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The Materials Genome Initiative, the interplay of experiment, theory and computation

Juan J. de Pablo [a,*], Barbara Jones [b], Cora Lind Kovacs [c], Vidvuds Ozolins [d], Arthur P. Ramirez [e]

[a] Institute for Molecular Engineering, University of Chicago, 5747 S. Ellis Ave., Chicago, IL 60637, United States
[b] IBM Research – Almaden, 650 Harry Road, San Jose, CA 95120, United States
[c] Department of Chemistry and Biochemistry, The University of Toledo, 2801 W. Bancroft, Toledo, OH 43606, United States
[d] Department of Materials Science and Engineering, University of California – Los Angeles, Los Angeles, CA 90095, United States
[e] Jack Baskin School of Engineering, University of California – Santa Cruz, Santa Cruz, CA 95064, United States

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ABSTRACT

Advances in theoretical, computational and experimental materials science and engineering offer not only the promise to accelerate the pace at which new materials are discovered, but also to reduce the time required to bring new products to market. The so-called Materials Genome Initiative seeks to capitalize on that promise by identifying innovative research paradigms that integrate theory, computation, synthesis, and characterization in manners that, until recently, were not possible. A workshop was held at the National Science Foundation in December of 2013 to identify some of the central challenges and opportunities facing materials research within the context of that initiative. This article summarizes the findings of the workshop, and presents a series of concrete recommendations with the potential to facilitate its implementation. It also provides an overview of timely fundamental, technical and logistical challenges, organized according to distinct classes of materials, whose solution could have significant practical and societal benefits.

1. Introduction

Railroad, highways, and the Internet transformed the way we think, the way we live, and the way we grew. These three coordinated national initiatives changed the country and the world. Railroads cut the time to traverse the US from three months to three days. The interstate highway system led to unprecedented mobility so that people could essentially travel anywhere, anytime. The Internet cut the time to send information to another city from days to milliseconds. Entire industries, and indeed society as a whole, were transformed. But today, much communication among researchers still occurs at the speed of the peer-reviewed publication, which may be months or even years. While peer-review remains an essential aspect of all of science, many pre-review activities work at peer-review pace and these can be sped up. By allowing code, experimental results, simulation output, hypotheses, and human expertise to be communicated instantaneously and freely among researchers, the proposed Materials Genome Initiative (MGI) [1] has the potential to achieve an inflection point in the pace of discovery within materials science and engineering that may be comparable to that achieved by earlier, once-in-a-generation infrastructure developments listed above.

The materials genome is known; it comprises all the elements in the periodic table. What we do not know in detail is how function depends on the genome. We have come a long way using empirical methods, and more recently, quantitative methods, to develop materials theories (thermodynamics, quantum mechanics, collective phenomena such as crystallization and self-assembly, magnetism, superconductivity, ferroelectricity, multiferroics, surfaces and interface properties). Some areas have developed adequate theories to predict function and control complexity, and examples of their benefits our found in the steel, semiconductor, and polymer industries.

What we miss is a “grand theory” of how function emerges from assembling the right atoms in the right way, as well as a theory that tells us how to make a material. Organic chemistry has been very successful in developing site specific methods that allow building complex molecules, with the number of synthesis steps often exceeding twenty or more. More complex molecules are synthesized by bio-molecular systems (bio-engineering), where bacteria are programmed to produce, for instance, insulin or interferon.

* Corresponding author. Tel.: +1 (773) 702 7791.
E-mail address: depablo@uchicago.edu (J.J. de Pablo).

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The enterprise of bio- and genetic engineering is based on understanding how the genome is interpreted and processed, and how the information on building a protein can be controlled. In the same vein, the Materials Genome Initiative attempts to create the knowledge to move towards the rational design and discovery of advanced materials having superior, or even hitherto unknown, functions and capabilities.

The improved ability to simulate not just materials structure but also collective properties has placed computational science alongside synthesis, analytical theory, and experiment as the four essential legs of an integrated approach towards deploying new materials. It is essential that teams of scientists be assembled that integrate computational science into a coherent research approach. To gauge the magnitude of the challenge represented by the MGI, we note that while the human genome is constructed of four base pairs, synthetic materials employ nearly the entire periodic table, about one hundred different elements. The algorithms that form the physical basis for the human genome, encoded in the DNA molecule, are understood. However, the structure-property relations that translate a DNA sequence or mutation into a disease are not known, and continue to be the subject of much research. In the context of the MGI, there is no similar set of algorithms for synthesizing materials with predictable macroscopic properties from the elements using first principles. As condensed matter scientists work towards a "grand theory" of materials, computation will play a pivotal role, for calculating structure, properties, and even for providing big data organization of known materials and methods [2,3]. At the same time, high throughput synthesis of promising candidates identified by theory, followed by preparation of highest quality single crystalline materials or carefully prepared amorphous materials to measure pristine intrinsic materials' properties, will be crucial. The MGI has clearly multiple elements; recent reports have highlighted the need for data and standards [4], as well as the promise of computational approaches for predictive materials design over multiple length and time scales [2,3]. Building on these past studies, this report focuses on the interplay between theory, computation and experiment, and how a tight integration of these three elements of materials research will accelerate the discovery and deployment of new materials.

The ultimate return on investment will be profound. The advances afforded by the Materials Genome Initiative will guide the development of more effective pharmaceuticals, new medical technologies, new industries, more effective manufacturing processes. They will bring about enormous improvements to multiple technologies, with higher density computer memory, faster integrated circuits, faster communications, smart plastics for high-performance applications, high-efficiency semiconductor solar cells, inexpensive and abundant systems for energy storage, flexible displays, optical motors and adaptive optical cloaks, or stronger, lighter weight, and more durable structural materials. One can only imagine the benefits to society and our economy.

2. Vision of how the MGI might function

Consider a university researcher with an idea for a new battery material potentially capable of storing energy at a much higher density than currently possible [5]. She queries a large database of experimental and computational data to identify candidate materials and then accesses an online simulation service to perform more detailed quantum-mechanical calculations and mesoscale simulations that suggest other promising compounds, perhaps those that do not require strategic materials. She hands off these new leads to collaborators at other institutions who tackle problems of synthesis and costs. They make some of the materials identified in the calculations and upload energy storage performance data to the database. These results are seen by other computational researchers, who refine the calculations and show why the new materials are effective. The new energy-storage material is made in several labs and performance results are independently verified, thereby stimulating industry to explore commercialization. Key aspects of commercial scale fabrication and scale-up are taken into consideration by industrial scientists and engineers as the materials are being developed, thereby ensuring that the products of nanoscale research can be produced by the ton. All of this happens faster than the time it takes for a single research paper to be published today. This is the scientific and engineering communities' vision of how materials may be developed in the not-too-distant future.

Implementing a framework that enables such a vision faces enormous technical and logistical challenges. Intellectual property considerations must be phased into that process; the data base mentioned above does not exist; the results of calculations and experiments must be validated and peer-reviewed at blazing speeds; and the proper attribution of authorship must be respected, to name a few. But if these challenges can be worked out, new, inexpensive batteries for applications in transportation could be developed in months. New coatings with light-harvesting capabilities could become a reality. High-definition flexible screens could become common place. Materials for ultra-high density data storage, capable of holding a thousand-fold more information in devices the size of a key chain, would soon become available. Energy-efficient refrigeration systems based on entirely new principles could be developed. Taken together, all of these advances would usher a new era for technology in the US. The outcomes for the vision of the MGI would be simply extraordinary, and would breed a new generation of pioneers and inventors that could sustain US economic growth for decades.

This vision can only be realized with strategic investments in research, education and infrastructure. The materials research community needs roadmaps and a framework that allow the US to escape existing, primitive technologies. The Materials Genome Initiative (MGI) could provide that framework, and the resources required for such investments.

3. Logistical recommendations

3.1. Promote an all-encompassing MGI mode of research

As the MGI facilitates the ability of researchers to communicate and collaborate, materials research should be democratized, with projects driven by broad science goals rather than the expertise of individuals. Multi-scale modeling should be adopted from the outset, and prototyping and scale-up should be viewed as routine matters. Repositories of software at national laboratories or large centers should be the norm, with significant development activities and the capacity to maintain community software. It is important to provide financial support for such activities.

3.2. Create networks of experts from different disciplines and industries

Reliance on local expertise with a particular research discipline is limiting. Advances in one area of research could revolutionize a completely different discipline, provided the right tools were easily available. This is particularly true for industry, where financial constraints necessarily limit the pool of technical expertise to that required by a particular industry. Cyber tools, including software and access to databases, are not subject to the physical boundaries that separate industries and laboratories. They are particularly amenable to exchange between disciplines, but mechanisms to