DOE MGI-Related Basic Energy Sciences Research

NSF / DOE Principal Investigators' Meeting

January 11, 2016

Linda Horton and Jim Davenport
Materials Sciences and Engineering Division
Office of Basic Energy Sciences, Office of Science
U.S. Department of Energy

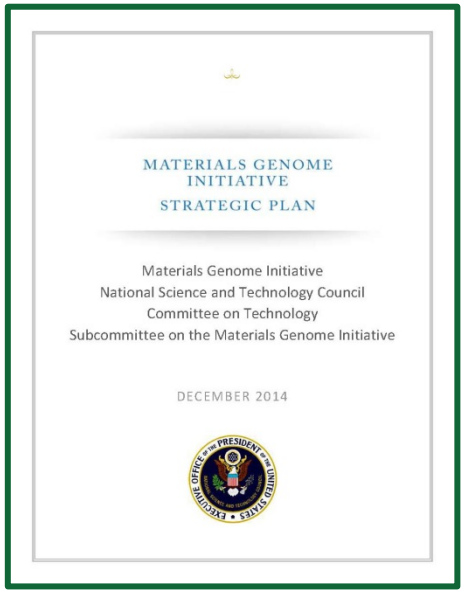
Materials Genome Initiative (MGI)

- MGI was announced by the President in 2011
- The Vision:

  MGI will enable discovery, development, manufacturing, and deployment of advanced materials at least twice as fast as possible today, at a fraction of the cost.
- Multiagency initiative coordinated by the MGI Subcommittee of the OSTP Committee on Technology
  - Cross-agency coordination, including workshops and PI meetings
- Strategic Plan was released in December 2014
- Key Challenges:
  - Leading a culture shift in materials research:

    Integrated team approach that links computation, data, and experiment and crosses boundaries from academia to federal laboratories to industry
  - Integrating experiment, computation, and theory:

    Advanced tools and techniques
  - Making digital data accessible: Combining data from experiment and computation
  - Creating a world-class materials workforce
- Federal MGI funding supports over 500 scientists in 200 companies, universities and national laboratories (White House, June 2014)


MATERIALS GENOME INITIATIVE
STRATEGIC PLAN

Materials Genome Initiative
National Science and Technology Council
Committee on Technology
Subcommittee on the Materials Genome Initiative

DECEMBER 2014

http://www.whitehouse.gov/mgi
www.mgi.gov

U.S. DEPARTMENT OF ENERGY

Secretary
Ernest Moniz

Deputy Secretary
Elizabeth Sherwood-Randall

Under Secretary for Nuclear Security
Frank G. Klotz

- Defense Nuclear Nonproliferation
- Defense Programs
- Naval Reactors
- Counter-terrorism
- Defense Nuclear Security
- Emergency Operations

Under Secretary for Science & Energy
Franklin Orr

Office of Science
Cherry Murray
Patricia Dehmer

- Basic Energy Sciences — Harriet Kung
- Advanced Scientific Computing Research — Steve Binkley
- Biological & Environmental Research — Sharlene Weatherwax
- SBIR/STTR — Manny Oliver
- High Energy Physics — James Siegrist
- Nuclear Physics — Tim Hallman
- Fusion Energy Sciences — Ed Synakowski
- Workforce Develop. for Teachers & Scientists — Jim Glownia

Under Secretary for Management & Performance
David Klaus (A)

- Energy Efficiency & Renewable Energy — David Danielson
- Fossil Energy — Christopher Smith
- Nuclear Energy — John Kotek (A)
- Electricity Delivery & Energy Reliability — Pat Hoffman

Advanced Research Projects Agency – Energy
Ellen Williams

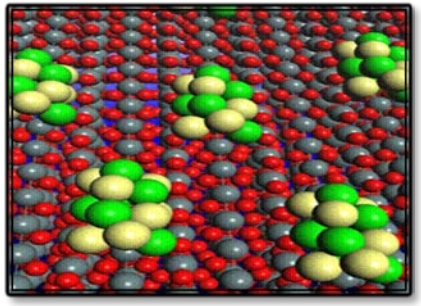
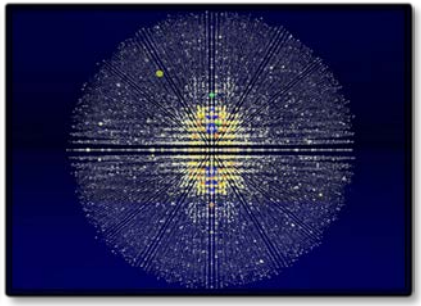
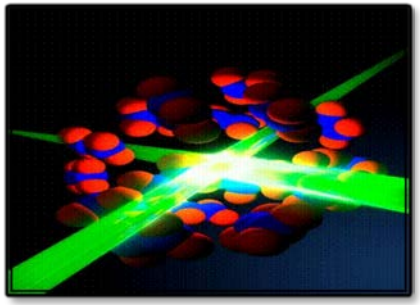
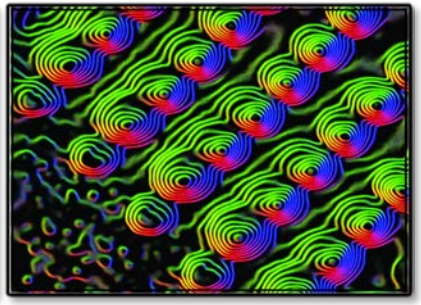
EERE also supports MGI-related research

Basic Energy Sciences Mission
Focus on Transformational Science

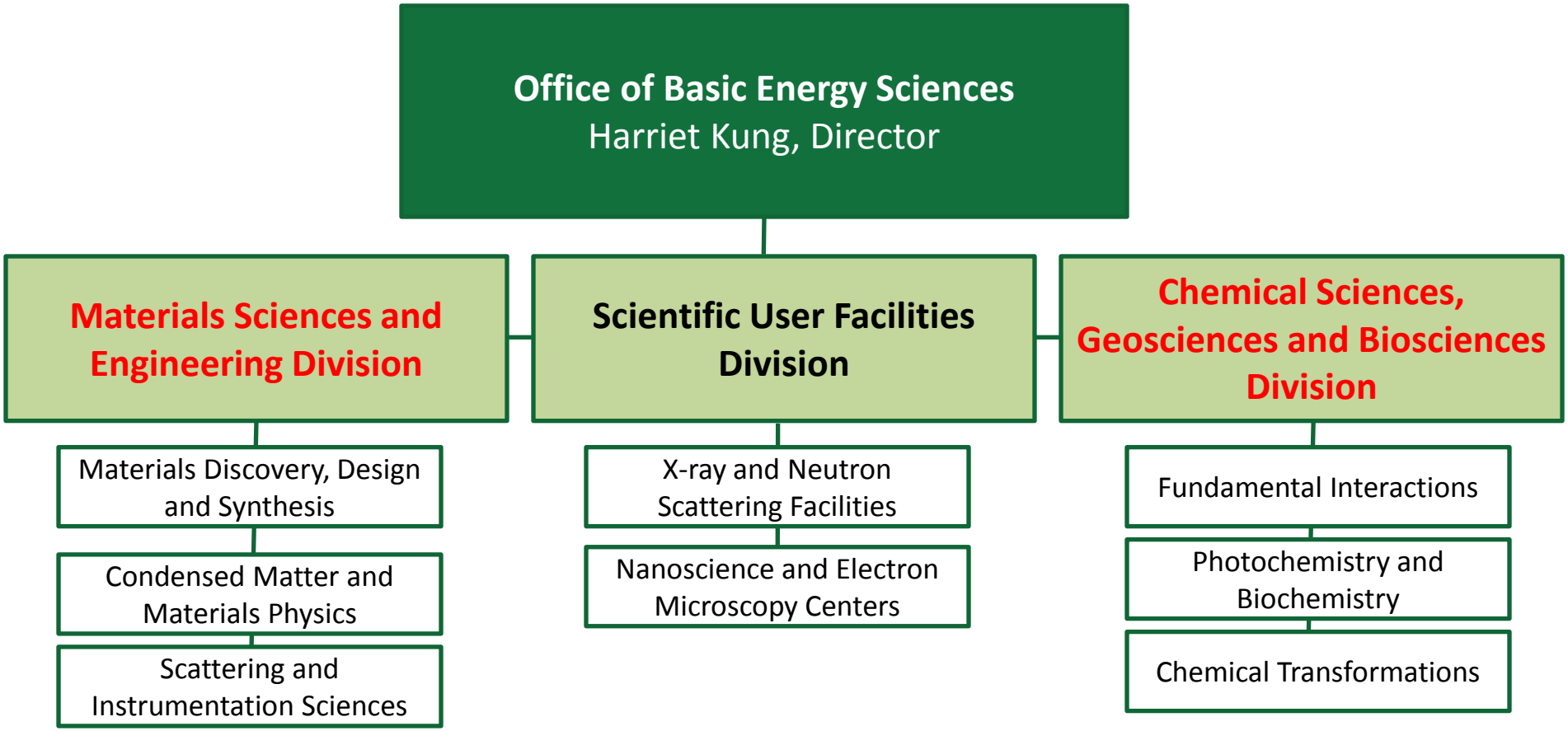
- **Fundamental research** to understand, predict, and ultimately control matter and energy at the electronic, atomic, and molecular levels

- 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

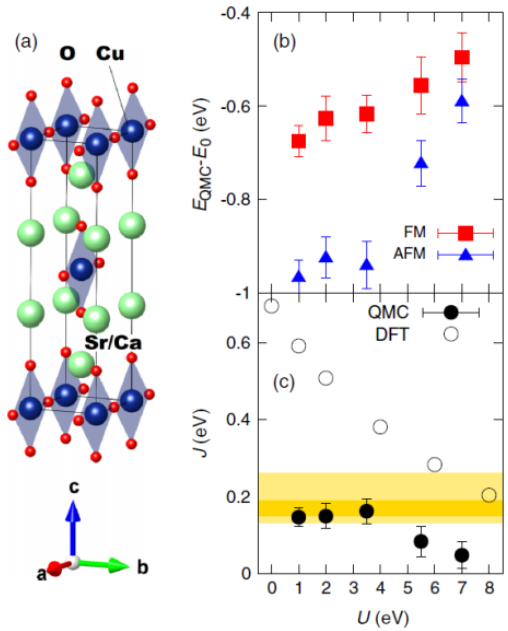





Office of Basic Energy Sciences



Both Materials and Chemical Sciences Divisions support MGI-related awards

Access to Computational Capabilities Supported by Advanced Scientific Computer Research is Critical to MGI-related Research

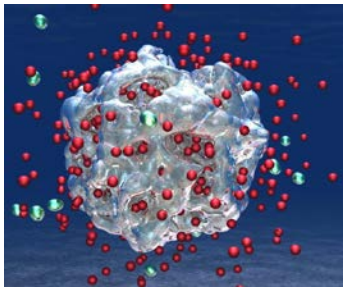


Ab-initio Quantum Monte Carlo calculations of spin superexchange in the cuprate Ca_2CuO_3 with variational Hubbard parameter U.

K. Foyevtsova et al., PRX 4, 031003 (2014); QMC calculations performed on Titan at OLCF.

- More than 300 Projects at NERSC
- 900 Million core hours allocated at NERSC in 2015
- 1.5 Billion core hours requested at NERSC for 2016
- Almost 2 Billion core hours awarded via INCITE program at Argonne and ORNL in 2015

Molecular dynamics simulation of hydrogen-on-demand using metallic alloy nanoparticles in water. H_2 molecules (green) produced by an Al (silver)-Li (red) nanoparticle.
K. Shimamura et al., Nano Lett. 14, 4090 (2014); MD calculations performed at IBM Blue Gene/Q at ALCF.

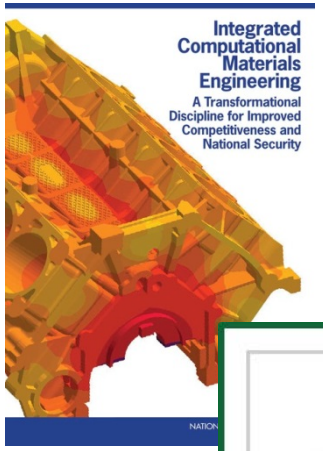


20 Peta-FLOPS; 299,008 CPUs + GPUs

10 Peta-FLOPS; 768,432 CPUs

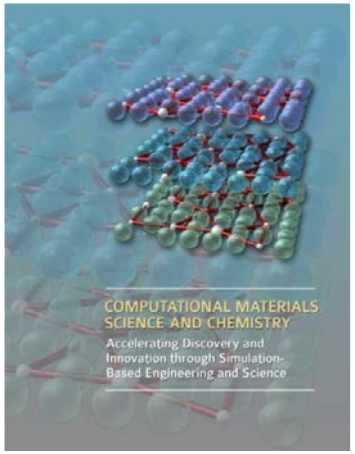
2.57 Peta-FLOPS; 133,824 CPUs

Defining the Scientific Program:
Strategic Planning for Materials Genome Initiative

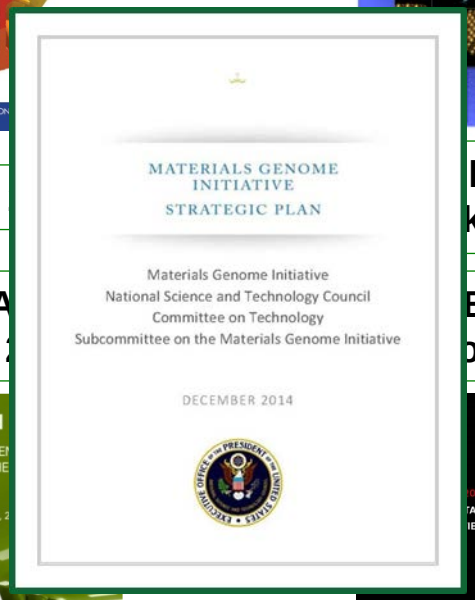


NRC ICME

lti-agency
kshop 2009



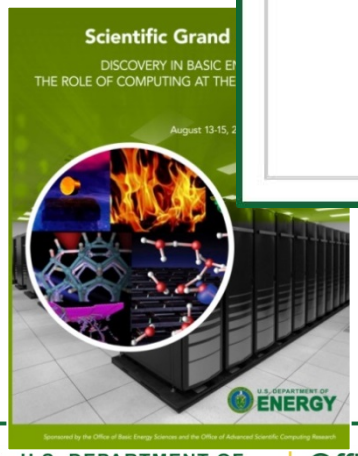
DOE BES-ASCR
Workshop 2010

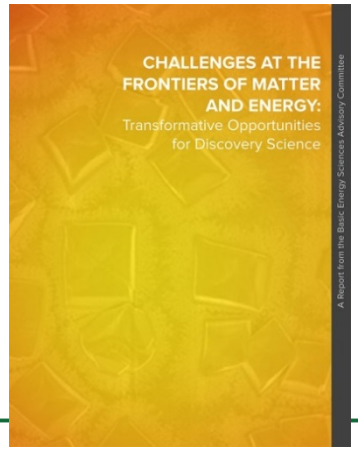


DOE BES-A
Workshop

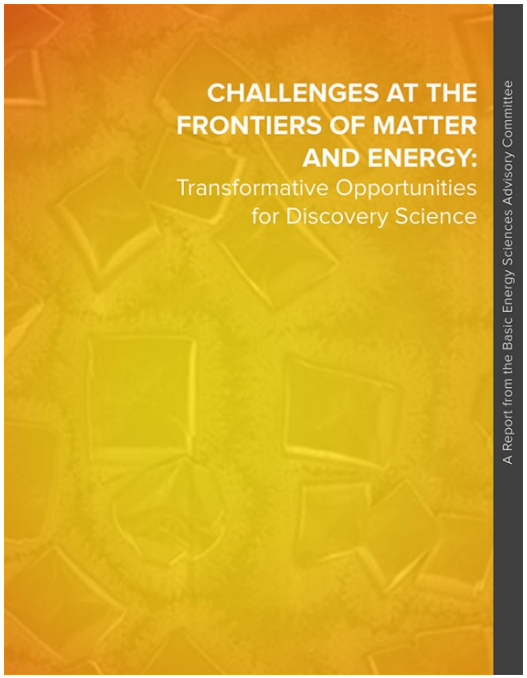
BESAC
oScale 2012

BESAC Grand
Challenges 2015





Latest BESAC Report: New Transformative Opportunities have Foundations in the 2007 Grand Challenges



New transformative opportunities

- Mastering hierarchical architectures and beyond-equilibrium matter
- Beyond ideal materials and systems: Understanding the critical roles of heterogeneity, interfaces and disorder
- Harnessing coherence in light and matter

New crosscutting opportunities

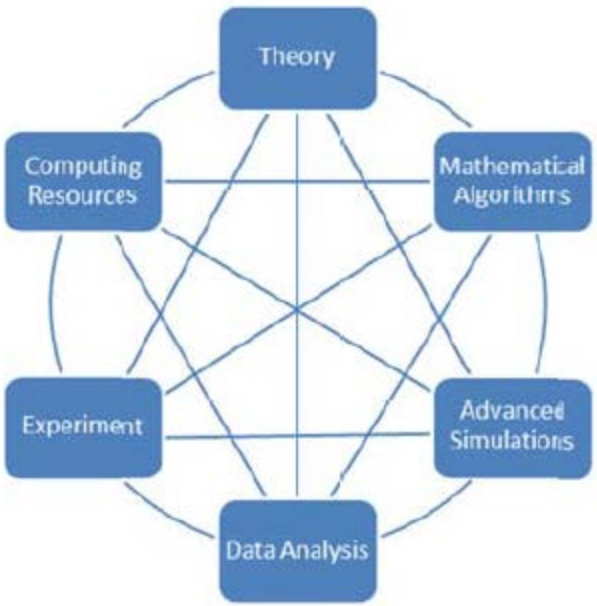
- Revolutionary advances in models, mathematics, algorithms, data, and computing
- Exploiting transformative advances in imaging capabilities across multiple scales

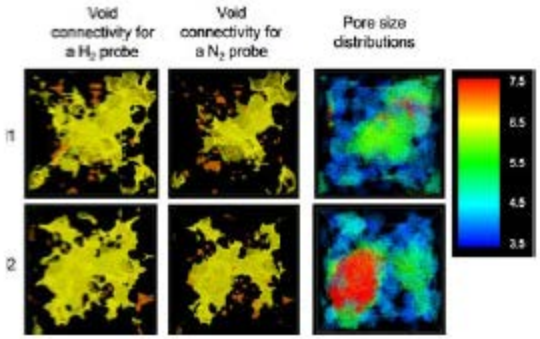
Existing grand challenges (still work to be done)

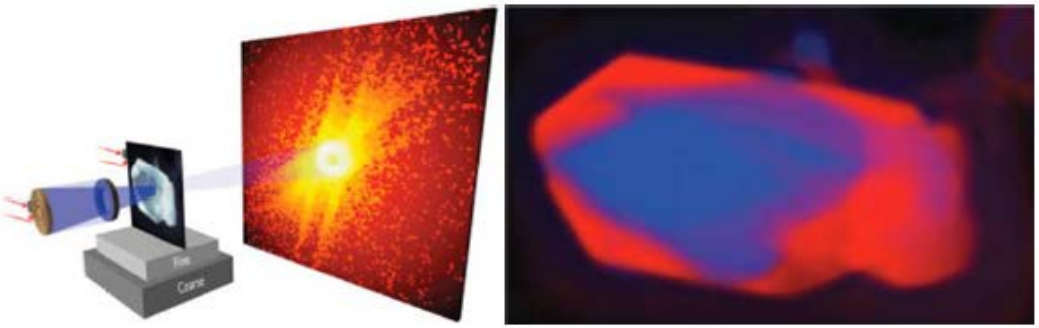
- Control at the level of electrons
- Efficient synthesis for tailored properties
- Correlated systems
- Energy and information on the nanoscale
- Systems away from equilibrium

Revolutionary Advances in Models, Mathematics, Algorithms, Data, and Computing

A "perfect storm" of theoretical, mathematical, computational, and experimental capabilities are poised to greatly accelerate our ability to find, predict, and control new materials, understand complex matter across a range of scales, and steer experiments towards illuminating deep scientific insights.







DOE BES MGI-related Portfolio

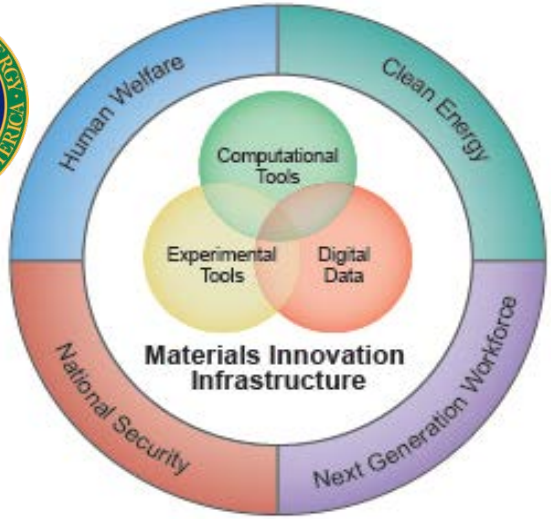
- **Predictive Theory and Modeling, FY 2012**
  - 19 Awards, $13 million/year (Materials & Chemistry); 3 & 5 Year awards
  - 5 Year Awards:
    - Light Weight Alloys (Allison, U Michigan)
    - Quantum Monte Carlo (Kent, ORNL)
    - Oxide Catalysts (Norskov, SLAC)
    - Materials Project (Persson, LBNL)
    - MOFs (Siepmann, U Minn)
- **SciDAC, FY 2012**
  - 7 Awards, $6 million/year (BES & ASCR funding)
  - 5 year awards, not renewable
- **Ultrafast Materials and Chemical Sciences**
- **Energy Frontier Research Centers**
- **Computational Materials Sciences**
- **Graduate Student Awards**

MGI & Materials Project: Achievements to Date

Materials Genome Initiative

2011: "*make the process of* ***discovery & development of advanced materials faster, less expensive, more predictable***"

"solutions in most pressing areas require advanced materials"



High-Quality Materials DATA

- > **60,000 relaxed compounds:** validated energy, phase diagrams
- > **70,000 Pourbaix diagrams:** world's largest set
- > **40,000 band structures** + higher accuracy 2,700 band gaps
- > **2,000 elastic tensors:** world's largest data set

Rapid DISSEMINATION

- **Ten Apps** enabling material searching and design
- **First Materials data API** ; community download > 8 million data
- **MPContribs framework:** platform for data sharing
- **Over 15,000 registered users !**

State-of-the-art OPEN SOURCE CODES

DESIGN

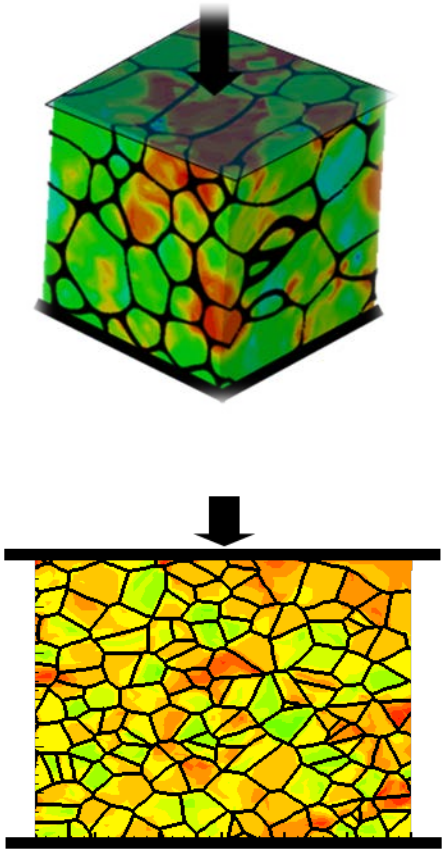
Design of **novel functional materials** (photocatalysts, thermoelectrics, cathodes/electrolytes)

https://materialsproject.org/ https://github.com/materialsproject

Predictive Theory and Modeling

Integrated Multi-Scale Modeling of Structural Materials

- Software Center devoted to light alloys for transportation – magnesium
- Headed by John Allison, University of Michigan, plus 10 faculty, 4 staff, 9 post-doctoral researchers/grad students
- Theme – modeling across scales
  - Atomistic, first principles, statistical mechanics, phase field modeling, plasticity, fatigue & ductility
- Validation – atom probe tomography, 3-D microstructure, property measurements
- 'Materials Commons'
  - Data repository, experimental & simulation data
  - Open source

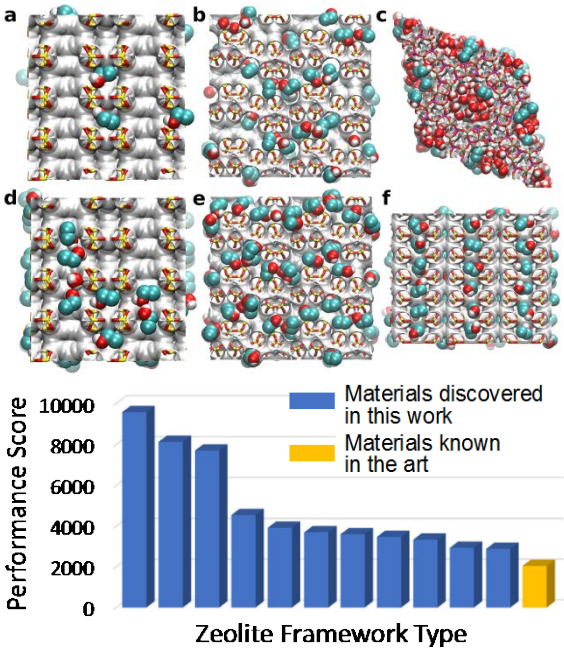


Modeling microstructures for deformation and failure modes

NANOPOROUS MATERIALS GENOME CENTER – Ilja Siepmann (U Minn)

Discovery of Zeolites for Ethanol Purification

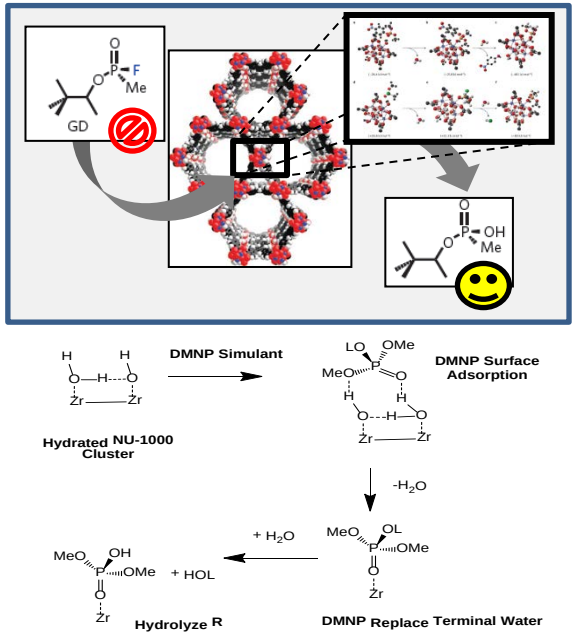
- **Predictive chemical simulations** using one day on *ALCC's Mira* and a hierarchical approach bypass decades of experimental effort.
- **Single-step adsorption process** from fermentation broth to fuel-grade ethanol.



Bai, Jeon, Ren, Knight, **Deem**, **Tsapatsis** & **Siepmann**, *Nature Commun.* **6**, 5912 (2015).

MOFs for Hydrolysis of Organophosphonates

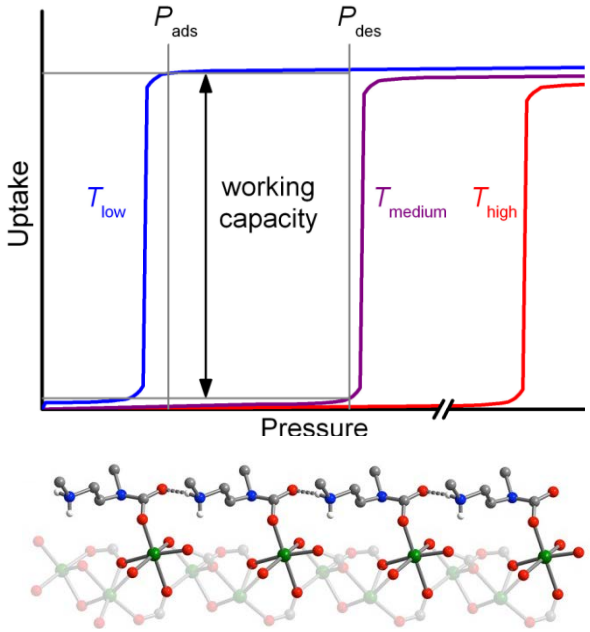
- **Chemical design** yields catalysts for destruction of chemical warfare agents yielding only the *non*-toxic product of VX hydrolysis.
- Experiment & computation demonstrate **concerted action of Zr^{IV} nodes.**



Mondloch, …, **Snurr**, **Cramer**, **Hupp** & **Farha**, *Nature Mats.* **14**, 512 (2015).

Functionalized MOF for Carbon Capture

- **Chemical design** yields sorbent reducing energy cost of capture & release through step-shaped adsorption isotherm.
- Experiment & computation show **cooperative insertion of CO_2** in diamine-appended MOFs.

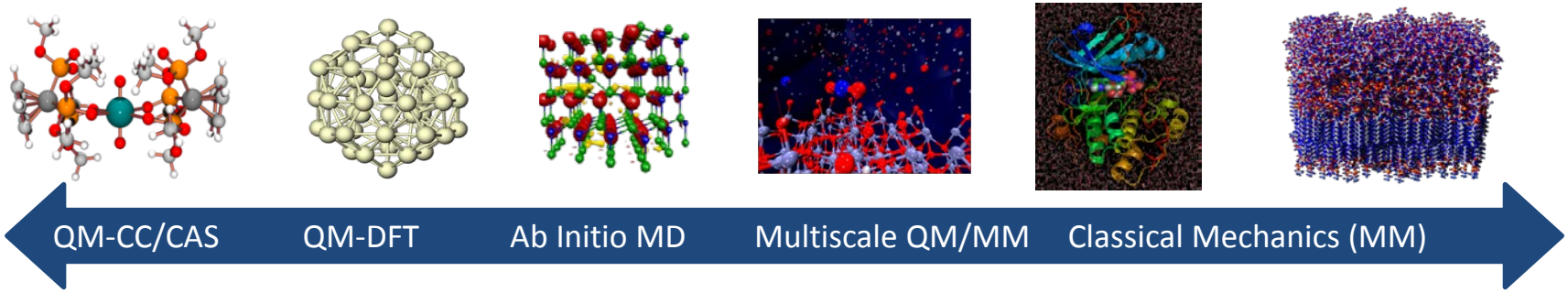


McDonald, …, **Neaton**, **Smit**, **Gagliardi** & **Long**, *Nature* **519**, 303 (2015).

U.S. DEPARTMENT OF ENERGY | Office of Science
University of Minnesota | Berkeley University of California | Berkeley Lab | Georgia Institute of Technology | Northwestern University | Rice | Washington State University

BES/ASCR SciDAC Award:
Charge Transfer and Charge Transport in Photo-Activated Systems

Problem: Finding the optimal solar-harvesting “needle” in the materials-genome “haystack” requires methods for determining how materials absorb light



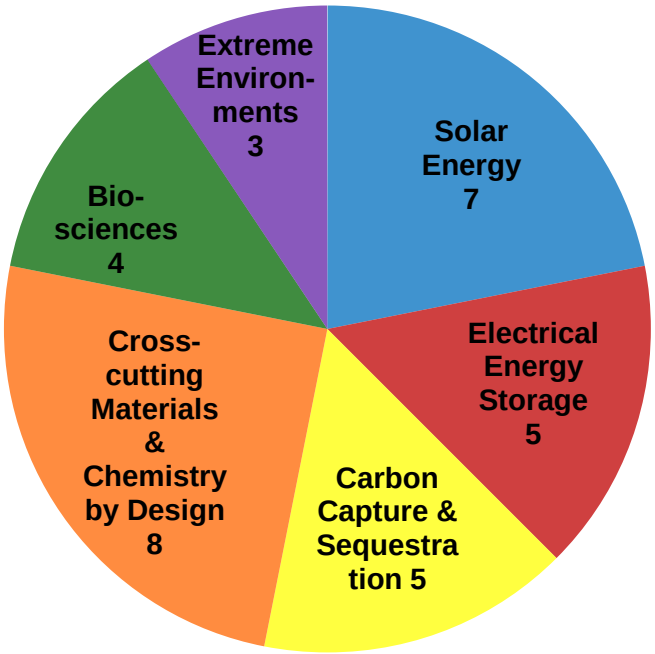
Approach: Develop publically available methods, algorithms, and software tools for reliable modeling of excited-state charge transfer and charge transport in photo-activated systems on leadership class computational platforms.

Impact: Improved computational treatment of excited-states on the molecular scale is required for predictive simulation of materials that convert solar energy to electricity or fuels.

Collaboration with two SciDAC institutes. PI: Chris Cramer, University of Minnesota.

Energy Frontier Research Centers
FY 2014 Recompetition

- Solicitation requested applications that included
  - Areas of energy-relevant research identified by recent BES and BESAC workshops
  - **Research to advance the rate of materials and chemical discovery**
  - Mesoscale science
- 32 EFRCs: 22 Renewal + 10 New



Participants in today's meeting include:

Center for Computational Design of Functional Layered Materials
John Perdew (Temple University)

Center for Emergent Superconductivity
Peter Johnson (Brookhaven National Laboratory)

Center for Next Generation Materials by Design
Bill Tumas (National Renewable Energy Laboratory)

Inorganometallic Catalyst Design Center
Randall Snurr (Northwestern)

Computational Materials Sciences – FY 2015

What is Different? What is Needed?

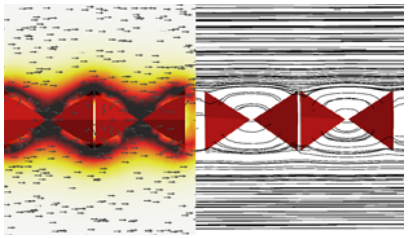
- Move theory and computation from research-use by experts to more general use by the community --- then industry
- Fund teams of theorists, experimentalists and computational scientists with the express purpose of accelerating the development and delivery of experimentally validated computational software
  - Fill in theoretical and scientific knowledge gaps
    - Current codes fail for strategic functional materials – magnets, thermal materials, superconductors, advanced semiconductors, catalysts
  - Open source software, maintained for broad-use
    - Enhance speed and complexity by taking full advantage of today's super computers and future generation of exascale leadership computing capabilities
- Build on the current portfolio of theory research and experimental characterization facilities, including user facilities
  - Seamlessly integrate codes with databases of validated information from both theory and experiment

Computational Materials Sciences
FY 2015 = $8M; FY 2016 = $12M

- Deliverable: Robust, open-source community software and databases for predictive design of functional materials within the Materials Genome Initiative for Global Competitiveness

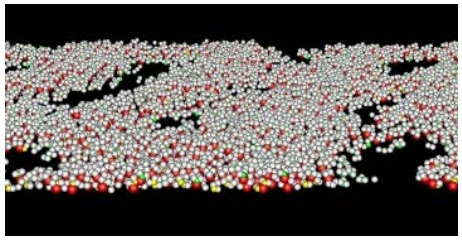
- Support began in FY 2015 for 3 teams for 4-year awards; Additional FY 2016 funds (+$4M)
- Deliver research codes and data for design of functional materials to the materials sciences communities in academia, labs, and industry
- Use integrated teams combining expertise in materials theory, modeling, computation, synthesis, characterization, and processing/fabrication
- Use facilities and tools for synthesis, characterization, simulation, and computation, relying especially on the SC scientific user facilities and leadership class computing

FY 2015 Awards:



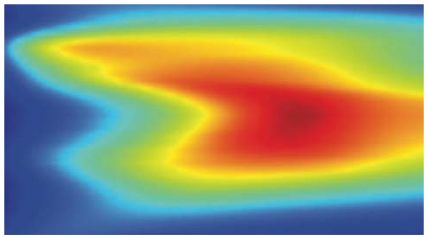
Experimental & Calculated Images of Ordered Nanoparticle Chains

Functional Materials Design for Energy Conversion
Galli, Argonne National Laboratory



Structure and Dynamics in Self-Assembled Monolayers

Computational Synthesis of Layered Materials
Vashishta, University of Southern California



Inelastic Neutron Response Predicted by Dynamical Mean Field Theory

Computational Design of Correlated Materials
Kotliar, Brookhaven National Laboratory

Computational Materials Sciences

FY 2016 Funding Request (+ $4M compared to FY 2015)

- "..to support research for functional material topics not supported in FY 2015. Each research team will focus on a different area of functional materials."

Funding Opportunity Announcement in FY 2015

- Applications in FY 2015 required:
  - Address a specific class of functional materials; Proposals focused on structural materials are not considered responsive
  - For more details see Funding Opportunity Number: DE-FOA-0001276
- Funding level per application: $2M to $4M per year for 4 years
  - $8M appropriated for FY 2015
- Only one Letter of Intent and subsequent application were accepted from any institution and from any lead PI/Director
- Important dates:
  - Issue Date: 1/26/2015
  - Required Letter of Intent Due: 2/23/2015 at 5:00 PM ET
  - Application Due: 4/17/2015 at 11:59 PM ET

DOE Office of Science Graduate Student Research (SCGSR) Program

The SCGSR Program provides supplemental awards to outstanding graduate students to spend 3 to 12 months conducting part of their doctoral thesis/dissertation research at a DOE national laboratory in collaboration with a DOE laboratory scientist.

- Gradua
- The ap udent's thesis a
- Studen GSR priority
  - BE
  - Ap

A topic on "Predictive Materials Sciences and Chemistry" has been included since the program began in FY 2014

FY 2014: 19 awards

FY 2015: 8 awards to date

(FY 2015-2 applications are under review)

FY 2016 – 1 opens in February 2016

Award Be

- A mont general living expenses
- Reimbursement of inbound/outbound traveling expenses to/from the DOE laboratory of up to $2,000.

(Award payments are provided directly to the student.)

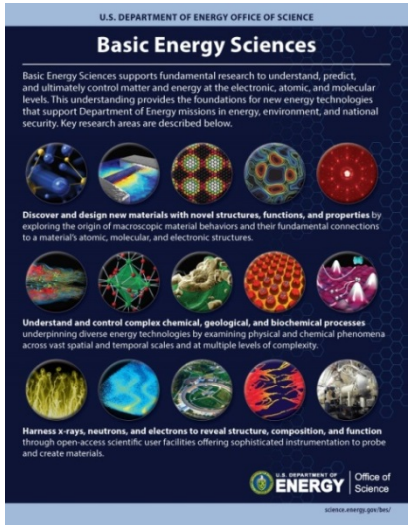
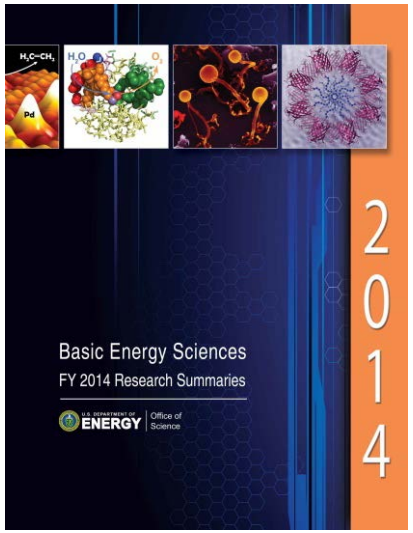
- Qualified graduate program & Ph.D. Candidacy
- Graduate research aligned with an SCGSR priority research area
- Establishment of a collaborating DOE laboratory scientist at the time of application

2016 Solicitation 1 – Applications Open: February 2016

Full details, requirements, FAQs, and link to application at: http://science.energy.gov/wdts/scgsr/

Newest Online Resources

- **BES Brochure**
  - 11”x17” brochure describing BES-supported research, tools, and facilities
  - Examples illustrate BES investments in:
    - research ranging from discovery science to science for energy technologies, and
    - tools including laboratory equipment, theory and experiment, and large user facilities.



- **BES Research Summaries**
  - Report describing over 1,200 BES-supported research projects in FY 2014
  - Each entry includes the title, senior investigators, number of students and postdocs, institutions, funding level, program scope, and FY 2014 highlights.