/operation, selectively probing the active sites.

II. Infrastructure Gaps

- Train researchers to think in terms of MGI workflows. Mechanisms suggested are: MGI workshops (with case studies) held on a regular basis by recognized MGI centers; development of new courses at universities; and targeted exchange of personnel between academia/industry/national labs within specific MGI-focused large projects.
- Need for support mechanisms to allow catalysis and separations researchers to better coordinate and share existing instrumentation in order to enable MGI workflows.
- Likewise, new “national” facilities that allow characterization of catalysts and separation materials under “close-to-industrial” conditions (e.g., presence of toxic/corrosive components that cannot be easily handled in academic labs).
- Create mechanisms to bridge between materials discovery at lab-scale and implementation/deployment at bench scale/prototype scale.

III. Strategy for Road Mapping the Accelerator Network

- Establish a working group to select key specific MGI targets with high societal value in order to develop a draft work flows. Successful implementation will enable stakeholder engagement and support.
- Establish mechanisms to fund exchanges of chemical industry and faculty in order to start discussions/work on MGI-related problems.
- Understand the key barriers in the chemical industry towards creating a viable value proposition for MGI, perhaps through meetings/workshops.

IV. Grand Challenge Themes and Foundational Problems were Considered for Catalysis:

- Catalysts by design — structure and function:
  - Discovery and lead generation, improvement targets.
  - Develop materials, from model to industrial scale, that incorporate multiple functions defined at the molecular level.
  - Cross cutting need for significantly advanced tools: computational, experimental, spectroscopic, etc.
- Translation to technology:
  - Realization of design — new synthesis strategies, scale-up, aging, etc.
  - Realize benefits from the same tools for better understanding and scientific design.

IV. Grand Challenge Themes and Foundational Problems were Considered for Catalysis (continued):

- Modeling and characterization tools that advance the entire continuum from discovery, design, and translation to practice:
  - Reaching longer length and time scales with higher accuracy, representing complex environments, complex reaction networks, improved methods for uncertainty quantification.
  - Build better science base, experimental, and computational definitions of active sites and their function while accelerating application.
  - Go significantly beyond what conventional DFT can do today.
- Database development and implementation as a key enabler of all of the above.

Session 5: Biomaterials and Bio-Enabled Materials

I. Critical Issues and Technology Gaps

- Standard test methods to enable comparability:
  - Developing effective biomaterials requires comparable measurements of biological response (protein adsorption, bacterial or mammalian cell response in vitro, tissue response in vivo).
  - For predictive modeling, large data sets of comparable, reproducible data are needed.
  - Requires consensus standard test methods and reference materials to enable the field to advance without slowing innovation. Standards for reporting are required.
- High-throughput screening of protein/cell/bacteria/tissue interactions with materials, including instrumentation, characterization of cells, and materials.
- Resources for sharing data to facilitate collaboration:
  - Standard annotations and metadata, data storage and transfer, collaborative environments, cloud solutions, big data solutions, data analysis, databases.
- Predictive modeling directed at biomaterials (long length and time scales); addressing the first three gaps above will enable this to occur.
- Uniquely designed interdisciplinary MGI biomaterials educational offerings.

II. Infrastructure Gaps

- Establishment of laboratories for collecting data and training (vertical).
- Establishment of interdisciplinary, “pipeline” laboratories (horizontal, cross-cutting).
- High-performance computing center for modeling.
- Center for fabrication, nanoscale features, additive manufacturing.

III. Strategy for Road Mapping the Accelerator Network

- Incentivize establishment of interdisciplinary teams of practice.
- Strategy for road mapping: establish working groups, first charge for each is to identify near term goals.

Session 6: Inorganic Optical and Electronic Materials

I. Critical Issues and Technology Gaps

- Bringing data and data analysis together in repositories:
  - It is not clear how the efforts in data collection and analytics will fit into the current space of verification, peer review, and intellectual property, which seems to govern the actions of our current processes.
  - Need standardization for data collection to facilitate tracking and analyzing such data.
  - An international panel or some of the professional societies might take the lead to help establish the format for reporting certain types of data.
  - Information regarding calculations or experimental assumptions (metadata) needs to be attached to the datasets.
  - The publishing world is an economic enterprise, not a data repository.
  - Do we wait for Google® to help develop databases and search tools or do we push/incentivize publishers to do this?

- Technology gaps are also seen in the areas of theory, experiments, and simulations.
  - Support engineering applications and aim for more predictive and quantitative character.
  - Would it be possible to have a “mail-in” sample approach where a scientist can simply drop a sample in the mail, ship to a facility, and get the data quickly?
  - Some techniques need to be able to analyze thousands to tens of thousands of samples where others are used to analyze only a few samples in detail.
  - Judicious screening experiments are needed to circumvent potential bottlenecks in the techniques.
  - Uncertainty analysis is critical to the entire process, both in modeling/simulation and experimentation.
  - Aspects such as interfaces and impurities are very important and hard to control. Their measurement can be challenging.
  - We tend to have initial demos that show promise in a material, but it is difficult to find money to follow up and scale/understand new semiconductor materials (e.g., 2D materials, perovskites, etc.).
- Discovery tools:
  - User facilities for computational resources or experiments/characterization are lacking.
  - Problems in this space are deeply rooted in physics with transport of electrons, phonons, and photons, which must be understood in order to design electronics/optoelectronics. Finding or creating the appropriate tools needed to bridge length scales within this multiphysical space remains a daunting challenge.
  - Can “crowd sourcing” play a role in this area? If so, how do we harness this resource for funding and analysis in MGI?

II. Infrastructure Gaps

- Research infrastructure should support genuine collaboration between theory and experiments. The following are needed:
  - Cloud resources.
  - Virtual collaboration resources.
  - High-throughput synthesis resources.
  - Tools for interrogating and analyzing data.
  - Better computational tools for the atomistic scale domain.
- Should the necessary infrastructure follow the NNIN model? What is the balance of national laboratory scale user facilities versus distributed facilities?
  - Focusing on grand challenge problems can help guide the topics for investment in the MGI.
- Mechanisms are needed for collaborations with industry without fear of IP issues. How can incentives be developed?
  - There were also issues of domestic vs. international industry. We are falling behind foreign sources of materials in this area.
  - We need to establish a national center for crystal and material synthesis for semiconductor materials like those found around the globe.
- Address how to impact the educational and training process for people entering the MGI workforce.

III. Strategy for Road Mapping the Accelerator Network

- The network requires high-throughput synthesis and processing, rapid screening, and appropriate education and training tools.
- It was pointed out that although the NNIN is a distributed resource model, it does not promote data sharing. This is a major deficiency when considering MGI.
  - Can other networks be included to build a “network of networks?”
  - The discussion should be expanded to include SRC, DARPA, Mantech, ITRS, etc., which have roadmaps for electronics and optoelectronics, as well data analytics.
- Find nucleation points for MGI, starting with a few activities and using them as pathfinder programs from which subsequent activities can learn.
- Address IP and sharing issues to ensure outreach and connectivity to industry. Due to the complexity of this area, there is a potential for high cost and high risk, but high reward.

Recommended Path Forward in Road Mapping the Accelerator Network

The cross-cutting recommendations compiled on page 9 provide an insight into issues and challenges facing this Initiative, as well as possible remedies and solutions that may be instituted in order to realize the vision of the Materials Genome Initiative. Because the materials classes/application domains were quite distinct, this input is unique in terms of formulating action items on the path forward to establishing a MGI Accelerator Network. The suggestions below attempt to "drill down" into possible solutions that could be developed and even enacted with additional support sought out by the initial host universities of the Accelerator Network. There will also be an expanding role and involvement of working groups and other stakeholders (academia, industry, and government research laboratories).

1. Explore ways in which the Accelerator Network might assist the development of MGI by building on existing Foundational Engineering Problems (FEPs)[1] and defining new FEPs to pursue nationally collaborative MGI-relevant efforts in selected materials domains. The FEPs should be framed by working groups formed by the Materials Accelerator Network within several of the workshop materials classes/application domains and should be based on additional support for this activity. The area of structural materials already appears to be invested in such FEPs through national laboratory and professional society leadership.
2. Focus on requirements/specifications-driven materials development that connects to industry needs and the materials supply chain to achieve culture shift in materials research and development. This shift should involve the integration of experiment, theory, computation, and data sciences/analytics. Hosting workshops and forming working groups in materials classes should start with those classes with the strongest support for these efforts. This can be assessed by "Requests for Information" calls from the Materials Accelerator Network to the various communities involved through the Materials Accelerator Network website. This establishes the basis for joint proposals to develop case studies that demonstrate success for high throughput materials development along with the formation of associated MGI domain-specific stakeholder networks.
3. Provide links to major MGI efforts, including the compilation being conducted by the National Science and Technology Council's Committee on Technology Subcommittee of the Materials Genome Initiative (Draft Strategic Plan, June 2014). Provide capabilities for self-identification of MGI activities on the Materials Accelerator Network website[2].

4 Foster development of a world-class current and future MGI workforce:

- Introduce MGI-relevant curricula at higher education institutions, collaborative short courses, and conference workshops.
- Foster focus articles on MGI in special issues of journals, trade, and industry publications, as well as new, emerging venues such as the TMS journal *Integrating Materials and Manufacturing Innovation*.

5. Promote development of the materials infrastructure for high-throughput synthesis, processing, characterization, property measurement, and computational screening. Also promote the development of shared resources for three-dimensional, in-situ, and time resolved experimental methods to understand mechanisms at the level required for materials development and to develop and validate supportive modeling approaches.

6 The Accelerator Network should promote linkage of the MGI community with distributed modeling and simulation tools and data analytics with efforts to generate and archive materials data (materials data infrastructure) as emphasized in the draft MGI Strategic Plan issued by the NSTC in June 2014.

7. Establish the Accelerator Network and pursue resources to enable sustainable efforts like those listed above.

1 Foundational Engineering Problems (FEPs) are defined in the National Academy of Engineering Report Integrated Computational Materials Engineering, ISBN978-0-309-11999-3 (2008). http://www.nae.edu/19582/Reports/25043.aspx

2 www.acceleratornetwork.org

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Materials Accelerator Network