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Computational materials science and MRS



Bruce M. Clemens
2012 MRS President

Computational materials science represents an important slice of the field of materials science. The goal of computational materials science, of course, is to design new materials by integrating first-principles methods with a wide array of computational techniques, such as *ab initio*, finite element, and Monte Carlo and phase field methods. At a more macroscopic level, information from quantum mechanical data can be combined with atomistic and mesoscale data along with experimental data to predict bulk properties. Simulations across multiple length scales are increasingly being used for materials design. With continuing rapid development of appropriate algorithms as well as hardware, computational materials science is playing an increasingly crucial role in developing new materials and improving the properties of existing materials.

Given its importance, it is not surprising that computational materials science is a focal point of programming at MRS Meetings as well as an important aspect of MRS publications. A perusal of recent as well as upcoming symposia at the MRS Spring and Fall Meetings reveals several dedicated to aspects of computational materials research, including simulations, modeling, and informatics. On the publications side, the May 2012 issue of *MRS Bulletin* expounded on “Three decades of many-body potentials in materials research” while the theme of the March 2011 *MRS Bulletin* issue was “High-performance computing for materials design to advance energy science.” In addition, computational materials science clearly weaves across research presented through other MRS avenues.

The Materials Research Society’s support for the development of computational materials science extends beyond technical symposia and publications; most notably the Society’s recent advocacy efforts supported the Materials Genome Initiative (MGI) that was announced in June 2011, and which is further described in an article by Ashley White in this issue of *MRS Bulletin* (see p. 715). The goal of MGI is to promote the use of computational tools, experimental data, and models to streamline the design and discovery of critical new materials. The initiative’s stated goals are to “discover, develop, manufacture, and deploy advanced materials at least twice as fast as is possible today, at a fraction of the cost” to address some of the most pressing current needs including clean energy, national security, and human welfare.

Months prior to the formal announcement of MGI in mid-2011, the MRS executive leadership and Government Affairs Committee leadership were asked, by the White House Office of Science and Technology Policy (OSTP), to comment and add suggestions to the development of the Materials Genome Initiative. We were pleased to be selected as one of the potential stakeholders and very glad to be able to comment on the ideas and concepts being developed within MGI. That same level of cooperation was maintained both last year and throughout 2012 as MGI moved from concept stage to formal research calls for proposals, and as the overall initiative took more formal shape. We continue to look for ways to promote and support the MGI as it continues to evolve.



MRS provided a direct letter of support to the White House on the initiative, and also participated as co-lead on a separate letter-writing effort to obtain endorsements by many other professional societies and supporting organizations. A symposium X session at the 2011 MRS Fall Meeting in Boston was dedicated to a series of presentations by the senior leadership on MGI from OSTP, the National Science Foundation (NSF), and the Department of Energy's Basic Energy Sciences (DOE BES) outlining the concept and the importance of the new paradigms that were being implemented under the MGI framework. The MRS Government Affairs Committee also developed a focused session with federal government agency materials leadership on MGI in January 2012 to explore how MRS and other professional materials societies—including The Minerals, Metals & Materials Society (TMS), ASM International, the American Ceramic Society, and the Society for Advancement of Material and Process Engineering—could work together to better promote and engage the materials community.

MRS Bulletin articles have helped to disseminate information to the materials community to explain and outline the federal plan for MGI. At both the 2011 MRS Fall Meeting and the 2012 MRS Spring Meeting, the government agency presentations, particularly by NSF and DOE BES, have deliberately highlighted the priority and attention being given to the initiative. At the 2012 MRS Spring Meeting, a dedicated workshop titled “Advancing infrastructure for materials design and application” was held on MGI software tools as well as on research at the Massachusetts Institute of Technology associated with their “Materials Project.” MRS leaders have also participated in multi-society meetings, led by TMS, regarding MGI.

In order to expand to a broader community, MRS formally introduced the Society of Industrial and Applied Mathematics and Autodesk, a 3D software producer, to the leadership at OSTP on MGI. Both of these introductions have benefited their respective organizations and created new opportunities. We continue to explore how we can expand further relationship in support of MGI and the materials research community. These collaborative efforts are examples of MRS advocating on behalf of the initiative and facilitating a wider reach for the program.

The article by Ashley White in this issue of *MRS Bulletin* provides an overview of MGI, the current stage of development, and some of the challenges. Other communications are planned by MRS in the coming months and into next year. An education symposium is currently being planned on MGI for the 2013 MRS Spring Meeting on the “discovery-to-commercialization” process. The MRS Government Affairs Committee will continue to play an important role in the support of MGI both within MRS and externally as the research funding for this initiative will require long-term commitment by Congress.

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