U.S. DEPARTMENT OF ENERGY | Office of Science

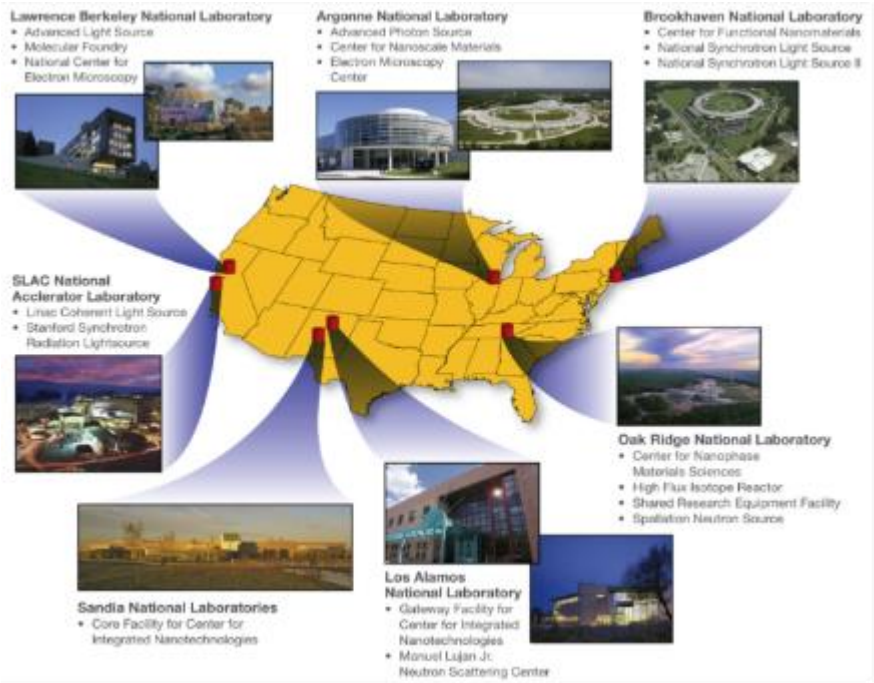
BES Introduction
SciDAC-4 PI Meeting

Rockville, MD
July 23, 2018

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

DOE Office of Basic Energy Sciences: Scientific User Facilities

Nearly 16,000 users in FY 2017



- ✸ **Available to all researchers *at no cost* for non-proprietary research, regardless of affiliation, nationality, or source of research support**
- ✸ **Access based on external peer merit review of brief proposals**
- ✸ **Coordinated access to co-located facilities to accelerate research cycles**
- ✸ **Collaboration with facility scientists an optional potential benefit**
- ✸ **Instrument and technique workshops offered periodically**
- ✸ **A variety of on-line, on-site, and hands-on training available**
- ✸ **Proprietary research may be performed at full-cost recovery**

Neutron Sources

- High Flux Isotope Reactor (ORNL)
- Spallation Neutron Source (ORNL)

Light Sources

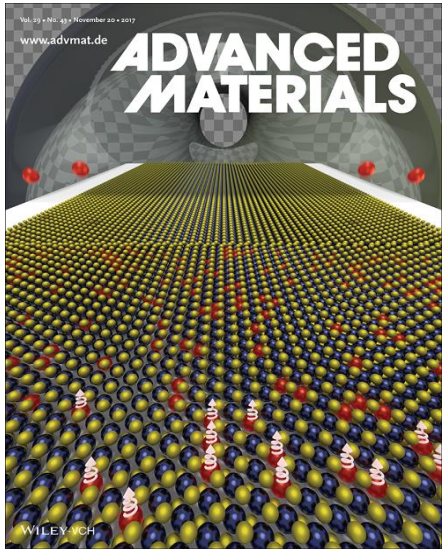
- Advanced Light Source (LBNL)
- Advanced Photon Source (ANL)
- Linac Coherent Light Source (SLAC)
- National Synchrotron Light Source-II (BNL)
- Stanford Synchrotron Radiation Laboratory (SLAC)

Nanoscale Science Research Centers

- Center for Functional Nanomaterials (BNL)
- Center for Integrated Nanotechnologies (SNL & LANL)
- Center for Nanophase Materials Sciences (ORNL)
- Center for Nanoscale Materials (ANL)
- Molecular Foundry (LBNL)

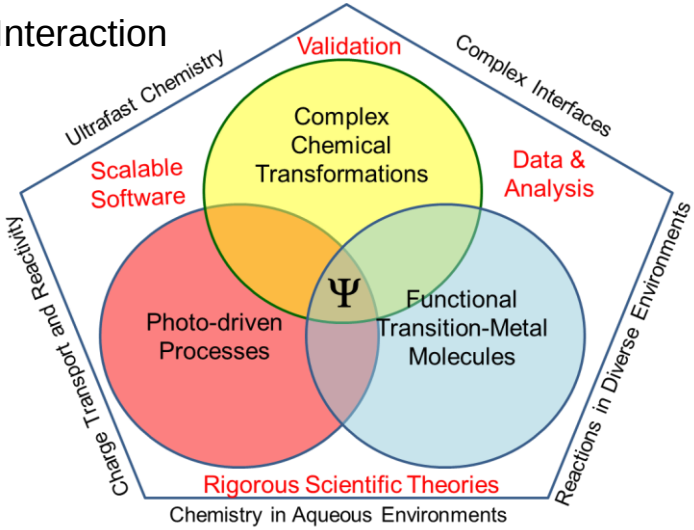
DOE/BES Computational Materials Sciences

- **5 CMS Centers** → Functional Materials, Open Source Software, Experimental Validation
  - **C2SEPEM**, Steve Louie, LBNL/UC Berkeley, Many Body Perturbation Theory, BerkeleyGW
  - **COMSCOPE**, Gabi Kotliar, BNL/Rutgers; Dynamical Mean Field Theory, Spectroscopy
  - **CPSFM**, Paul Kent, ORNL, Quantum Monte Carlo
  - **MAGICS,** Priya Vashishta, U Southern California, 2-d synthesis
  - **MICCoM**, Giulia Galli, ANL/U Chicago, NanoScale Assemblies
    - 1st Principles MD, Qbox, West, SSAGES
- **Materials Project**, Kristen Persson, LBNL/UC Berkeley
  - Large Collection of Computed Data & Properties, Analysis Software
  - See ShyuePing Ong, Anubhav Jain
- **PRISMS**, John Allison, U Michigan, Structural Materials, Mg Alloys
  - MultiScale Modeling, Phase Field, See Katsuyo Thornton
- **TIMES**: Tom Devereaux, SLAC, dynamics, time dependent response, Also Brian Moritz, Chunjing Jia



DOE/BES Computational Chemical Sciences

- **4 CCS Centers** → Chemical Processes, Open Source Software, Experimental Validation
  - **SPEC**, Sotiris Xantheas (PNNL), Excitations and Correlated Phenomena
  - **Computational Tools for Complex Chemical Systems**, Judit Zador (SNL), Catalysis
  - **NGMC**, Ilja Siepman (U Minnesota), Chemical Separations and Transformations
  - **FLO-SIC,** Koblar Jackson (Michigan State), DFT Without Self-Interaction
- **2 CCS Small Groups**
  - **Interfacial Charge Transfer Dynamics**, Barry Dunietz (Kent State), Margaret Cheung (U Houston), Eitan Geva (U Michigan), Post-Marcus Theory
  - **Molecular Magnets**, Ed Barnes, Sophia Economu, Kyungwha Park, Nick Mayhill (VA Tech)



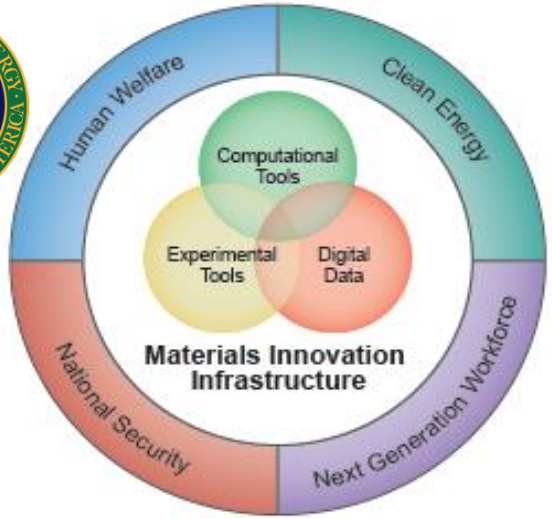
- **11 CCS Single-PI projects**
  - **Transition Metals**, Heather Kulik (MIT); Angela Wilson (Michigan State); Serdur Ogut (UIC)
  - **Excited States/Nonadiabatic Processes**: Piotr Piecuch (Michigan State); Michele Pavanello (Rutgers); Jerzy Leszczynski (Jackson State); Lasse Jensen (Penn State); Christine Aikens (Kansas State); Marivi Fernandez-Serra (Stony Brook); Arun Yethiraj (U Wisconsin)

Materials Project: Kristin Persson, LBNL

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

- > **67,000 relaxed compounds:** validated energy, phase diagrams
- > **530,000 NanoPorous Materials**
- > **46,000 band structures** + higher accuracy 2,700 band gaps
- > **4,000 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

BES Roundtables on Quantum Information Sciences

- Opportunities for Basic Research for Next-Generation Quantum Systems
  - October 30-31, 2017 (1.5 days)
  - Chair – David Awschalom (U Chicago/ANL)

    Co-chair – Hans Christen (ORNL)
  - Identify opportunities for basic materials and chemical sciences, including nanoscale research, to enable the next-generation of quantum devices and systems.
- Opportunities for Quantum Computing in Chemical and Materials Sciences
  - October 31 – November 1 (1.5 days)
  - Chair – Joel Moore (UC-Berkeley/LBNL)

    Co-chair – Alan Aspuru-Guzik (Harvard U)
  - Identify opportunities for quantum computing (QC) to enable significant and impactful advances in understanding of important fundamental challenges in chemical and materials sciences

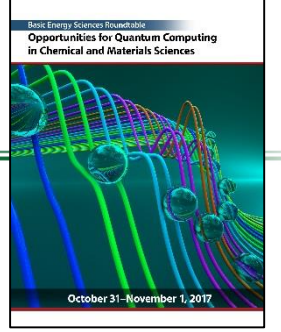
FY 2018 – FY 2019 BES Research Priorities

- **Quantum Information Science (QIS)**
  - By exploiting the intricate quantum mechanical phenomena, QIS will create fundamentally new ways of obtaining and processing information and open new vistas of science discovery and technology innovation. Research priorities were identified in two QIS roundtables held in October 2017.
- **Ultrafast Science**
  - Ultrafast science remains a priority in both research divisions to position the U.S. leadership in this critical field of science and in anticipation of the completion of the LCLS-II construction project. Research priorities were identified in a roundtable held October 2017.
- **Computational Materials and Chemical Sciences**
  - Computational Materials Sciences (CMS) and Computational Chemical Sciences (CCS) are maintained in support of the Exascale Computing Initiative. CCS was funded in FY 2017 and is moved to a new budget line in the FY 2019 Request.
- **Materials and Chemical Sciences for Future Nuclear Energy**
  - Research will be supported to achieve a multi-scale spatial and temporal understanding of fundamental physical and chemical processes that govern the properties and performance of novel material systems and fuels required for advanced reactors.
- **Priorities identified by Advisory Committee and Basic Research Needs Reports**
  - Both the core research and EFRCs will emphasize emerging high priorities identified by the Basic Energy Sciences Advisory Committee and recent Basic Research Needs workshop reports.

BES SciDAC Presentations

- Tom Devereaux, SLAC and Stanford University
  - Superconductivity and CDWs in the Doped Hubbard & t-J Models: Pairing without Quasiparticles
- Martin Head-Gordon, LBNL and UC Berkeley
  - Advancing Catalysis Modeling: From Atomistic Chemistry to Whole System Simulation
- Thomas Maier, ORNL and University of Tennessee
  - S-wave pairing from repulsive interactions: Quantum Monte Carlo study of systems with incipient bands
- Todd Martinez, SLAC and Stanford University
  - Scaling Quantum Mechanics and First Principles Dynamics for Accuracy and Efficiency
- Today 1:30 – 3:30 Followed by Posters

Quantum Information Science: Quantum Computing Opportunities in Chemical and Materials Sciences



Roundtable in October 2017 defined a BES research agenda for emerging quantum computing and provided input on priority research opportunities:

- Controlling the quantum dynamics of nonequilibrium chemical and materials systems
  - Elucidate the fundamental principles underlying chemical reactions and catalytic pathways; discover dynamical phases of matter; and understand how to prepare entangled states across many quantum degrees of freedom
- Unraveling the physics and chemistry of strongly correlated electron systems
  - Enable a correct description of the quantum behavior of strongly entangled electrons to allow discovery of the principles controlling superconductivity, magnetic states and the dynamics of electronic states
- Embedding quantum hardware in classical frameworks
  - Develop efficient hybrid algorithms that embed quantum computing for strongly correlated quantum components in classical computing for more weakly correlated parts, thus enabling simulations of molecular and materials problems containing thousands of atoms
- Bridging the classical–quantum computing divide
  - Improve the efficiency of quantum computing using approximate results from classical computing as input, and improve the accuracy of classical computing using high-accuracy results from quantum computing to parameterize and optimize complex models

Quantum Information Science: Opportunities for Basic Research for Next Generation Quantum Systems

Roundtable in October 2017 defined a BES research agenda for quantum systems for QIS and provided input on priority research opportunities:

- Advance artificial quantum-coherent systems with unprecedented functionality
  - Develop new capabilities for synthesis that couple theoretical predictions and real-time measurements of targeted quantum characteristics, including coherence
  - Explore robotic synthesis of layered materials, design of quantum properties for hybrid (organic and inorganic) systems, creation of topological states of matter, and precise control to position atomic defects
- Enhance creation and control of coherence in quantum systems
  - Understand scaling of coherence lengths and times with system size and complexity, and identify new signatures of quantum states in artificial quantum-coherent systems
  - Investigate mechanisms to prevent decoherence, leading to discovery and exploitation of novel entangled excitations
- Discover novel approaches for quantum-to-quantum transduction
  - Advance new capabilites for coherent transfer of complete wavefunctions between disparate physical systems, the core of quantum measurement and information processing
  - Develop new techniques for generation and stabilization of nonclassical states of light and matter; high fidelity transfer of quantum wavefunctions; and quantum state replication and entanglement
- Implement new quantum methods for advanced sensing and process control
  - Design new quantum-based sensors, detectors, and imaging systems for precise measurements of time, space, and fields to probe material properties and chemical processes
  - Create novel methods to use squeezed states for metrology and understand the connections of entanglement, thermodynamics, and many-body localization/diffusion

Office of Science Early Career Research Program

Office of Science Early Career Research Program – Started in FY 2010

- Purpose: To support individual research programs of outstanding scientists early in their careers and to stimulate research careers in the disciplines supported by the Office of Science
- Eligibility: Within 10 years of receiving a Ph.D., either untenured academic assistant or associate professors on the tenure track or full-time DOE national lab employees
- 5-Yr Awards: University grants $150,000/yr, National lab awards $500,000/yr min

FY 2017 Program

- 700 Office of Science proposals received, 21 Basic Energy Sciences (19 universities, 2 Labs) awards out of a total of 59 awards for the Office of Science (10 in BES-Materials Sciences and Engineering)

FY 2018 Program

- **Awards announced – see website for more information.**
- **Annual FOA will be released in FY 2019 for the next opportunity. FOAs cover different topics than the annual FOA for BES – important to read the details!**

Office of Science Graduate Student Research (SCGSR) Program

Prepare graduate students for STEM careers critically important to the DOE Office of Science mission. (~ 100-120 participants)

- Graduate students conduct a part of their graduate thesis research at a DOE lab with a collaborating principal investigator.
- Award terms range from 3 months to 1 year and can begin any time between the earliest and latest start dates specified in the solicitation.
- Graduate students pursuing Ph.D. degrees in areas of physics, chemistry, material sciences, biology (non-medical), mathematics, engineering, computer or computational sciences, or specific areas of environmental sciences that are aligned with the mission of the Office of Science are eligible to apply for the supplemental research awards provided by the SCGSR program.
- Specific areas of interest deemed to be of high program priority/workforce need. The areas may change slightly from year to year, depending on program determinations of workforce need.

Award Benefits:

- A monthly stipend of up to $3,000/month for 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.)

Eligibility:

- U.S. Citizen or Lawful Permanent Resident
- Qualified graduate program & Ph.D. Candidacy
- Research aligned with a SCGSR priority research topic
- Establishment of a collaborating DOE laboratory scientist at the time of application

See website for details: https://science.energy.gov/wdts/scgsr/