Dear Colleagues,

The Materials Genome Initiative (MGI), announced by President Obama in 2011, aims to support US institutions to discover, develop, and deploy advanced materials twice as fast, at reduced cost. While much progress has been made in computational design of materials, discovery, deployment, and commercialization of new materials would benefit greatly from the increased support of experimental data.

High-throughput experimental techniques, where hundreds of samples are synthesized, characterized, and catalogued for their functional properties, provide an important tool toward these aims. In May of 2014 a workshop was held in San Francisco, CA, and it was attended by more than 90 experts in the field of high-throughput experimentation. The workshop was organized by Applied Materials, Inc. and the University of South Carolina, and was supported by the National Science Foundation, National Institute of Standards and Technology, and the White House Office of Science and Technology Policy. The purpose was to determine the most effective means of leveraging the existing high-throughput materials science infrastructure to support the MGI, identify common needs within the community, and create a comprehensive roadmap that would ensure future US competiveness in fields of technological priority.

The expert group identified the need for experimental and data standards as well as increased access to high-throughput device characterization tools as some of the most significant opportunities to realize the full potential of high-throughput experimentation for materials commercialization. This group proposes a nationwide experimental effort incorporating multiple public–private efforts to accelerate commercialization of advanced electronic materials, catalysts, and materials for energy, with centers equipped with novel interface/device measurement techniques and data management tools. This coordinated national effort will provide the scientific community with increased access to high-throughput tools, expertise, and data, driving materials innovation forward by complementing existing theoretical achievements with systematic experimental validations.

Moving forward, there is a clear-cut case for the inclusion of high-throughput methodologies as the experimental workhorse to complement and help inspire the future computational efforts in the MGI.

The Organizing Committee


| | |
|---|---|
| **Dr. Martin L. Green (Technical Conference Chair)**<br>National Institute of Standards and Technology, Gaithersburg, MD | **Prof. Jason R. Hattrick-Simpers**<br>University of South Carolina, Columbia, SC |
| **Prof. Ichiro Takeuchi**<br>University of Maryland<br>College Park MD | **Dr. Sara C. Barron**<br>National Institute of Standards and Technology, Gaithersburg, MD |
| **Dr. Ajey M. Joshi**<br>Applied Materials, Inc.<br>Santa Clara, CA | **Dr. Tony Chiang**<br>Intermolecular<br>San Jose, CA |
| **Dr. Albert Davydov**<br>National Institute of Standards and Technology, Gaithersburg, MD | **Dr. Apurva Mehta**<br>Stanford Synchrotron Radiation Lightsource<br>Menlo Park, CA |

**Fulfilling the Promise of the Materials Genome Initiative via High-Throughput Experimentation**

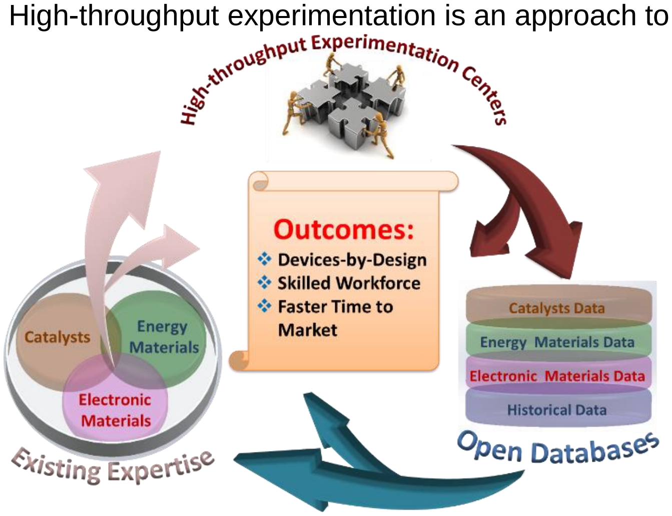
The Materials Genome Initiative (MGI), announced by President Obama in 2011, aims to accelerate the process of materials discovery and design and halve the time to commercialization of advanced materials. Thus far, the MGI has resulted in significant progress in computational simulation, modeling, and predictions of materials properties. However, prodigious amounts of experimental data are necessary to inform and validate these computational models. High-throughput experimental methodologies, which allow accelerated synthesis and testing of materials for optimized performance, are uniquely suited to rapidly generate high-quality experimental data, and hence represent the key experimental counterpart to bring the computational materials design efforts of the MGI to fruition.

Today, the nation faces challenges in numerous arenas such as increased competition in manufacturing, renewable energy generation, and access to natural resources. Advanced materials solutions to these challenges are possible and must be discovered and deployed at unprecedented speed. The development of low-cost solar cells, for example, is limited by the necessity to identify and optimize combinations of up to six property-matched materials and integrate them into a complex multi-layered device structure with specific performance metrics.

***Here, a national effort is proposed to launch the high-throughput materials research infrastructure required for a complete MGI approach to materials solutions in technology areas of national and global interest. The result will be the discovery of innovative materials, and their integration into the novel devices driving future economic growth in technological sectors such as energy, advanced electronics, aerospace, defense, and catalysis. This accelerated innovation capability will ensure the global competitiveness of the United States in high-tech manufacturing in the 21st century, and foster a highly skilled national workforce trained in high-throughput materials techniques.***

**The Experimental High-Throughput Materials Superhighway**

High-throughput experimentation is an approach to materials research and development where sample "libraries" containing hundreds of different materials (and materials combinations) are prepared and rapidly evaluated for selected properties; examples include light absorption in a photovoltaic material, or selectivity of a catalyst for methane activation. By combining rapid library synthesis and characterization, the high-throughput approach can provide experimental realization of materials designed for specific functionalities by computational approaches.




Vision for a national effort in high-throughput experimentation to accelerate materials development in the Materials Genome Initiative

To maximize the impact of this effort on the MGI, there needs to be widespread adoption of standards for *materials synthesis*, *characterization,* and *data management*. Standard library architectures will facilitate the use of shared experimental tools, and standard data formats will permit use of analysis software and informatics platforms. Both will increase researchers' productivity and impact by expediting the generation, dissemination, and utilization of results through databases of experimental materials properties. There must also be a community effort to develop new methodologies that expand the scope of high-throughput studies to characterizing materials interfaces, which serve as the basis for device functionality.

**Required Consortium and Infrastructure**

Leveraging the existing network of practitioners of high-throughput experiments will maximize scientific impact and return on public investment. The network will be mobilized to address urgent, high-impact, and materials-constrained technological gaps such as advanced electronic materials, materials for clean and sustainable energy, and catalysis. Individual topics will reflect the diversity of each field; for example, novel transparent conductors encompass light-emitting diodes, solar cells, and smart-glass.

To minimize barriers to materials discovery and collaboration in these fields, the network would benefit from centralized shared access facilities developing core high-throughput experimental and data handling workflows. These high-throughput experimentation centers (HTECs) would have on-site library synthesis, processing, and structural characterization capabilities, as well as staff with expertise in experimental design, fabrication, analysis, data management, and materials informatics. Because structural and compositional analyses are the foundations of materials exploration, advanced characterization facilities such as synchrotron beam lines are ideal launching points for HTECs. These facilities will make high-throughput techniques available to the broader research community and increase the quantity and statistical significance of data by enabling sharing among researchers in standard formats. These HTECs would also provide venues for experimentalists and theorists to collaborate and for materials informatics platforms and analysis software to be vetted on diverse datasets. Importantly, the resources of the HTECs must be accessible to industry seeking high-throughput solutions to materials discovery or device optimization.

The highly diverse nature of university-based materials exploration efforts makes the participation of academic institutions critical to the success of these HTECs. Universities also form the core training grounds for a diverse and flexible MGI-ready workforce capable of coalescing workflows involving theory, experimentation, and data science. A consortium of educators, who are experts in the field, will collaborate to develop web-based video tutorials on experimental best practices, experimental and data-driven materials science courses, MGI lectures, and MGI-based virtual “labs” based on emerging materials problems.

Through this effort, openly accessible databases of useful materials properties will be developed and populated with data from high-throughput materials research. Making diverse and high-quality materials synthesis protocols and property data readily accessible in standardized digital formats will enhance coupling with computational materials models, predictions, and data-mining algorithms that have been the workhorse of MGI-driven materials development thus far.

**Path Forward and Measuring Impact**

Engaging and expanding the network of high-throughput experimental expertise for each technological topic and launching the first HTECs can be accomplished in two years by prioritizing MGI projects that incorporate experimental high-throughput techniques. Specific high-impact topics must be selected that align with near- and intermediate-term industrial goals. Examples of such topics include solid-state batteries, ultrahigh-temperature metals for turbines in next-generation natural gas power plants, and low-power multiplexed sensors for flexible electronics. Ultimately, the success of this effort, and that of the greater MGI, will be evaluated by the quality and time-to-market of advanced materials-based technologies.