LA-SiGMA

Louisiana Alliance for Simulation-Guided Materials Applications

Materials Genome Initiative

Mark Jarrell

This new national initiative is expected to be of the same size and scope as the National Nanoscale Initiative

Report from White House Office of Science Policy

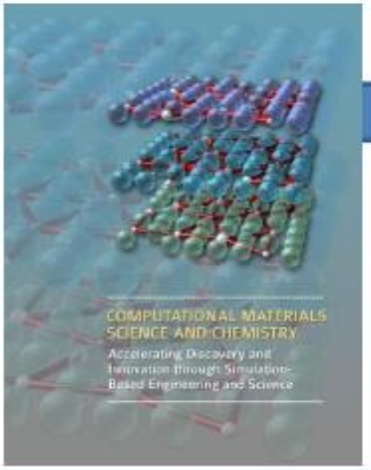
$100M in WH FY12 Budget
- NSF, DOE, NIST

Support for development of
- Computational tools
- Software
- New methods for material characterization
- Open standards and databases

http://www.whitehouse.gov/sites/default/files/microsites/ostp/materials_genome_initiative-final.pdf

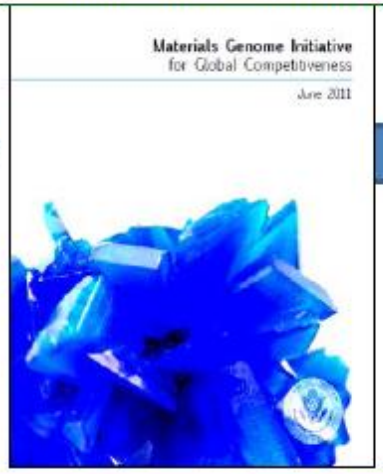
Materials by Design – Materials Genome Initiative – American Manufacturing

Joint BES-ASCR Workshop, July 2010



"We are at the threshold of a new era where predictive modeling will transform our ability to design new materials and chemical processes, thereby enabling rational discovery strategies for systems that were not tractable a few years ago."

National Science and Technology Council, Office of Science and Technology Policy



The Materials Genome Initiative will create a new era of materials innovation that will serve as a foundation for strengthening domestic industries …and offers a unique opportunity for the United States to discover, develop, manufacture, and deploy advanced materials at least twice as fast as possible today, at a fraction of the cost.

A Renaissance in American Manufacturing, President Obama Speech on June 24, 2011

*President Obama kicks off the **Advanced Manufacturing Partnership** (AMP), a national collaboration between the government, industries, and universities to invest in cutting-edge technologies, create new jobs and bring about a renaissance in American manufacturing. As part of his new AMP, the President is announcing an ambitious plan, the **Materials Genome Initiative**, to double the speed with which we discover, develop, and manufacture new materials.*

Thomas Kalil, Deputy Director for Policy: White House Office of Science and Technology Policy

Responsible for the Nanotechnology Initiative while in the Clinton Wh
Responsible for the Materials Genome Initiative while in the Obama W

http://www.ornl.gov/sci/cmsinn/talks/9_kalil.pdf

http://www.npr.org/templates/story/story.php?storyId=

http://www.ornl.gov/sci/cmsinn/talks/9_kalil.pdf

Goals

- High-level goals
  - Reduce time/cost to discover, invent and optimize new materials with desired functionality and performance
  - Reduce time/cost from invention to commercialization/ manufacturing
- Mid-level goals
  - Particular applications (e.g. energy, water, health, national security, electronics, advanced manufacturing, etc.)
  - Many of these goals are urgent

http://www.ornl.gov/sci/cmsinn/talks/9_kalil.pdf

Types of Support

- Integrated teams – (e.g. experiment, theory, CS) interested in making progress on particular challenge such as energy storage or conversion
  - Beyond the "staple job" – maximizing the respective contribution of the different members of the team to solving the problem
  - Supplements to existing grants?
  - Industrial collaboration
- Information storage, curation, analysis, and retrieval
  - What is the materials science equivalent of National Center for Biotechnology Information?
  - What kinds of databases would have the biggest impact on the field?

http://www.ornl.gov/sci/cmsinn/talks/9_kalil.pdf

Types of Support

- Development of new and improved models, methods, and tools
  - Increase accuracy of our ability to predict materials properties, expand the number of properties that can be predicted
  - Application of machine learning, data mining, data visualization
  - Better modeling and simulation for materials synthesis, processing, manufacturing
  - Validation and verification
  - Investments needed to exploit current and future computational platforms (manycore, cloud computing, advances in high-performance computing)

http://materialsinnovation.tms.org/genome.aspx

MATERIALSINNOVATION @TMS

Accelerating the discovery, development, and deployment of materials systems.

MGI Goals

•Materials for national security, including high strength, lightweight alloys for transportation systems

•Materials for human health and welfare, including protective gear for increased safety

•Materials for clean energy systems, including synthetic materials that replicate photosynthesis

Long term goals

•Lower-cost insertion of advanced materials into U.S. manufacturing

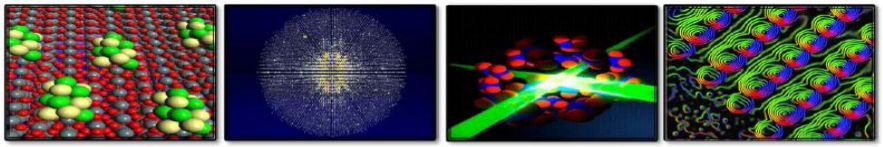
•Rapid deployment of materials solutions to meet national challenges

•Consolidation of scattered research and development efforts for a more cohesive, efficient approach to materials advancement (centers)

Department of Energy

Basic Energy Sciences Mission
Focus on Transformational Science

- **Fundamental research** to understand, predict, and ultimately control matter and energy at the electronic, atomic, and molecular levels
- Provide the **foundations for new energy technologies** to support DOE's missions in energy, environment, and national security
- Plan, construct, and operate world-leading scientific user **facilities** for the Nation



U.S. DEPARTMENT OF ENERGY | Office of Science

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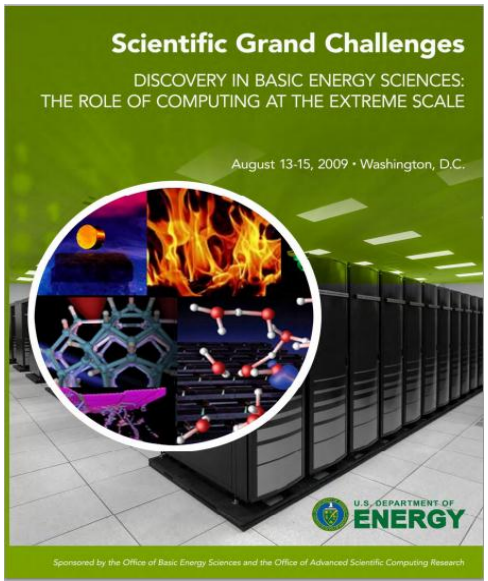
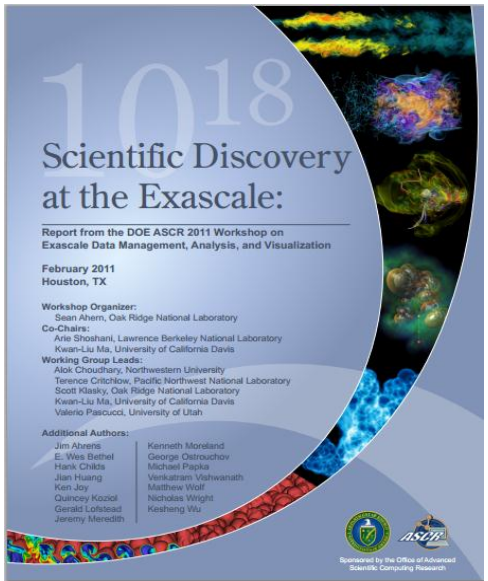
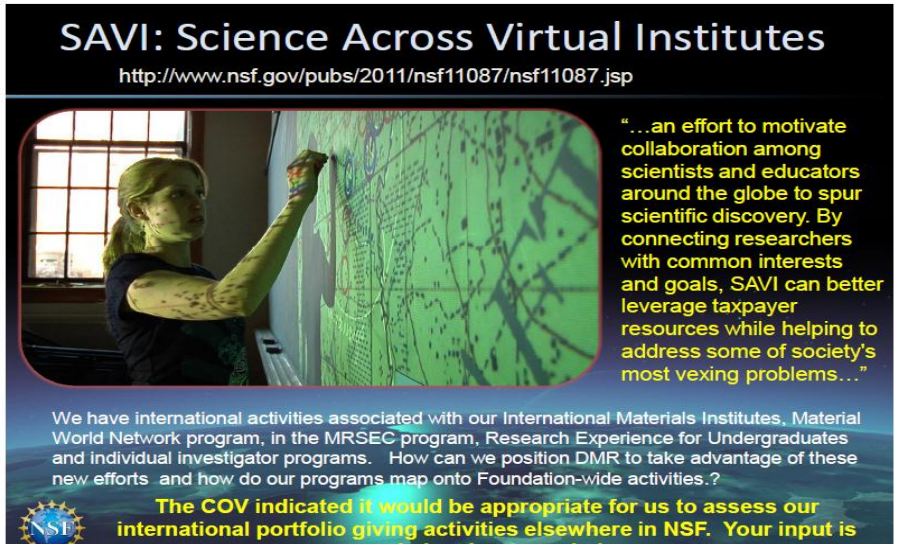




MGI funds in two directorates

- Basic Energy Sciences ($40M FY12)
- Predictive Theory and Modeling
- Pre Proposal March 1
- Full Proposals May 10
- Theory Modeling and Simulation
- ASCR
- SciDAC Partnerships in Materials and Chemical Sciences
- With BES
- Due March 12
- See Program Documents
- http://science.energy.gov/ascr/news-and-resources/program-documents/

National Science Foundation



Upcoming "DMR" Deadlines

- **Anytime:** Science Across Virtual Institutes (SAVI)
- **Anytime:** Career-Life-Balance
- **Anytime:** other supplemental requests
- **Nov. 10:** Materials World Network (MWN)
- **Nov. 14-18:** Grad. Res. Fellows
- **Dec. 5:** SEES Fellows: post-docs.
- **Dec. 15** closes: (every 4 mos.): Innovation Corps (I-Corps): training and seed $
- **Jan. 15** opens: (1 mo. window) DMREF (Materials Genome Initiative): DCL re. FRG
- **Jan. 26:** Major Res. Instrumentation (MRI)
- **Feb. 1:** Sustainable Energy Pathways (SEP): teams
- **Soon:** Cyberinfrastructure Framework for 21st Century Science and Engineering (CIF21)
- **Soon:** The Interface of the Biological, Mathematical, and Physical Sciences (BioMaPS)
- **Soon:** Cultural Heritage Science (previously SCIART)
- **May 1**: IGERT
- **May 14:** PIRE
- **July 23+:** CAREER
- **Aug. 22**: REU Sites
- **Sept 1** opens: (2 mos. window) DMR Unsolicited Proposals (incl. GOALI, RUI, FRG)

http://www.mrfn.org/8-2-Rieker.pdf

MGI: 3 NSF Divisions

- Divisions of Materials Research (DMR) in MPS
- Civil, Mechanical, Manufacturing Innovation (CMMI)
- Chemical, Bioengineering, Environmental and Transport Systems (CBET) in ENG

Dear Colleague Letter

- Designing Materials to Revolutionize and Engineer our Future (DMREF)
- http://www.nsf.gov/pubs/2011/nsf11089/nsf11089.jsp

Less emphasis on new programs than DOE

Materials Genome Initiative

Develop the ability to search for new materials on the computer

- Software to leverage the nations cyberinfrastructure
- Data
- Interdisciplinary research teams

MGI should be of the same size and scope as the NNI, and involve many agencies

- NSF
- DOE
- NIST
- ONR
- Air Force

MGI has the potential to greatly increase funding for computational materials science and chemistry