U.S. DEPARTMENT OF ENERGY

DOE-BES
Materials Sciences and Engineering
Physical Behavior Program

activities in

Thermoelectrics

Refik Kortan
Program Manager

Division of Materials Sciences and Engineering
Office of Basic Energy Sciences, Office of Science
U.S. Department of Energy

DOE 3rd Thermoelectrics Applications Workshop,
Baltimore, 20 March 2012

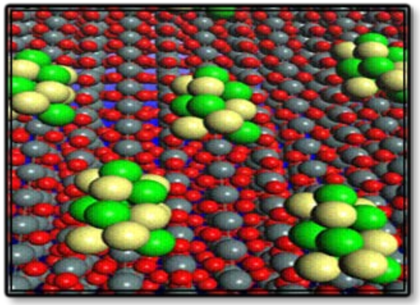
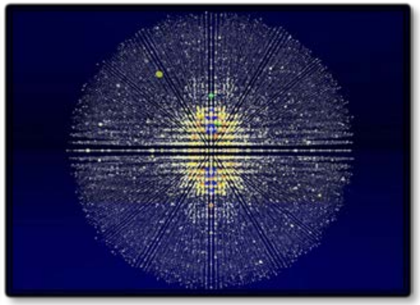
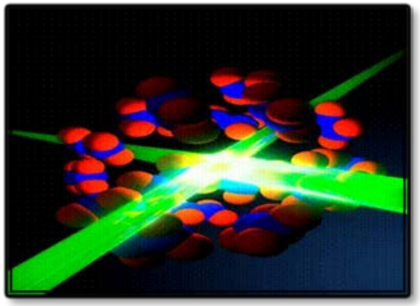
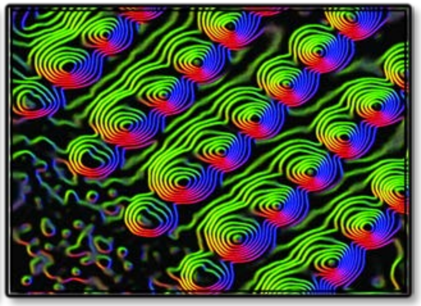
DOE Missions

DOE Secretary, Dr. Steven Chu

- Sustain basic research, discovery and mission driven
- Catalyze a transformation of the national/global energy system
- Enhance nuclear security
- Contribute to US competitiveness and jobs

Basic Energy Sciences Mission

- 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

BRNs: Basic Research Needs Documents

Disruptive, Transformational Advances Require "Control"

Control of materials properties and functionalities through electronic and atomic design

- New materials discovery, design, development, and fabrication, especially materials that perform well under extreme conditions
- "Control" of photon, electron, spin, phonon, and ion transport in materials
- Science at the nanoscale, especially low-dimensional systems
- Designed catalysts
- Designed interfaces and membranes
- Structure-function relationships
- Bio-materials and bio-interfaces, especially at the nanoscale
- New tools for spatial characterization, temporal characterization, and for theory/modeling/computation

http://science.energy.gov/bes/news-and-resources/reports/

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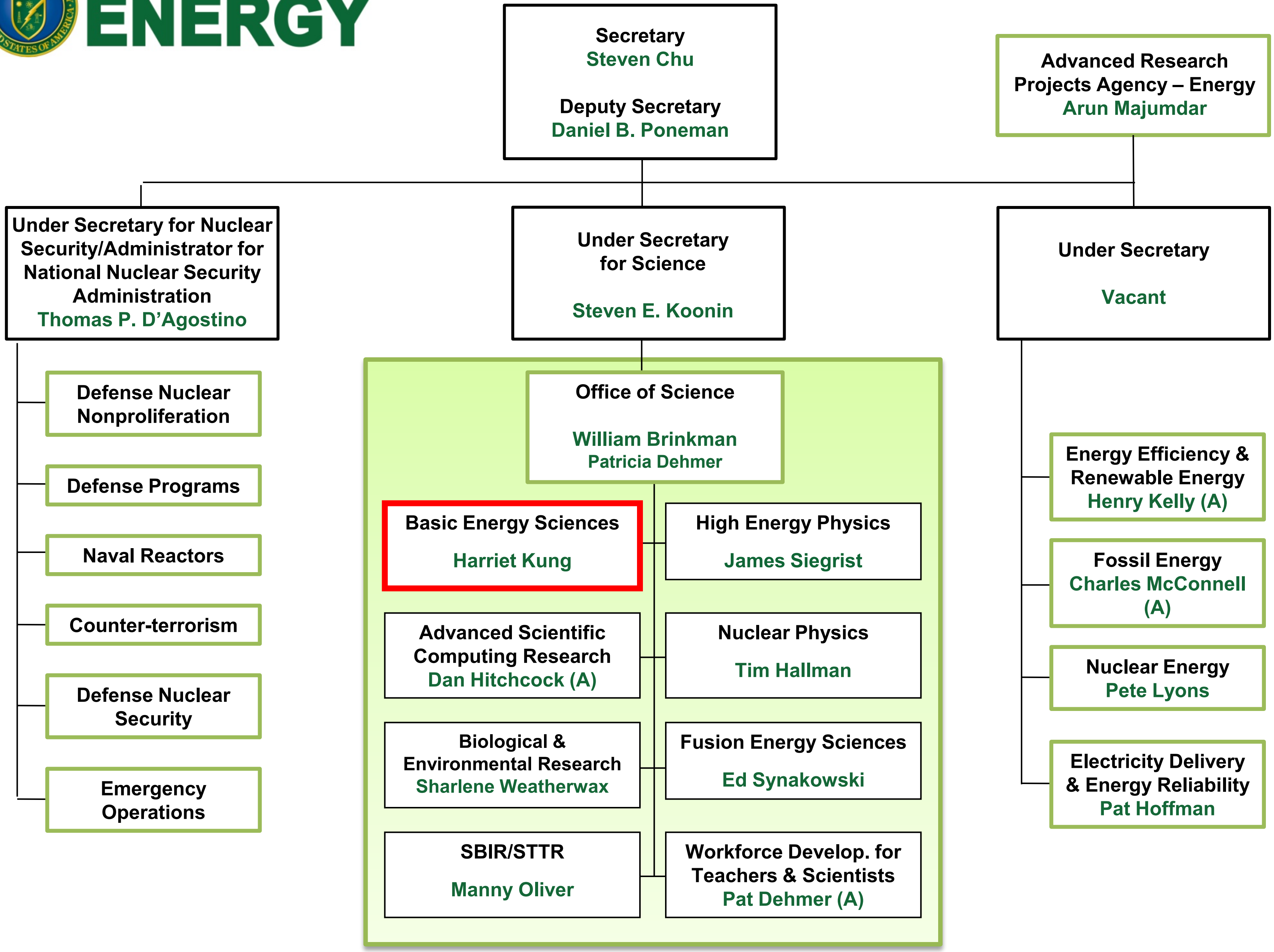


Office of Basic Energy Sciences

Office of Basic Energy Sciences
Harriet Kung, Director

- **Materials Sciences and Engineering Division**
  - Materials Discovery, Design and Synthesis
  - Condensed Matter and Materials Physics
  - Scattering and Instrumentation Sciences
- **Scientific User Facilities Division**
  - X-Ray and Neutron Scattering Facilities
  - Nanoscience and Electron Microscopy Centers
- **Chemical Sciences, Geosciences and Biosciences Division**
  - Fundamental Interactions
  - Photochemistry and Biochemistry
  - Chemical Transformations

Research grouped by scientific topics
-- not by specific energy technologies

Office of Basic Energy Sciences

Harriet Kung, Director

Wanda Smith, Administrative Specialist

BES Budget and Planning
- Bob Astheimer, Senior Technical Advisor
- Margie Davis, Financial Management

BES Operations
- Dawn Adin, AAAS Fellow
- Kerry Gorey, Program Support Specialist
- Robin Hayes, Program Manager
- Natalia Melcer, Program Manager
- Katie Perine, Program Analyst / BESAC
- Ken Rivera, Laboratory Infrastructure / ES&H

Materials Sciences and Engineering Division

Linda Horton, Director

Teresa Crockett, Program Analyst
Vacant

Materials Discovery, Design, and Synthesis — Arvind Kini; Jorge Mariani, P.A.
- Materials Chemistry — Craig Henderson, Michael Sennett
- Biomolecular Materials — Mike Markowitz
- Synthesis and Processing Science — Bonnie Gersten
- Technology Coordination Program Management — Craig Henderson, John Vetrano

Condensed Matter and Materials Physics — Jim Horwitz; Marsophia Agnant, P.A.
- Experimental Condensed Matter Physics — Andy Schwartz
- Theoretical Condensed Matter Physics — Jim Davenport
- Physical Behavior of Materials — Refik Kortan
- Mechanical Behavior and Radiation Effects — John Vetrano

Scattering and Instrumentation Sciences — Helen Kerch; Cheryl Howard, P.A.
- X-ray Scattering — Lane Wilson
- Neutron Scattering — Thiyaga P. Thiyagarajan
- Electron and Scanning Probe Microscopies — Jane Zhu
- Experimental Program to Stimulate Competitive Research (DOE EPSCoR) — Tim Fitzsimmons

Scientific User Facilities Division

Harriet Kung, Acting Director

Linda Cerrone, Program Support Specialist
Rocio Meneses, Program Assistant

Operations
- X-ray and Neutron Scattering Facilities — Peter Lee, Vacant, ◆ James Murphy, BNL
- NSRCs and EBMCs* — Mihal Gross, ☆ Tof Carim
- Accelerator and Detector Research — Eliane Lessner
- Facilities Coordination; Metrics; Assessment — Van Nguyen

Construction
- National Synchrotron Light Source-II — Phil Kraushaar
- Facilities Upgrades and Major Items of Equipment (MIE) Projects — Joe May, Phil Kraushaar

*Nanoscale Science Research Centers and Electron-beam Microcharacterization Centers

Chemical Sciences, Geosciences, and Biosciences Division

Eric Rohlfing, Director

Diane Marceau, Program Analyst
Michaelene Kyler-Leon, Program Assistant

Fundamental Interactions — Michael Casassa; Robin Felder, P.A.
- Atomic, Molecular, and Optical Sciences — Jeff Krause
- Gas Phase Chemical Physics — Wade Sisk
- Condensed Phase and Interfacial Molecular Science — Gregory Fiechtner
- Computational and Theoretical Chemistry — Mark Pederson

Photochemistry and Biochemistry — Rich Greene; Sharron Watson, P.A.
- Solar Photochemistry — Mark Spitler, ◆ Margaret Ryan, PNNL
- Photosynthetic Systems — Gail McLean
- Physical Biosciences — Robert Stack
- Fuels from Sunlight Energy Innovation Hub — Carol Bessel

Chemical Transformations — John Miller; Vacant, P.A.
- Catalysis Science — Paul Maupin, Raul Miranda, ◆ Jan Hrbek, BNL
- Separations and Analysis — Larry Rahn
- Heavy Element Chemistry — Philip Wilk
- Geosciences — Nick Woodward
- Technology Office Coordination — Marvin Singer

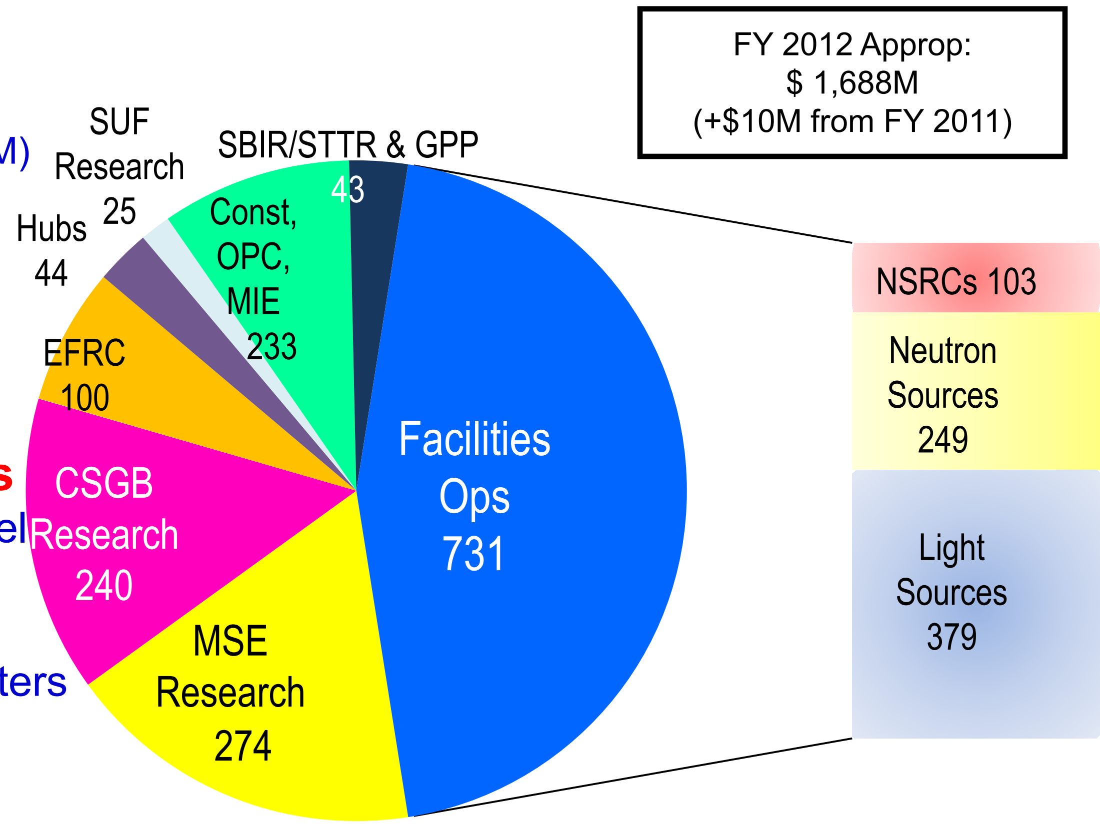
LEGEND

◆ Detailee (from DOE laboratories)
☆ On Detail to OSTP
P.A. Program Assistant

February 2012

FY 2012 BES Budget Appropriation

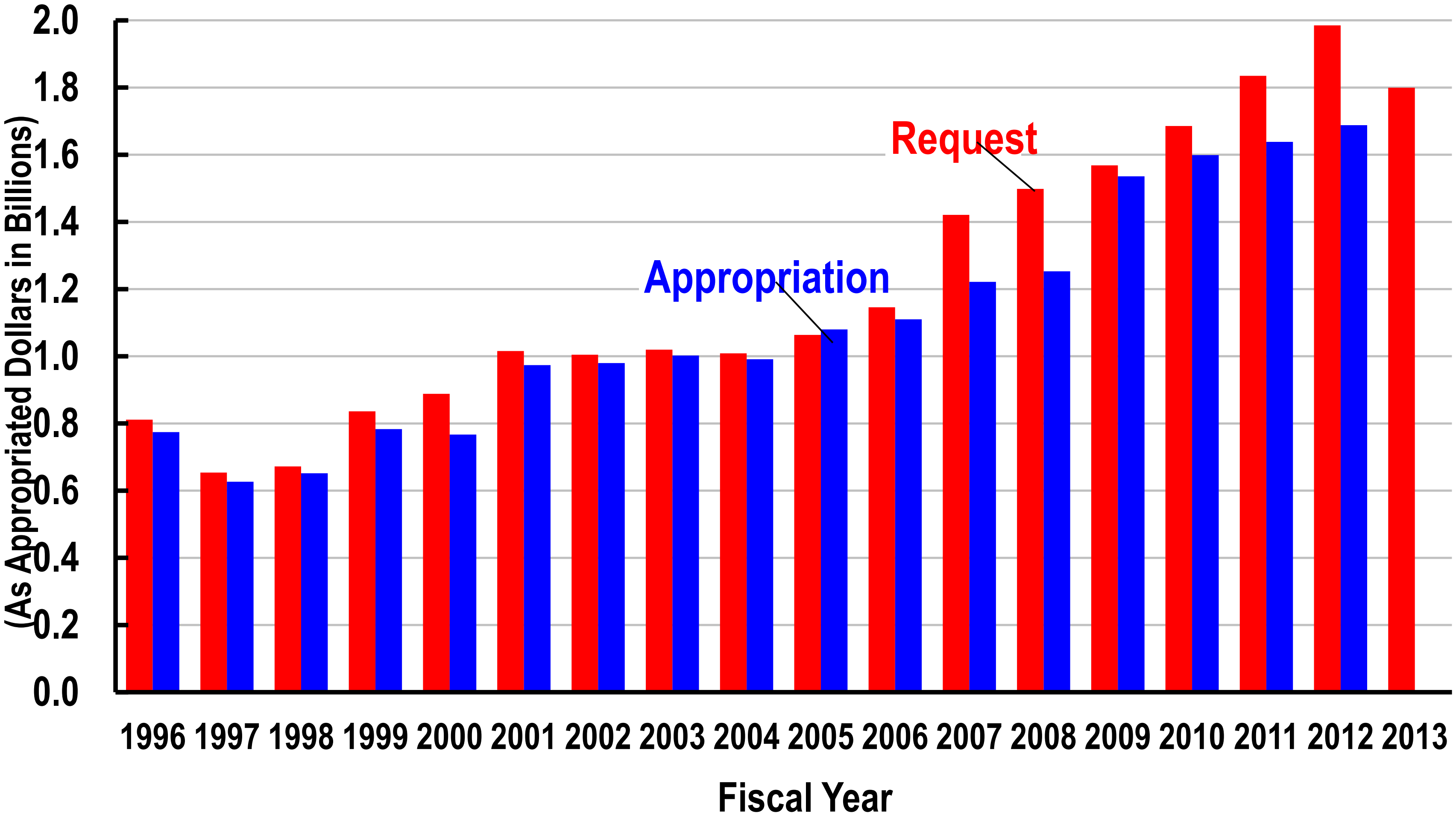
- **Research programs**
  - Energy Innovation Hubs
    - Battery and Energy Storage Hub (+$20M)
  - Energy Frontier Research Centers
  - Core Research
    - Plan to initiate new projects in materials and chemistry by design



- **Scientific user facilities operations**
  - All facilities operate below optimum level
    - Synchrotron light sources
    - Neutron scattering facilities
    - Nanoscale Science Research Centers

- **Construction and instrumentation**
  - National Synchrotron Light Source-II ($159M) and NEXT instrumentation ($12M)
  - Spallation Neutron Source instruments ($12M)
  - Advanced Photon Source upgrade ($20M)
  - Linac Coherent Light Source-II ($30M)

History of BES Request vs. Appropriation



BES Research — Science for Discovery & National Needs

Three Major Types of Research Thrusts

Increasing progression of scientific scope and level of effort

- **Core Research (many)**

  Support single investigator and small group projects to pursue their specific research interests

- **Energy Frontier Research Centers (46)**

  $2-5 million-per-year research centers, established in 2009, focus on fundamental research related to energy

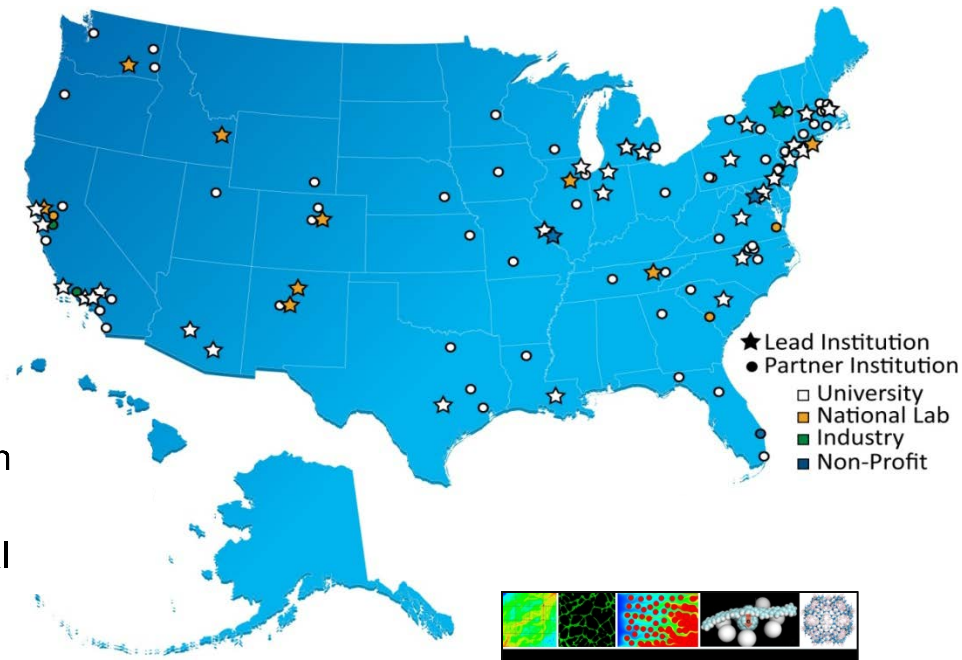
- **Energy Innovation Hubs (1 in BES)**

  $20 million+ -per-year research centers focus on integrating basic & applied research with technology development to enable transformational energy applications

Energy Frontier Research Centers

46 EFRCs in 35 States launched in Fall 2009

- ~860 senior investigators and ~2,000 students, postdoctoral fellows, and technical staff at ~115 institutions
- > 250 scientific advisory board members from 12 countries and > 35 companies

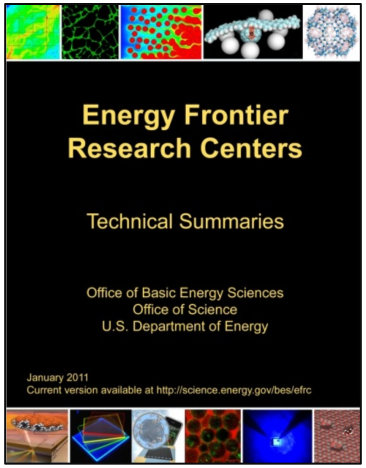


Impact to date:

- >1,000 peer-reviewed papers including more than 30 publications in *Science* and *Nature*.
- > 40 patents applications and nearly 50 additional patent/invention disclosures by 28 of the EFRCs.
- at least 3 start-up companies with EFRC contributions

Assessment of progress:

- All EFRCs are undergoing mid-term peer review to assess progress towards goals and plans for the next 2 years of R&D.



http://science.energy.gov/bes/efrc/

Physical Behavior of Materials Program

Supports fundamental research on the functional properties of materials. Emphasis is on the behavior of complex materials in response to external stimuli often encountered in energy-related applications and to develop scientifically rigorous models to improve understanding of mechanisms controlling physical behavior of materials – to predict and control the physical behavior of materials and design new materials with desired behaviors. (28 Lab, 48 University Projects)

Focus Topics : Magnetic, Electronic and Photonic Materials, Materials for Hydrogen Storage and Fuel Cells, Surfaces and Interfaces, Transport in Materials, Thermophysics and Thermochemistry (2 Lab, 7 Univ. on Thermoelectrics and Thermal transport)

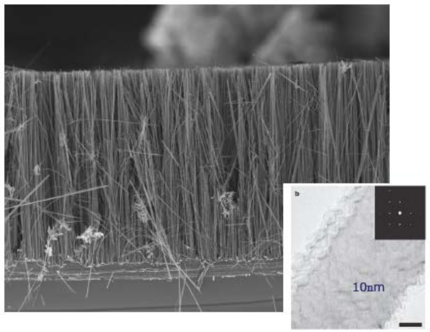
Understanding Fundamentals of Charge and Heat Transport is a high priority for the Physical Behavior Program

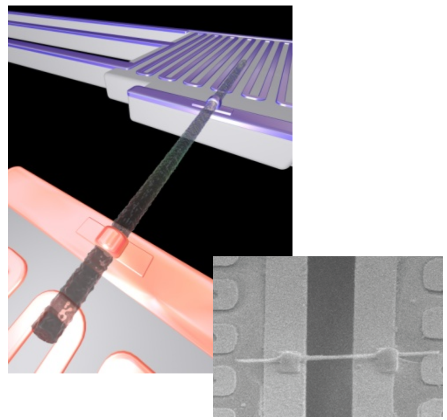
Thermoelectrics is the ultimate playground for physical sciences, overlapping;

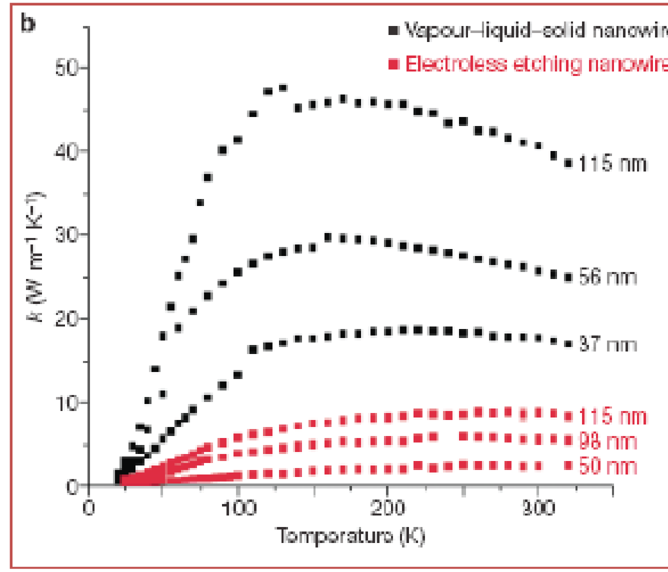
- **Physics, Chemistry, Electrical and Mechanical Engineering**
- **Thermodynamics**
- **Nano materials**

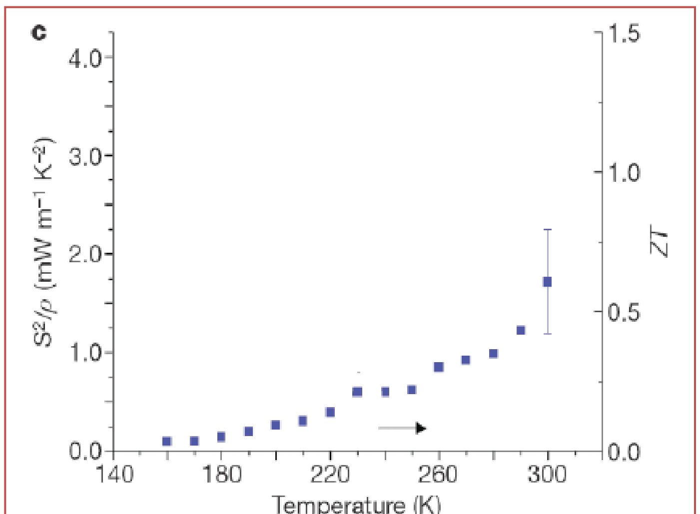
Potential Game Changer : Silicon Nanowire Thermoelectrics

Nature, 45, 163, (2008) *A. Hochbaum, A. Majumdar, P. Yang, (LBNL)*

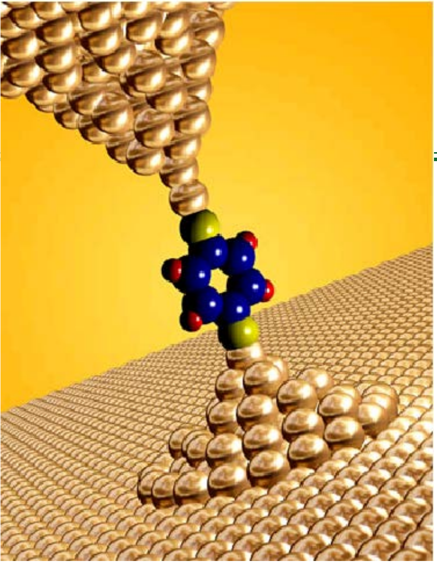






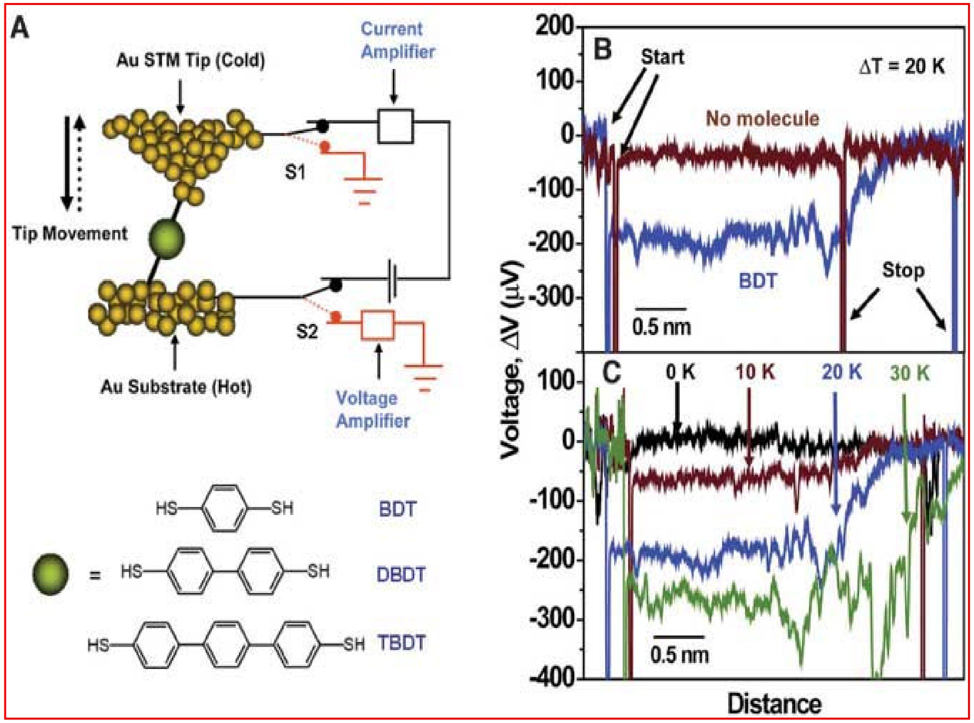


- Smallest diameter rough Si nanowire k comparable to bulk Silica.
- ZT is a thermoelectric figure of merit which balances heat-driven electrical conductivity and thermal conductivity. (larger values are desirable and only a few exotic materials are known to have ZT > 1)
- 0. 48 nm rough Si nanowires have a room temperature (300 K) ZT of 0.6 compared to ~0.01 for bulk Si.



Thermoelectricity in Molecular Junctions

Science 315, 1568, 2007 P. Reddy, P-Y.Jang, R.Segalman, A. Majumdar



- By trapping molecules between two gold electrodes with a temperature difference across them, the junction Seebeck coefficients of **1,4-benzenedithiol** (BDT), 4,4′-dibenzenedithiol, and 4,4″-tribenzenedithiol in contact with gold were measured at room temperature to be +8.7 ± 2.1 microvolts per kelvin (μV/K), +12.9 ± 2.2 μV/K, and +14.2 ± 3.2 μV/K, respectively (where the error is the full width half maximum of the statistical distributions).

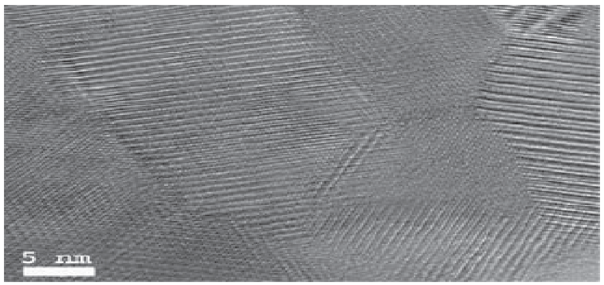
- The positive sign unambiguously indicates p-type (hole) conduction in these heterojunctions, whereas the Au Fermi level position for Au-BDT-Au junctions was identified to be 1.2 eV above the highest occupied molecular orbital level of BDT.

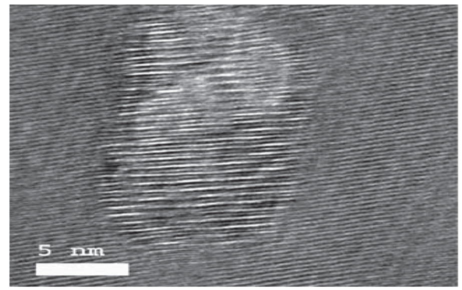
- The ability to study thermoelectricity in molecular junctions provides the opportunity to address these fundamental unanswered questions about their electronic structure and to begin exploring molecular thermoelectric energy conversion.

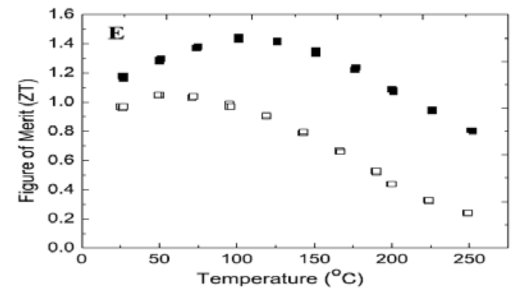
Nano-Enabled Thermoelectric Behavior (ZT) Improvement (> 40%)

Science 320, 634 (2008) G. Z. Ren (BU), Chen (MIT)

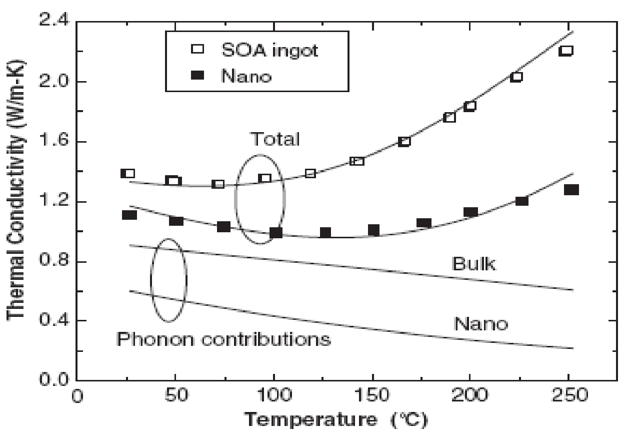
Ideal thermoelectric materials are known to have good electrical and poor thermal conductions. It is now discovered that by preparing nano-sized particles of BiSbTe alloy, and hot pressing them the thermal conduction of the material significantly decreased. The elementary carriers of heat, phonons scatter strongly at the grain boundaries giving rise to the observed phenomenon.

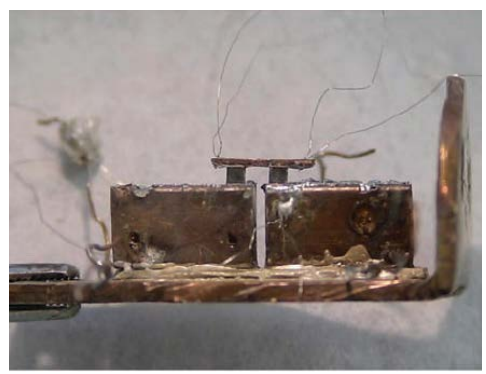


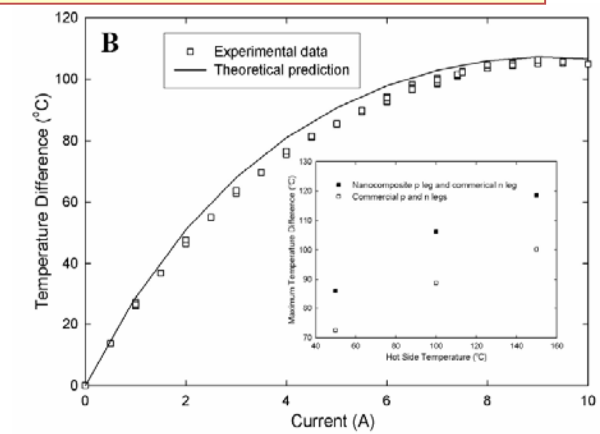




Nano grains with clean grain boundaries (left), nano inclusion in a single grain (middle), and temperature-dependent ZT (right).



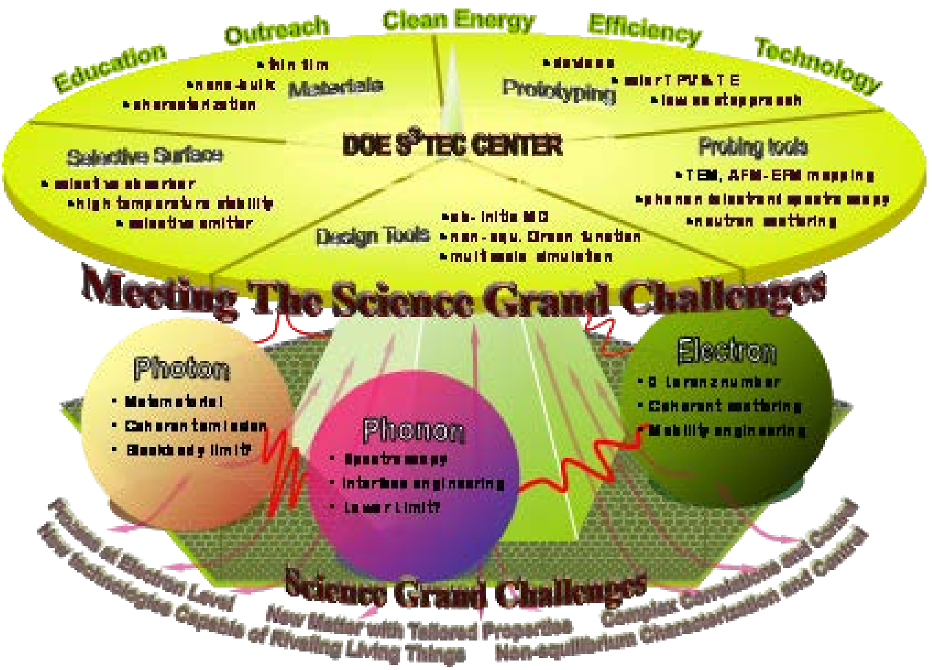




Thermal conductivity reduction (left), a two-leg Peltier cooling device (middle), and the cooling performance (right).

Solid-State Solar Thermal Energy Conversion Center (S^{3}TEC)
Gang Chen (MIT)

S^{3}TEC Center aims at developing transformational solid-state energy technologies to convert solar energy into electricity via heat, by advancing fundamental science of energy carrier coupling and transport, designing new materials, and inventing cost-effective manufacturing processes, and training energy workforce.



RESEARCH PLAN AND DIRECTIONS

(1) Engineering electron and phonon transport in nanostructures to achieve high performance thermoelectric materials,

(2) controlling photon absorption and emission for materials working at high temperatures, and

(3) device prototyping to demonstrate the high efficiency and low cost potential of the solar thermal energy conversion technologies.

U.S. DEPARTMENT OF ENERGY | Office of Science

Massachusetts Institute of Technology

OAK RIDGE National Laboratory

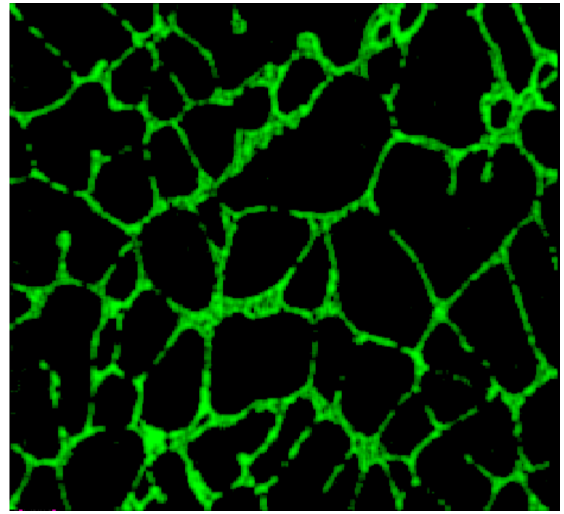
RPI

[efrc] RMSSEC
Revolutionary Materials for Solid State Energy Conversion

Revolutionary Materials for Solid State Energy Conversion

Donald T. Morelli (Michigan State University)

The Center for Revolutionary Materials for Solid State Energy Conversion will focus on the fundamental science of thermoelectricity. It will combine experimental, theoretical, and computational approaches to synthesize, characterize, and understand the nature of the thermo-electric energy conversion process.



Auger map of boron (green) decorating grain boundaries in a Co-Si alloy.

High resolution TEM image showing spinodally decomposed regions in PbTe-16%PbS.

RESEARCH PLAN AND DIRECTIONS

Challenges: Create "contraindicated" properties in solids

Approaches: Synthesis of novel structures, compounds, and alloys; computational and theoretical investigations

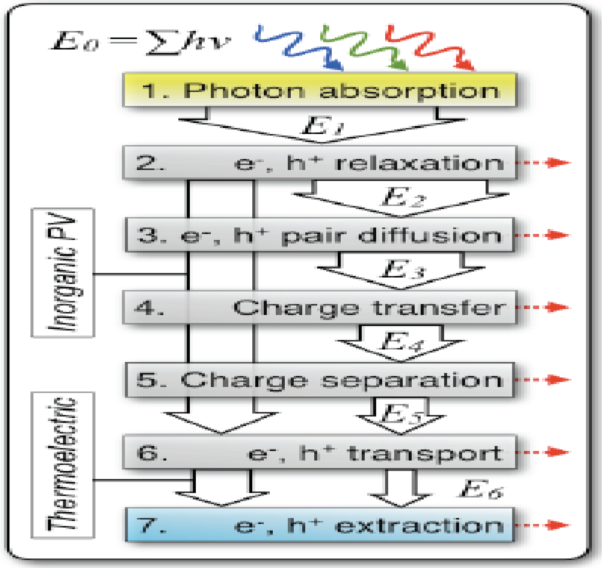
Uniqueness: Nanoscience, self-assembly of nanostructures

Outcomes: Deeper understanding of thermoelectric energy conversion

MICHIGAN STATE UNIVERSITY · OAK RIDGE NATIONAL LABORATORY (Managed by UT-Battelle for the Department of Energy) · NORTHWESTERN UNIVERSITY · THE OHIO STATE UNIVERSITY · M · UCLA · WAYNE STATE UNIVERSITY

Peter F. Green (University of Michigan)

Researchers in the center for thermal and solar energy conversion (CSTEC) investigate fundamental processes that govern the efficiency of solar and thermal energy conversion in nanostructured, complex, and low-dimensional inorganic, hybrid, and organic materials



RESEARCH PLAN AND DIRECTIONS

Research is conducted in three areas:

(1) Inorganic PV investigations of site-controlled nanostructured materials: absorption phenomena and carrier transport;

(2) Thermoelectric properties of single molecular junctions, quantum dots, wires, thin films and bulk skutterudites;

(3) Organic and Hybrid PV materials: Absorption phenomena, molecular design (caged molecules, self-aligning polythiophene derivative molecules), nanoscale characterization, devices

More Information? http://science.energy.gov/bes/ *

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* Or just Google "DOE BES"